



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:17 PM UTC

PDB ID : 3Q84 / pdb_00003q84
Title : Crystal structure of human PACSIN 1 F-BAR domain
Authors : Bai, X.
Deposited on : 2011-01-06
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

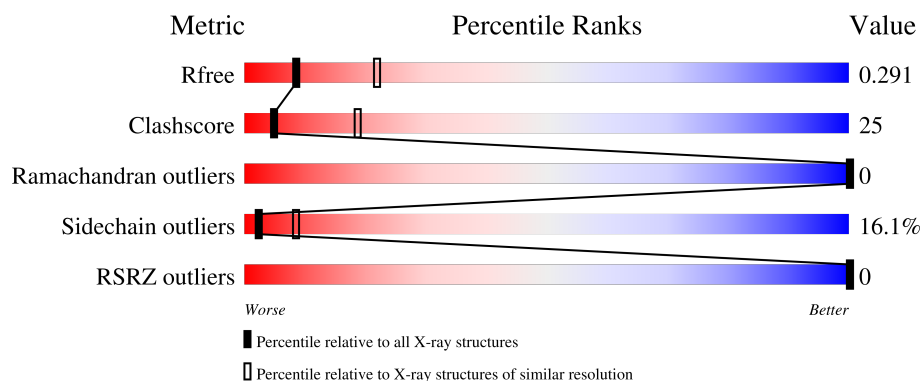
1 Overall quality at a glance ⓘ

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	295	52% 35% 10% .
1	B	295	59% 29% 7% ..
1	G	295	63% 24% 10% .
1	H	295	58% 31% 8% .
1	M	295	45% 37% 8% .. 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	N	295	54% 31% 6% • 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14091 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 Protein kinase C and casein kinase substrate in neurons protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	Se	0	0	0
			2350	1478	415	442	5	10			
1	B	285	Total	C	N	O	S	Se	0	0	0
			2353	1475	418	445	5	10			
1	G	287	Total	C	N	O	S	Se	0	0	0
			2353	1475	419	444	5	10			
1	H	288	Total	C	N	O	S	Se	0	0	0
			2375	1492	421	447	5	10			
1	M	271	Total	C	N	O	S	Se	0	0	0
			2227	1401	395	418	5	8			
1	N	272	Total	C	N	O	S	Se	0	0	0
			2216	1390	395	418	5	8			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	G	1	Total	Ca	0	0
			1	1		
2	M	1	Total	Ca	0	0
			1	1		
2	N	1	Total	Ca	0	0
			1	1		

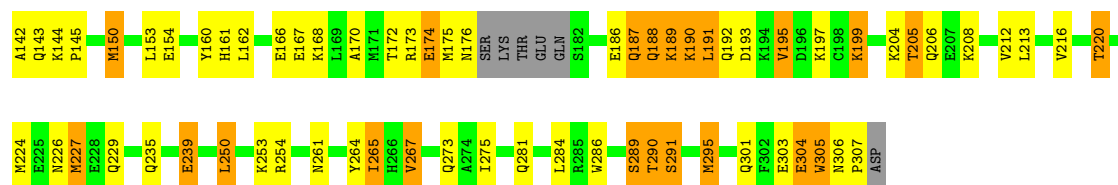
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	44	Total	O	0	0
			44	44		
3	B	44	Total	O	0	0
			44	44		

Continued on next page...

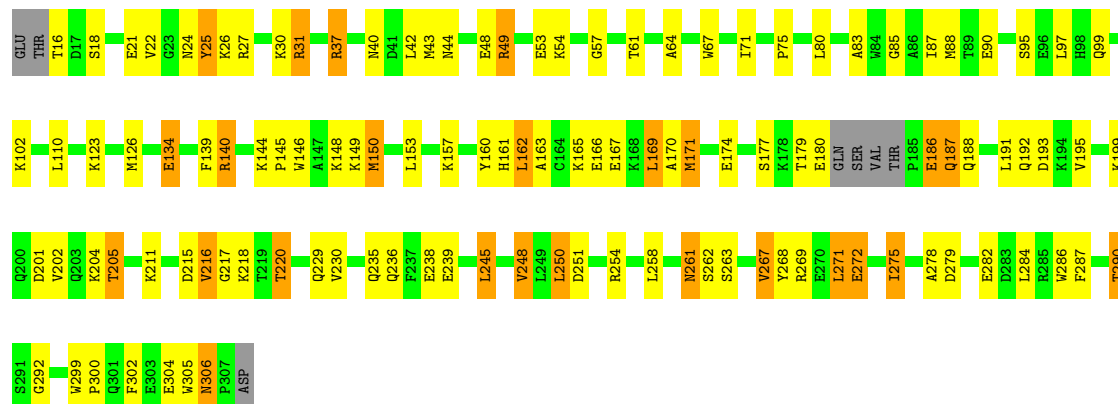
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	40	Total 40	O 40	0	0
3	H	32	Total 32	O 32	0	0
3	M	23	Total 23	O 23	0	0
3	N	30	Total 30	O 30	0	0



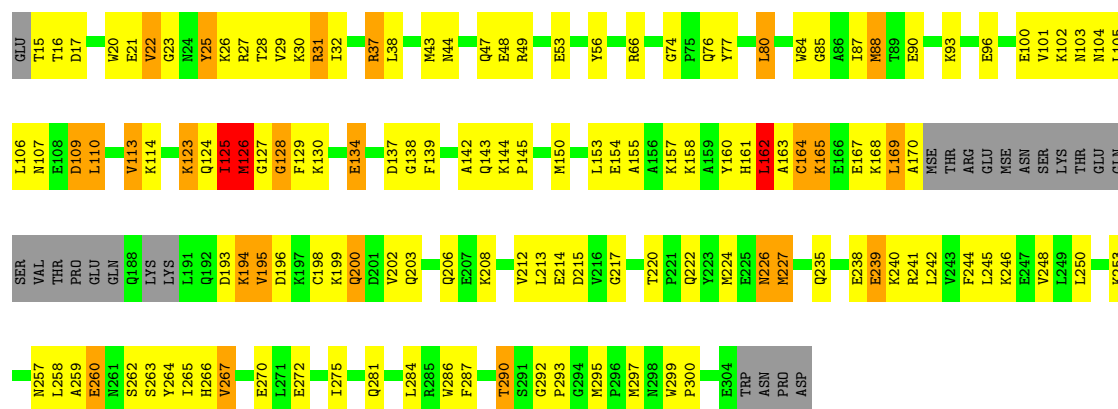
- Molecule 1: Protein kinase C and casein kinase substrate in neurons protein 1

Chain H: 58% 31% 8% .



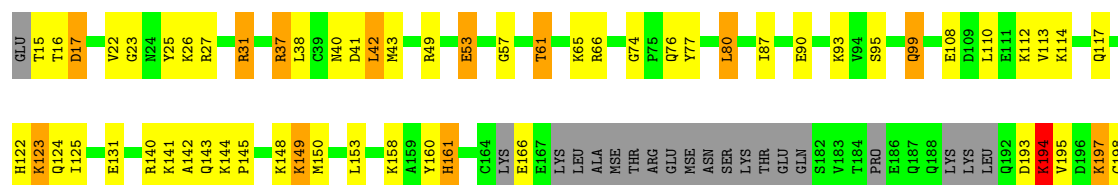
- Molecule 1: Protein kinase C and casein kinase substrate in neurons protein 1

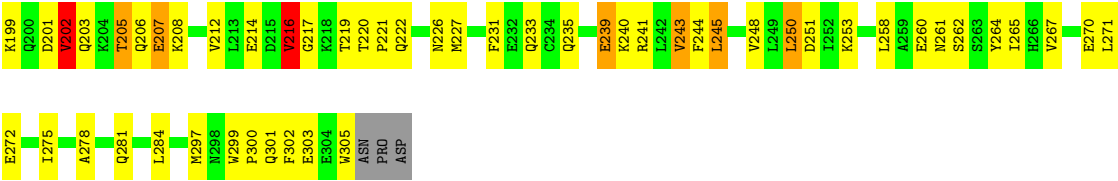
Chain M: 45% 37% 8% . 8%



- Molecule 1: Protein kinase C and casein kinase substrate in neurons protein 1

Chain N: 54% 31% 6% . 8%





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	86.35Å 154.29Å 215.45Å 90.00° 90.34° 90.00°	Depositor
Resolution (Å)	29.06 – 2.80 29.06 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.2 (29.06-2.80) 94.6 (29.06-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.33 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.221 , 0.294 0.234 , 0.291	Depositor DCC
R_{free} test set	3358 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	53.5	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -1/2*h-1/2*k,-3/2*h+1/2*k,-l 0.012 for -1/2*h+1/2*k,3/2*h+1/2*k,-l 0.003 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.005 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.447 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14091	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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: CA

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	1.45	11/2384 (0.5%)	1.32	19/3178 (0.6%)
1	B	1.30	9/2387 (0.4%)	1.22	15/3184 (0.5%)
1	G	1.29	1/2386 (0.0%)	1.19	10/3180 (0.3%)
1	H	1.33	4/2411 (0.2%)	1.22	8/3215 (0.2%)
1	M	1.29	3/2261 (0.1%)	1.27	21/3019 (0.7%)
1	N	1.05	0/2247	1.20	11/2998 (0.4%)
All	All	1.29	28/14076 (0.2%)	1.24	84/18774 (0.4%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	GLU	CA-C	-6.45	1.45	1.52
1	B	288	ARG	C-O	-6.28	1.16	1.24
1	B	44	ASN	C-O	-5.90	1.17	1.24
1	B	281	GLN	C-O	-5.83	1.17	1.24
1	M	56	TYR	C-O	-5.81	1.17	1.24
1	M	103	ASN	C-O	-5.75	1.17	1.24
1	A	101	VAL	C-O	-5.69	1.17	1.24
1	B	287	PHE	C-O	-5.68	1.17	1.24
1	A	103	ASN	C-O	-5.67	1.17	1.24
1	B	86	ALA	CA-CB	-5.67	1.44	1.53
1	G	40	ASN	C-O	-5.66	1.17	1.24
1	A	86	ALA	CA-CB	-5.61	1.44	1.53
1	B	128	GLY	C-O	-5.58	1.18	1.23
1	A	109	ASP	CA-C	-5.47	1.45	1.52
1	M	107	ASN	CA-C	-5.47	1.45	1.52
1	B	291	SER	CA-C	-5.45	1.46	1.52
1	A	71	ILE	CA-C	-5.40	1.46	1.52
1	H	287	PHE	C-O	-5.39	1.17	1.24
1	B	281	GLN	CA-C	-5.34	1.45	1.52
1	A	104	ASN	C-O	-5.29	1.18	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	295	MSE	CG-SE	-5.28	1.79	1.95
1	A	84	TRP	C-O	-5.26	1.18	1.24
1	H	64	ALA	CA-CB	-5.22	1.45	1.53
1	A	67	TRP	C-O	-5.15	1.17	1.24
1	A	275	ILE	C-O	-5.14	1.18	1.24
1	H	97	LEU	C-O	-5.11	1.18	1.24
1	A	87	ILE	C-O	-5.10	1.18	1.24
1	H	275	ILE	C-O	-5.03	1.18	1.24

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	305	TRP	N-CA-C	-13.48	96.59	111.28
1	A	73	LYS	N-CA-C	-12.94	97.47	113.38
1	M	126	MSE	N-CA-C	-10.00	96.55	110.35
1	B	304	GLU	N-CA-C	9.60	122.22	110.41
1	M	25	TYR	N-CA-C	-8.74	102.63	113.20
1	A	106	LEU	N-CA-C	8.45	120.49	111.28
1	M	109	ASP	N-CA-C	8.14	119.78	111.07
1	A	74	GLY	CA-C-N	8.07	128.26	119.87
1	A	74	GLY	C-N-CA	8.07	128.26	119.87
1	B	125	ILE	N-CA-C	7.70	118.47	110.62
1	A	172	THR	N-CA-C	-7.43	103.19	111.28
1	M	195	VAL	N-CA-C	7.42	120.32	111.05
1	A	240	LYS	N-CA-C	-7.32	103.38	111.36
1	M	164	CYS	N-CA-C	-7.27	103.36	111.28
1	M	165	LYS	N-CA-C	7.16	119.16	111.36
1	N	197	LYS	N-CA-C	-7.11	103.53	111.28
1	H	22	VAL	N-CA-C	7.06	118.55	109.30
1	B	280	ALA	N-CA-C	6.99	118.55	111.07
1	N	264	TYR	N-CA-C	6.96	118.52	111.07
1	M	101	VAL	CB-CA-C	-6.90	102.82	112.14
1	H	25	TYR	N-CA-C	-6.88	104.88	113.20
1	A	199	LYS	N-CA-C	-6.87	103.90	112.90
1	B	128	GLY	N-CA-C	-6.80	102.22	112.41
1	A	78	GLY	N-CA-C	6.61	124.53	112.37
1	M	125	ILE	CB-CA-C	-6.37	103.82	111.97
1	A	248	VAL	N-CA-C	-6.33	104.33	110.72
1	M	106	LEU	N-CA-C	6.30	118.22	111.36
1	M	162	LEU	N-CA-C	-6.29	104.50	111.36
1	M	128	GLY	N-CA-C	6.24	119.28	112.29
1	G	295	MSE	N-CA-C	6.24	118.69	110.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	22	VAL	N-CA-C	6.13	117.32	109.30
1	B	262	SER	CB-CA-C	-6.04	101.31	110.92
1	G	189	LYS	CA-C-N	-6.01	112.62	120.44
1	G	189	LYS	C-N-CA	-6.01	112.62	120.44
1	A	109	ASP	N-CA-C	5.95	119.00	111.69
1	G	109	ASP	N-CA-C	5.89	117.56	111.03
1	A	104	ASN	CA-C-N	-5.82	112.88	120.44
1	A	104	ASN	C-N-CA	-5.82	112.88	120.44
1	B	109	ASP	N-CA-C	5.76	117.64	111.36
1	G	304	GLU	N-CA-C	-5.73	104.01	111.74
1	N	202	VAL	CB-CA-C	-5.72	104.42	112.14
1	N	194	LYS	N-CA-C	5.71	120.25	113.28
1	H	97	LEU	N-CA-C	5.69	117.48	111.28
1	H	292	GLY	CA-C-N	5.69	125.79	119.87
1	H	292	GLY	C-N-CA	5.69	125.79	119.87
1	N	74	GLY	CA-C-N	5.67	125.19	119.19
1	N	74	GLY	C-N-CA	5.67	125.19	119.19
1	A	168	LYS	N-CA-C	-5.66	105.11	111.28
1	G	94	VAL	N-CA-C	-5.56	105.10	110.72
1	M	260	GLU	N-CA-C	-5.53	106.37	113.01
1	M	107	ASN	CA-C-N	-5.52	114.28	122.56
1	M	107	ASN	C-N-CA	-5.52	114.28	122.56
1	B	110	LEU	CA-C-N	5.49	127.64	120.28
1	B	110	LEU	C-N-CA	5.49	127.64	120.28
1	M	265	ILE	N-CA-C	-5.48	105.03	110.62
1	M	195	VAL	CB-CA-C	-5.47	103.69	112.16
1	N	260	GLU	CA-C-N	5.46	130.01	121.76
1	N	260	GLU	C-N-CA	5.46	130.01	121.76
1	H	248	VAL	N-CA-C	-5.41	105.26	110.72
1	N	260	GLU	O-C-N	5.39	128.76	122.67
1	B	126	MSE	N-CA-C	5.33	117.09	111.28
1	B	288	ARG	CA-C-N	-5.29	113.56	120.44
1	B	288	ARG	C-N-CA	-5.29	113.56	120.44
1	G	188	GLN	N-CA-C	5.24	119.30	113.01
1	M	300	PRO	N-CA-C	5.23	119.09	111.03
1	A	81	GLU	N-CA-C	-5.21	105.60	111.28
1	G	39	CYS	N-CA-C	-5.20	105.61	111.28
1	A	90	GLU	N-CA-CB	5.20	117.76	110.12
1	B	290	THR	N-CA-C	5.19	117.61	111.33
1	A	304	GLU	N-CA-C	-5.17	103.20	110.50
1	N	216	VAL	N-CA-CB	5.16	116.24	110.62
1	B	106	LEU	N-CA-C	5.14	116.69	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	74	GLY	CA-C-N	5.12	124.81	119.64
1	M	74	GLY	C-N-CA	5.12	124.81	119.64
1	M	21	GLU	N-CA-C	-5.11	102.82	110.23
1	N	243	VAL	N-CA-C	-5.11	105.56	110.72
1	G	32	ILE	CB-CA-C	-5.10	105.26	112.14
1	H	75	PRO	N-CA-C	5.07	119.95	114.68
1	B	230	VAL	N-CA-C	-5.06	105.61	110.72
1	A	303	GLU	N-CA-C	5.05	116.64	108.41
1	A	107	ASN	CA-C-N	-5.04	113.39	122.46
1	A	107	ASN	C-N-CA	-5.04	113.39	122.46
1	H	110	LEU	N-CA-C	-5.03	106.31	112.90
1	B	92	ASP	N-CA-C	5.01	116.74	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2350	0	2286	130	1
1	B	2353	0	2288	109	1
1	G	2353	0	2285	149	1
1	H	2375	0	2313	101	1
1	M	2227	0	2171	153	0
1	N	2216	0	2134	111	0
2	B	1	0	0	0	0
2	G	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
3	A	44	0	0	0	0
3	B	44	0	0	1	0
3	G	40	0	0	2	0
3	H	32	0	0	1	0
3	M	23	0	0	0	0
3	N	30	0	0	2	0
All	All	14091	0	13477	691	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (691) 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:H:177:SER:CB	1:H:191:LEU:HD13	1.51	1.40
1:N:43:MSE:HE1	1:N:114:LYS:CB	1.53	1.38
1:A:169:LEU:HD13	1:A:170:ALA:N	1.41	1.33
1:M:160:TYR:HE1	1:M:206:GLN:NE2	1.28	1.29
1:G:191:LEU:HD12	1:G:192:GLN:N	1.45	1.28
1:H:169:LEU:C	1:H:169:LEU:HD23	1.54	1.28
1:N:43:MSE:CE	1:N:114:LYS:HB2	1.62	1.28
1:B:110:LEU:HD23	1:B:110:LEU:O	1.33	1.27
1:M:161:HIS:CD2	1:M:164:CYS:SG	2.29	1.25
1:H:85:GLY:HA2	1:H:88:MSE:CE	1.68	1.24
1:G:43:MSE:HE1	1:G:114:LYS:CA	1.66	1.24
1:A:162:LEU:C	1:A:162:LEU:HD23	1.60	1.23
1:N:43:MSE:HE3	1:N:114:LYS:N	1.52	1.23
1:N:43:MSE:HE1	1:N:114:LYS:CA	1.67	1.22
1:B:110:LEU:HD23	1:B:110:LEU:C	1.54	1.22
1:G:128:GLY:HA3	1:G:133:LYS:CE	1.70	1.19
1:H:177:SER:CB	1:H:191:LEU:CD1	2.20	1.19
1:M:125:ILE:H	1:M:125:ILE:CD1	1.49	1.18
1:G:174:GLU:HB3	1:G:191:LEU:CD2	1.73	1.18
1:A:169:LEU:HD22	1:A:169:LEU:O	1.39	1.17
1:M:43:MSE:CE	1:M:114:LYS:HB2	1.74	1.16
1:N:43:MSE:CE	1:N:114:LYS:CB	2.22	1.15
1:N:194:LYS:HD3	1:N:194:LYS:N	1.57	1.13
1:A:169:LEU:HD13	1:A:169:LEU:C	1.73	1.12
1:B:43:MSE:HE1	1:B:114:LYS:CA	1.78	1.13
1:G:128:GLY:CA	1:G:133:LYS:HE2	1.79	1.13
1:H:169:LEU:HD23	1:H:170:ALA:N	1.61	1.12
1:A:223:TYR:HE1	1:A:227:MSE:HE3	1.05	1.12
1:H:85:GLY:HA2	1:H:88:MSE:HE1	1.30	1.11
1:M:123:LYS:NZ	1:M:127:GLY:HA2	1.65	1.11
1:G:43:MSE:CE	1:G:114:LYS:N	2.14	1.10
1:A:37:ARG:HG2	1:A:37:ARG:HH21	1.00	1.10
1:G:167:GLU:OE1	1:G:199:LYS:HE3	1.52	1.10
1:G:174:GLU:CB	1:G:191:LEU:HD21	1.81	1.10
1:M:125:ILE:HD12	1:M:125:ILE:N	1.56	1.10
1:G:43:MSE:HE1	1:G:114:LYS:HA	1.14	1.09
1:A:143:GLN:HB2	1:A:227:MSE:HE1	1.11	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:43:MSE:HE1	1:M:114:LYS:CB	1.84	1.08
1:M:155:ALA:HA	1:M:158:LYS:HE2	1.26	1.08
1:B:43:MSE:HE1	1:B:114:LYS:HA	1.26	1.07
1:B:43:MSE:CE	1:B:114:LYS:CA	2.32	1.07
1:M:160:TYR:CE1	1:M:206:GLN:NE2	2.21	1.07
1:N:43:MSE:CE	1:N:114:LYS:CA	2.30	1.07
1:M:162:LEU:C	1:M:162:LEU:HD23	1.79	1.06
1:A:223:TYR:CE1	1:A:227:MSE:HE3	1.91	1.05
1:N:43:MSE:HE2	1:N:114:LYS:HB2	1.34	1.05
1:N:43:MSE:CE	1:N:114:LYS:N	2.19	1.05
1:B:110:LEU:C	1:B:110:LEU:CD2	2.30	1.04
1:A:162:LEU:C	1:A:162:LEU:CD2	2.30	1.04
1:G:191:LEU:CD1	1:G:191:LEU:C	2.30	1.03
1:G:43:MSE:CE	1:G:114:LYS:CA	2.36	1.02
1:A:162:LEU:HD23	1:A:162:LEU:O	1.56	1.02
1:G:43:MSE:HE3	1:G:113:VAL:HG22	1.38	1.02
1:M:154:GLU:O	1:M:158:LYS:HG2	1.60	1.01
1:M:198:CYS:SG	1:M:199:LYS:N	2.34	1.01
1:G:85:GLY:HA2	1:G:88:MSE:CE	1.90	1.00
1:H:171:MSE:SE	1:H:171:MSE:N	2.45	1.00
1:G:128:GLY:HA3	1:G:133:LYS:HE2	1.01	0.99
1:M:43:MSE:CE	1:M:114:LYS:CB	2.37	0.99
1:B:175:MSE:SE	1:B:176:ASN:OD1	2.29	0.99
1:B:43:MSE:HE3	1:B:114:LYS:N	1.76	0.98
1:H:126:MSE:H	1:H:126:MSE:SE	1.96	0.98
1:A:37:ARG:HH21	1:A:37:ARG:CG	1.76	0.98
1:G:190:LYS:HA	1:G:190:LYS:HZ2	1.27	0.98
1:G:85:GLY:HA2	1:G:88:MSE:HE2	1.41	0.98
1:G:186:GLU:CD	1:G:187:GLN:HA	1.88	0.98
1:H:160:TYR:HA	1:H:205:THR:HG23	1.42	0.97
1:B:43:MSE:CE	1:B:114:LYS:N	2.27	0.97
1:M:264:TYR:O	1:M:267:VAL:HG13	1.64	0.96
1:M:169:LEU:HD13	1:M:169:LEU:O	1.64	0.96
1:H:169:LEU:C	1:H:169:LEU:CD2	2.30	0.96
1:A:169:LEU:HD13	1:A:170:ALA:CA	1.95	0.96
1:G:191:LEU:HD12	1:G:191:LEU:C	1.89	0.96
1:H:169:LEU:CD2	1:H:170:ALA:N	2.30	0.95
1:A:169:LEU:CD1	1:A:170:ALA:N	2.29	0.94
1:G:191:LEU:CD1	1:G:192:GLN:N	2.30	0.94
1:B:43:MSE:HE2	1:B:114:LYS:HB2	1.49	0.94
1:A:143:GLN:CB	1:A:227:MSE:HE1	1.95	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:LEU:HD22	1:A:169:LEU:C	1.85	0.93
1:B:31:ARG:HH22	1:B:235:GLN:HE22	1.07	0.93
1:H:216:VAL:O	1:H:220:THR:HG22	1.69	0.93
1:M:43:MSE:HE1	1:M:114:LYS:CG	1.98	0.93
1:M:170:ALA:HB1	1:M:195:VAL:HG22	1.50	0.92
1:M:160:TYR:HE1	1:M:206:GLN:HE21	0.93	0.91
1:M:155:ALA:O	1:M:158:LYS:HG3	1.70	0.90
1:M:43:MSE:HE1	1:M:114:LYS:HG3	1.51	0.90
1:M:80:LEU:HD22	1:N:245:LEU:HD13	1.53	0.90
1:M:161:HIS:O	1:M:164:CYS:SG	2.29	0.90
1:G:189:LYS:C	1:G:190:LYS:NZ	2.30	0.90
1:A:143:GLN:HB2	1:A:227:MSE:CE	2.00	0.90
1:M:275:ILE:HG21	1:N:250:LEU:HD13	1.52	0.89
1:A:43:MSE:CG	1:A:113:VAL:HG21	2.04	0.88
1:B:85:GLY:HA2	1:B:88:MSE:HE2	1.56	0.88
1:G:186:GLU:OE1	1:G:187:GLN:HB2	1.73	0.87
1:H:170:ALA:HB1	1:H:195:VAL:HG22	1.56	0.87
1:B:85:GLY:HA2	1:B:88:MSE:CE	2.04	0.87
1:A:223:TYR:HE1	1:A:227:MSE:CE	1.86	0.86
1:A:37:ARG:HG2	1:A:37:ARG:NH2	1.81	0.86
1:N:194:LYS:N	1:N:194:LYS:CD	2.38	0.86
1:N:43:MSE:HE1	1:N:114:LYS:HA	1.55	0.85
1:M:123:LYS:HZ1	1:M:127:GLY:HA2	1.40	0.85
1:B:142:ALA:HB3	1:B:227:MSE:HE2	1.57	0.85
1:M:161:HIS:NE2	1:M:164:CYS:SG	2.48	0.85
1:H:160:TYR:HA	1:H:205:THR:CG2	2.07	0.85
1:N:43:MSE:HE3	1:N:114:LYS:H	1.40	0.85
1:A:43:MSE:CG	1:A:113:VAL:CG2	2.55	0.85
1:A:305:TRP:CG	1:A:305:TRP:O	2.30	0.84
1:G:31:ARG:HH22	1:G:235:GLN:HE22	1.25	0.84
1:B:43:MSE:CE	1:B:114:LYS:HB2	2.07	0.84
1:M:93:LYS:HE3	1:M:270:GLU:OE2	1.78	0.84
1:G:189:LYS:C	1:G:190:LYS:HZ3	1.84	0.84
1:A:206:GLN:O	1:A:210:GLU:HG3	1.78	0.84
1:G:142:ALA:HB3	1:G:227:MSE:HE1	1.58	0.84
1:M:125:ILE:H	1:M:125:ILE:HD12	0.72	0.84
1:A:31:ARG:NH2	1:A:235:GLN:HE21	1.75	0.83
1:B:43:MSE:CE	1:B:114:LYS:HA	2.01	0.83
1:A:85:GLY:O	1:A:88:MSE:HG2	1.77	0.83
1:B:43:MSE:CE	1:B:114:LYS:CB	2.56	0.83
1:B:261:ASN:HD22	1:B:261:ASN:C	1.85	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:174:GLU:HB3	1:G:191:LEU:HD21	0.89	0.82
1:G:187:GLN:HG2	1:G:187:GLN:O	1.76	0.82
1:G:190:LYS:HA	1:G:190:LYS:NZ	1.94	0.82
1:H:254:ARG:HD2	3:H:335:HOH:O	1.79	0.82
1:A:43:MSE:HG2	1:A:113:VAL:CG2	2.09	0.82
1:G:43:MSE:HE3	1:G:114:LYS:N	1.92	0.82
1:G:190:LYS:HZ3	1:G:190:LYS:N	1.77	0.82
1:A:170:ALA:HB1	1:A:195:VAL:HG22	1.62	0.82
1:M:161:HIS:HE1	1:N:305:TRP:CB	1.93	0.82
1:M:167:GLU:HG3	1:M:198:CYS:SG	2.20	0.82
1:A:261:ASN:C	1:A:261:ASN:HD22	1.88	0.82
1:H:169:LEU:HD23	1:H:170:ALA:CA	2.10	0.81
1:A:167:GLU:OE1	1:A:199:LYS:HG2	1.80	0.81
1:M:250:LEU:HD23	1:N:275:ILE:HG21	1.63	0.81
1:A:169:LEU:C	1:A:169:LEU:CD1	2.43	0.81
1:B:43:MSE:HE1	1:B:114:LYS:CB	2.10	0.80
1:G:190:LYS:NZ	1:G:190:LYS:N	2.30	0.80
1:A:18:SER:HA	1:B:295:MSE:HE2	1.64	0.80
1:M:264:TYR:O	1:M:267:VAL:CG1	2.30	0.80
1:H:179:THR:O	1:H:180:GLU:CB	2.30	0.80
1:G:186:GLU:CD	1:G:187:GLN:CA	2.55	0.79
1:M:169:LEU:O	1:M:169:LEU:CD1	2.30	0.79
1:A:43:MSE:HG2	1:A:113:VAL:HG21	1.63	0.79
1:B:175:MSE:CE	1:B:176:ASN:OD1	2.30	0.79
1:M:169:LEU:CD1	1:M:169:LEU:C	2.55	0.79
1:B:142:ALA:HB3	1:B:227:MSE:CE	2.12	0.79
1:B:142:ALA:HB1	1:B:226:ASN:HB3	1.64	0.79
1:G:186:GLU:OE1	1:G:187:GLN:CB	2.30	0.78
1:G:142:ALA:HB3	1:G:227:MSE:CE	2.13	0.78
1:H:261:ASN:ND2	1:H:263:SER:H	1.82	0.78
1:A:174:GLU:OE1	1:A:191:LEU:HD21	1.84	0.78
1:B:68:ARG:HD2	3:B:318:HOH:O	1.83	0.78
1:B:261:ASN:ND2	1:B:263:SER:H	1.82	0.78
1:N:202:VAL:CG2	1:N:203:GLN:N	2.47	0.77
1:G:224:MSE:HE2	1:H:299:TRP:CZ2	2.18	0.77
1:H:85:GLY:HA2	1:H:88:MSE:HE2	1.64	0.77
1:G:253:LYS:HG3	1:H:271:LEU:HD13	1.67	0.76
1:A:305:TRP:O	1:A:305:TRP:CD1	2.38	0.76
1:B:175:MSE:HE3	1:B:176:ASN:OD1	1.85	0.76
1:A:67:TRP:HB2	1:A:88:MSE:HE1	1.66	0.76
1:M:43:MSE:HE3	1:M:114:LYS:HB2	1.66	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:43:MSE:HE3	1:G:113:VAL:CG2	2.13	0.75
1:N:193:ASP:C	1:N:194:LYS:HD3	2.10	0.75
1:G:190:LYS:HZ2	1:G:190:LYS:CA	1.99	0.75
1:G:187:GLN:O	1:G:187:GLN:CG	2.34	0.75
1:B:175:MSE:C	1:B:177:SER:H	1.94	0.75
1:G:191:LEU:C	1:G:191:LEU:HD13	2.09	0.75
1:M:123:LYS:NZ	1:M:127:GLY:CA	2.47	0.75
1:M:245:LEU:HD23	1:N:80:LEU:HD22	1.68	0.75
1:M:76:GLN:HE21	1:M:77:TYR:H	1.35	0.74
1:G:142:ALA:CB	1:G:227:MSE:HE1	2.15	0.74
1:H:169:LEU:HD23	1:H:169:LEU:O	1.87	0.74
1:A:134:GLU:OE2	1:A:134:GLU:HA	1.87	0.74
1:H:201:ASP:O	1:H:205:THR:HB	1.87	0.74
1:G:227:MSE:HE2	1:G:227:MSE:HA	1.70	0.73
1:M:49:ARG:NH1	1:M:53:GLU:OE1	2.20	0.73
1:N:194:LYS:HD3	1:N:194:LYS:H	1.54	0.73
1:A:27:ARG:HD2	1:B:291:SER:HB3	1.70	0.73
1:G:186:GLU:OE1	1:G:187:GLN:HA	1.88	0.72
1:H:85:GLY:CA	1:H:88:MSE:CE	2.60	0.72
1:A:236:GLN:HE21	1:A:236:GLN:HA	1.54	0.72
1:G:190:LYS:NZ	1:G:190:LYS:CA	2.52	0.72
1:M:123:LYS:HZ2	1:M:127:GLY:HA2	1.53	0.72
1:A:307:PRO:O	1:A:308:ASP:C	2.31	0.72
1:H:177:SER:CB	1:H:191:LEU:HD11	2.18	0.72
1:M:162:LEU:C	1:M:162:LEU:CD2	2.57	0.72
1:M:163:ALA:HB1	1:M:202:VAL:HG22	1.70	0.72
1:M:161:HIS:CG	1:M:164:CYS:SG	2.82	0.72
1:M:195:VAL:O	1:M:198:CYS:SG	2.48	0.71
1:N:149:LYS:HE3	1:N:219:THR:HG21	1.71	0.71
1:B:175:MSE:HG3	1:B:176:ASN:N	2.05	0.71
1:A:167:GLU:O	1:A:171:MSE:HG3	1.91	0.71
1:G:142:ALA:CB	1:G:227:MSE:CE	2.68	0.71
1:N:43:MSE:HE1	1:N:114:LYS:CG	2.20	0.71
1:G:17:ASP:O	1:G:27:ARG:NH2	2.23	0.71
1:G:85:GLY:CA	1:G:88:MSE:HE2	2.21	0.70
1:G:216:VAL:O	1:G:220:THR:HG22	1.90	0.70
1:M:250:LEU:CD2	1:N:275:ILE:HG21	2.22	0.70
1:A:146:TRP:HZ3	1:A:220:THR:HG22	1.57	0.69
1:A:67:TRP:HB2	1:A:88:MSE:CE	2.21	0.69
1:H:146:TRP:CE2	1:H:150:MSE:HE3	2.28	0.69
1:M:272:GLU:HB2	1:N:253:LYS:HE3	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:126:MSE:HE2	1:M:126:MSE:HA	1.75	0.69
1:A:205:THR:O	1:A:208:LYS:HD2	1.94	0.68
1:G:43:MSE:HE1	1:G:114:LYS:CB	2.23	0.68
1:G:161:HIS:CD2	1:H:305:TRP:HA	2.29	0.68
1:N:31:ARG:HH22	1:N:235:GLN:HE22	1.39	0.68
1:A:99:GLN:HA	1:A:99:GLN:NE2	2.09	0.68
1:G:143:GLN:HG2	3:G:321:HOH:O	1.93	0.68
1:M:43:MSE:HE1	1:M:114:LYS:CA	2.23	0.68
1:A:43:MSE:HG3	1:A:113:VAL:HG21	1.74	0.68
1:A:43:MSE:SE	1:A:113:VAL:HG23	2.43	0.68
1:B:31:ARG:HH22	1:B:235:GLN:NE2	1.89	0.68
1:N:31:ARG:HH22	1:N:235:GLN:NE2	1.90	0.68
1:M:43:MSE:HG2	1:M:110:LEU:CD2	2.23	0.68
1:N:93:LYS:NZ	1:N:270:GLU:OE1	2.26	0.68
1:M:169:LEU:HD13	1:M:169:LEU:C	2.10	0.67
1:G:191:LEU:HD12	1:G:192:GLN:CA	2.25	0.67
1:M:164:CYS:SG	1:M:165:LYS:N	2.67	0.67
1:M:123:LYS:HZ1	1:M:127:GLY:CA	2.07	0.67
1:A:173:ARG:NH1	1:A:194:LYS:NZ	2.43	0.67
1:B:130:LYS:O	1:B:134:GLU:HG3	1.94	0.67
1:N:57:GLY:O	1:N:61:THR:HG23	1.95	0.67
1:N:301:GLN:HG2	1:N:302:PHE:N	2.08	0.67
1:G:186:GLU:OE1	1:G:187:GLN:CA	2.41	0.67
1:H:261:ASN:HD22	1:H:263:SER:H	1.41	0.67
1:A:162:LEU:CD2	1:A:163:ALA:N	2.58	0.66
1:G:43:MSE:CE	1:G:113:VAL:HG22	2.22	0.66
1:A:169:LEU:HD13	1:A:170:ALA:HA	1.77	0.66
1:B:71:ILE:HD12	1:B:88:MSE:HE1	1.76	0.66
1:H:174:GLU:HA	1:H:191:LEU:HD21	1.78	0.66
1:M:43:MSE:CE	1:M:114:LYS:CA	2.73	0.66
1:M:142:ALA:HB1	1:M:226:ASN:HB3	1.77	0.66
1:M:17:ASP:O	1:M:27:ARG:NH2	2.29	0.65
1:A:257:ASN:HD21	1:A:259:ALA:HB3	1.61	0.65
1:G:43:MSE:HE2	1:G:114:LYS:HB2	1.77	0.65
1:A:169:LEU:O	1:A:169:LEU:CD2	2.30	0.65
1:H:85:GLY:CA	1:H:88:MSE:HE1	2.19	0.65
1:A:143:GLN:CB	1:A:227:MSE:CE	2.70	0.65
1:A:305:TRP:CZ2	1:A:307:PRO:HG3	2.31	0.65
1:M:162:LEU:HD23	1:M:163:ALA:N	2.12	0.65
1:A:275:ILE:HG21	1:B:250:LEU:HD13	1.78	0.65
1:M:292:GLY:O	1:M:295:MSE:HB2	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:166:GLU:O	1:H:169:LEU:HB3	1.97	0.65
1:N:193:ASP:H	1:N:194:LYS:NZ	1.95	0.65
1:N:202:VAL:HG22	1:N:203:GLN:N	2.11	0.65
1:A:302:PHE:C	1:A:302:PHE:CD2	2.75	0.64
1:B:124:GLN:O	1:B:127:GLY:HA3	1.97	0.64
1:B:142:ALA:CB	1:B:227:MSE:HE2	2.26	0.64
1:G:186:GLU:CG	1:G:187:GLN:HA	2.27	0.64
1:G:304:GLU:O	1:G:305:TRP:C	2.37	0.64
1:H:261:ASN:HD22	1:H:261:ASN:C	2.06	0.64
1:A:216:VAL:O	1:A:220:THR:HG23	1.98	0.64
1:A:225:GLU:O	1:A:229:GLN:HG2	1.98	0.64
1:B:175:MSE:HG3	1:B:176:ASN:H	1.63	0.64
1:M:80:LEU:HD22	1:N:245:LEU:CD1	2.26	0.63
1:N:49:ARG:NH1	1:N:53:GLU:OE2	2.31	0.63
1:A:160:TYR:HA	1:A:205:THR:CG2	2.29	0.63
1:A:305:TRP:O	1:A:306:ASN:C	2.40	0.63
1:N:158:LYS:HA	1:N:161:HIS:HB2	1.80	0.63
1:B:238:GLU:OE2	1:B:241:ARG:NH2	2.32	0.62
1:B:261:ASN:ND2	1:B:263:SER:N	2.47	0.62
1:H:192:GLN:HA	1:H:195:VAL:HB	1.80	0.62
1:A:69:GLN:HG3	1:A:73:LYS:HE2	1.80	0.62
1:A:93:LYS:HE2	1:A:270:GLU:OE2	1.99	0.62
1:A:169:LEU:C	1:A:169:LEU:CD2	2.51	0.62
1:M:253:LYS:HE3	1:N:272:GLU:HB2	1.81	0.62
1:A:31:ARG:NH2	1:A:235:GLN:NE2	2.47	0.62
1:A:223:TYR:CE1	1:A:227:MSE:CE	2.71	0.62
1:B:17:ASP:O	1:B:27:ARG:NH2	2.31	0.62
1:B:261:ASN:HD21	1:B:263:SER:H	1.46	0.62
1:G:43:MSE:CE	1:G:114:LYS:CB	2.77	0.62
1:G:275:ILE:HG21	1:H:250:LEU:HD13	1.81	0.62
1:N:227:MSE:HE2	1:N:227:MSE:HA	1.80	0.62
1:G:43:MSE:CE	1:G:114:LYS:HB2	2.29	0.62
1:G:189:LYS:C	1:G:190:LYS:HZ2	2.08	0.62
1:B:175:MSE:CG	1:B:176:ASN:N	2.62	0.62
1:H:140:ARG:HG3	1:H:140:ARG:HH11	1.65	0.62
1:A:261:ASN:ND2	1:A:263:SER:H	1.98	0.61
1:G:261:ASN:O	1:G:265:ILE:HD13	1.99	0.61
1:H:267:VAL:HG22	1:H:268:TYR:CD2	2.34	0.61
1:H:54:LYS:HB2	1:H:102:LYS:HD3	1.82	0.61
1:G:212:VAL:O	1:G:216:VAL:HG23	2.00	0.61
1:H:126:MSE:SE	1:H:126:MSE:N	2.78	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:250:LEU:O	1:N:251:ASP:C	2.43	0.61
1:G:191:LEU:HD12	1:G:192:GLN:H	1.60	0.61
1:M:37:ARG:HG3	1:M:38:LEU:N	2.10	0.61
1:M:170:ALA:HB1	1:M:195:VAL:CG2	2.29	0.61
1:G:167:GLU:OE1	1:G:199:LYS:CE	2.40	0.61
1:B:261:ASN:C	1:B:261:ASN:ND2	2.56	0.61
1:M:157:LYS:NZ	1:N:303:GLU:CB	2.64	0.61
1:G:239:GLU:HG3	1:H:284:LEU:HD11	1.83	0.61
1:G:253:LYS:CD	1:H:272:GLU:HG3	2.31	0.60
1:M:43:MSE:HE3	1:M:114:LYS:N	2.15	0.60
1:G:43:MSE:HE2	1:G:114:LYS:N	2.16	0.60
1:G:162:LEU:HD23	1:G:162:LEU:O	2.01	0.60
1:N:123:LYS:HD2	1:N:124:GLN:O	2.00	0.60
1:A:99:GLN:HA	1:A:99:GLN:HE21	1.64	0.60
1:A:266:HIS:CE1	1:A:269:ARG:NH1	2.69	0.60
1:M:90:GLU:OE2	1:N:49:ARG:NH2	2.28	0.60
1:M:275:ILE:CG2	1:N:250:LEU:HD13	2.30	0.60
1:M:155:ALA:HA	1:M:158:LYS:CE	2.16	0.60
1:B:142:ALA:CB	1:B:227:MSE:CE	2.80	0.60
1:G:153:LEU:HD11	1:G:213:LEU:CD1	2.32	0.60
1:M:43:MSE:HE2	1:M:114:LYS:HB2	1.80	0.60
1:N:122:HIS:HE1	3:N:321:HOH:O	1.83	0.60
1:B:261:ASN:HD22	1:B:262:SER:N	1.99	0.60
1:N:37:ARG:O	1:N:40:ASN:HB2	2.02	0.59
1:A:162:LEU:HD23	1:A:163:ALA:N	2.12	0.59
1:H:169:LEU:HD23	1:H:170:ALA:HA	1.84	0.59
1:A:261:ASN:HD22	1:A:262:SER:N	2.00	0.59
1:N:43:MSE:CE	1:N:114:LYS:H	2.02	0.59
1:A:44:ASN:O	1:A:48:GLU:HG3	2.03	0.59
1:B:172:THR:O	1:B:175:MSE:HG3	2.02	0.59
1:M:241:ARG:HH12	1:N:76:GLN:HE22	1.50	0.59
1:M:226:ASN:N	1:M:226:ASN:HD22	2.00	0.59
1:A:80:LEU:HD12	1:B:245:LEU:HD13	1.85	0.59
1:A:160:TYR:HA	1:A:205:THR:HG23	1.84	0.59
1:A:153:LEU:HD23	1:A:153:LEU:C	2.26	0.59
1:G:43:MSE:CE	1:G:114:LYS:H	2.14	0.59
1:G:162:LEU:HD23	1:G:162:LEU:C	2.28	0.58
1:M:31:ARG:NH2	1:M:235:GLN:HE21	2.01	0.58
1:M:87:ILE:O	1:M:90:GLU:HG3	2.02	0.58
1:M:85:GLY:O	1:M:88:MSE:HG2	2.04	0.58
1:M:239:GLU:HG3	1:N:284:LEU:HD11	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:43:MSE:HE3	1:G:113:VAL:C	2.28	0.58
1:G:128:GLY:C	1:G:133:LYS:HE2	2.29	0.58
1:M:49:ARG:NH2	1:N:90:GLU:OE2	2.26	0.58
1:M:162:LEU:HD23	1:M:162:LEU:O	2.02	0.58
1:M:245:LEU:CD2	1:N:80:LEU:HD22	2.33	0.58
1:N:216:VAL:HA	1:N:219:THR:HG22	1.86	0.58
1:M:25:TYR:CD2	1:M:139:PHE:CB	2.87	0.58
1:M:109:ASP:O	1:M:113:VAL:HG13	2.04	0.58
1:B:175:MSE:C	1:B:177:SER:N	2.58	0.57
1:G:69:GLN:NE2	1:G:73:LYS:HG3	2.19	0.57
1:G:144:LYS:HB3	1:G:145:PRO:HD3	1.86	0.57
1:H:85:GLY:CA	1:H:88:MSE:HE2	2.33	0.57
1:M:281:GLN:H	1:M:281:GLN:NE2	2.01	0.57
1:G:153:LEU:HD11	1:G:213:LEU:HD12	1.85	0.57
1:G:160:TYR:HE1	1:G:206:GLN:HE21	1.52	0.57
1:H:87:ILE:O	1:H:90:GLU:HG3	2.04	0.57
1:M:242:LEU:HD22	1:N:80:LEU:HD13	1.86	0.57
1:B:64:ALA:HA	1:B:88:MSE:HG3	1.87	0.57
1:H:44:ASN:O	1:H:48:GLU:HG3	2.04	0.57
1:H:305:TRP:C	1:H:306:ASN:HD22	2.11	0.57
1:N:193:ASP:H	1:N:194:LYS:HZ2	1.52	0.57
1:B:179:THR:O	1:B:179:THR:HG22	2.05	0.57
1:G:150:MSE:HE1	1:H:300:PRO:HG3	1.86	0.57
1:M:170:ALA:CB	1:M:195:VAL:HG22	2.29	0.57
1:B:71:ILE:HD11	1:B:84:TRP:CE2	2.39	0.57
1:M:286:TRP:O	1:M:290:THR:HB	2.05	0.57
1:M:48:GLU:OE2	1:N:66:ARG:NH2	2.38	0.57
1:G:254:ARG:HD3	3:G:312:HOH:O	2.04	0.57
1:H:261:ASN:HD22	1:H:263:SER:N	2.01	0.56
1:M:123:LYS:HZ1	1:M:128:GLY:N	2.03	0.56
1:B:43:MSE:CE	1:B:114:LYS:H	2.16	0.56
1:B:175:MSE:O	1:B:177:SER:N	2.30	0.56
1:M:284:LEU:HD11	1:N:239:GLU:HB2	1.86	0.56
1:G:71:ILE:HD12	1:G:88:MSE:CE	2.35	0.56
1:M:22:VAL:HA	1:M:143:GLN:HE22	1.70	0.56
1:M:84:TRP:O	1:M:88:MSE:HE3	2.05	0.56
1:G:186:GLU:CD	1:G:187:GLN:CB	2.79	0.56
1:H:279:ASP:OD2	1:H:282:GLU:HB2	2.05	0.56
1:H:302:PHE:HE1	1:H:304:GLU:OE1	1.87	0.56
1:G:286:TRP:O	1:G:290:THR:HB	2.05	0.56
1:M:257:ASN:OD1	1:M:260:GLU:HG3	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:31:ARG:HH22	1:H:235:GLN:HE22	1.53	0.55
1:M:44:ASN:O	1:M:48:GLU:HG3	2.06	0.55
1:A:298:ASN:ND2	1:B:15:THR:HG23	2.21	0.55
1:B:126:MSE:N	1:B:127:GLY:HA2	2.22	0.55
1:H:238:GLU:HG3	1:H:238:GLU:O	2.05	0.55
1:M:123:LYS:HZ1	1:M:128:GLY:H	1.54	0.55
1:M:80:LEU:CD2	1:N:245:LEU:HD13	2.30	0.55
1:N:160:TYR:CB	3:N:6:HOH:O	2.55	0.55
1:A:307:PRO:HD2	1:A:308:ASP:H	1.72	0.55
1:G:220:THR:OG1	1:G:224:MSE:HE3	2.06	0.55
1:H:146:TRP:CD2	1:H:150:MSE:HE3	2.41	0.55
1:N:258:LEU:O	1:N:261:ASN:CB	2.54	0.55
1:A:185:PRO:N	1:A:188:GLN:HG2	2.22	0.55
1:H:83:ALA:HB2	1:H:278:ALA:HB2	1.87	0.55
1:A:216:VAL:O	1:A:220:THR:CG2	2.56	0.54
1:G:253:LYS:HD2	1:H:272:GLU:HG3	1.88	0.54
1:G:304:GLU:CA	1:H:161:HIS:NE2	2.70	0.54
1:A:261:ASN:C	1:A:261:ASN:ND2	2.57	0.54
1:A:281:GLN:H	1:A:281:GLN:NE2	2.05	0.54
1:B:125:ILE:HG23	1:B:126:MSE:SE	2.57	0.54
1:A:146:TRP:CZ3	1:A:220:THR:HG22	2.41	0.54
1:B:235:GLN:HE21	1:B:235:GLN:HA	1.73	0.54
1:A:303:GLU:O	1:B:161:HIS:HE1	1.89	0.54
1:G:264:TYR:OH	1:H:258:LEU:HB2	2.08	0.54
1:H:169:LEU:CD2	1:H:170:ALA:CA	2.82	0.54
1:M:93:LYS:CE	1:M:270:GLU:OE2	2.55	0.54
1:N:17:ASP:O	1:N:27:ARG:NH2	2.41	0.54
1:A:43:MSE:CG	1:A:113:VAL:HG23	2.38	0.54
1:M:227:MSE:HA	1:M:227:MSE:CE	2.38	0.54
1:A:76:GLN:HE21	1:A:77:TYR:H	1.56	0.53
1:A:275:ILE:CG2	1:B:250:LEU:HD13	2.38	0.53
1:M:124:GLN:O	1:M:126:MSE:O	2.26	0.53
1:G:161:HIS:HD2	1:H:305:TRP:HA	1.74	0.53
1:A:104:ASN:O	1:A:105:LEU:C	2.47	0.53
1:M:25:TYR:CE2	1:M:139:PHE:CB	2.92	0.53
1:M:241:ARG:NH1	1:N:76:GLN:HE22	2.06	0.53
1:G:190:LYS:HA	1:G:190:LYS:CE	2.39	0.53
1:A:266:HIS:ND1	1:A:269:ARG:NH1	2.57	0.52
1:H:31:ARG:HH12	1:H:235:GLN:HE21	1.56	0.52
1:B:143:GLN:NE2	1:B:223:TYR:OH	2.42	0.52
1:G:31:ARG:HH22	1:G:235:GLN:NE2	2.02	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:76:GLN:NE2	1:M:77:TYR:H	2.03	0.52
1:A:266:HIS:CE1	1:A:269:ARG:HH12	2.27	0.52
1:M:43:MSE:HE3	1:M:114:LYS:CA	2.40	0.52
1:A:173:ARG:NH1	1:A:194:LYS:HZ3	2.06	0.52
1:A:31:ARG:HH22	1:A:235:GLN:HE21	1.53	0.52
1:H:305:TRP:O	1:H:306:ASN:ND2	2.30	0.52
1:B:109:ASP:OD2	1:B:255:HIS:ND1	2.31	0.51
1:H:37:ARG:O	1:H:40:ASN:HB2	2.10	0.51
1:N:206:GLN:O	1:N:207:GLU:C	2.46	0.51
1:B:71:ILE:HD12	1:B:88:MSE:CE	2.39	0.51
1:G:261:ASN:C	1:G:261:ASN:OD1	2.52	0.51
1:M:257:ASN:HD21	1:M:259:ALA:HB3	1.76	0.51
1:B:160:TYR:O	1:B:161:HIS:C	2.52	0.51
1:G:80:LEU:HD22	1:H:245:LEU:HD13	1.92	0.51
1:N:108:GLU:O	1:N:112:LYS:HB2	2.10	0.51
1:N:194:LYS:CD	1:N:194:LYS:H	2.15	0.51
1:G:281:GLN:CD	1:G:281:GLN:H	2.17	0.51
1:H:171:MSE:SE	1:H:171:MSE:H	2.40	0.51
1:B:126:MSE:N	1:B:127:GLY:CA	2.73	0.51
1:G:43:MSE:CE	1:G:114:LYS:HA	2.06	0.51
1:H:67:TRP:O	1:H:71:ILE:HG13	2.11	0.51
1:M:196:ASP:O	1:M:200:GLN:HB2	2.11	0.51
1:N:258:LEU:O	1:N:261:ASN:HB2	2.11	0.51
1:A:174:GLU:OE1	1:A:191:LEU:HD11	2.11	0.51
1:B:31:ARG:NH2	1:B:235:GLN:HE22	1.91	0.51
1:M:123:LYS:NZ	1:M:128:GLY:N	2.58	0.51
1:M:25:TYR:CD2	1:M:139:PHE:CG	3.00	0.50
1:M:238:GLU:O	1:M:238:GLU:HG3	2.11	0.50
1:N:87:ILE:O	1:N:90:GLU:HG3	2.12	0.50
1:A:134:GLU:OE2	1:A:134:GLU:CA	2.54	0.50
1:B:281:GLN:HA	1:B:281:GLN:HE21	1.76	0.50
1:G:69:GLN:HE22	1:G:73:LYS:HD2	1.76	0.50
1:H:286:TRP:O	1:H:290:THR:OG1	2.30	0.50
1:G:154:GLU:OE2	1:G:154:GLU:HA	2.11	0.50
1:H:167:GLU:OE2	1:H:199:LYS:HG2	2.12	0.50
1:B:146:TRP:O	1:B:150:MSE:HB2	2.11	0.50
1:N:197:LYS:O	1:N:201:ASP:OD2	2.30	0.50
1:N:253:LYS:HD3	1:N:253:LYS:C	2.36	0.50
1:A:76:GLN:NE2	1:A:77:TYR:H	2.10	0.50
1:A:162:LEU:HD22	1:A:163:ALA:N	2.27	0.50
1:N:202:VAL:HG23	1:N:203:GLN:N	2.23	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:41:ASP:O	1:N:42:LEU:C	2.54	0.50
1:G:227:MSE:CE	1:G:227:MSE:HA	2.40	0.49
1:M:125:ILE:CD1	1:M:125:ILE:N	2.30	0.49
1:N:205:THR:O	1:N:208:LYS:HB3	2.12	0.49
1:B:176:ASN:O	1:B:177:SER:CB	2.60	0.49
1:G:187:GLN:O	1:G:187:GLN:OE1	2.30	0.49
1:G:304:GLU:O	1:G:306:ASN:O	2.30	0.49
1:A:307:PRO:O	1:A:308:ASP:O	2.30	0.49
1:G:71:ILE:HD11	1:G:84:TRP:CE2	2.47	0.49
1:M:43:MSE:CE	1:M:114:LYS:CG	2.81	0.49
1:N:301:GLN:CG	1:N:302:PHE:N	2.73	0.49
1:G:162:LEU:C	1:G:162:LEU:CD2	2.86	0.49
1:H:170:ALA:HB1	1:H:195:VAL:CG2	2.36	0.49
1:N:43:MSE:HE3	1:N:113:VAL:C	2.30	0.49
1:A:173:ARG:NH1	1:A:194:LYS:HZ2	2.10	0.49
1:M:169:LEU:C	1:M:169:LEU:HD12	2.37	0.49
1:A:201:ASP:O	1:A:205:THR:HB	2.13	0.49
1:M:25:TYR:CE2	1:M:139:PHE:HB2	2.48	0.49
1:M:25:TYR:H	1:M:25:TYR:HD1	1.56	0.49
1:M:194:LYS:NZ	1:M:194:LYS:HB3	2.28	0.49
1:N:202:VAL:O	1:N:205:THR:OG1	2.30	0.49
1:N:299:TRP:HE3	1:N:300:PRO:HD2	1.77	0.49
1:A:37:ARG:CG	1:A:37:ARG:NH2	2.50	0.48
1:G:110:LEU:C	1:G:110:LEU:CD2	2.87	0.48
1:G:235:GLN:HE21	1:G:235:GLN:HA	1.78	0.48
1:M:250:LEU:CD2	1:N:275:ILE:CG2	2.91	0.48
1:M:222:GLN:HA	1:M:222:GLN:NE2	2.28	0.48
1:G:208:LYS:O	1:G:212:VAL:HG23	2.14	0.48
1:B:286:TRP:O	1:B:290:THR:HB	2.14	0.48
1:H:25:TYR:CD1	1:H:25:TYR:C	2.91	0.48
1:M:43:MSE:HE1	1:M:114:LYS:HA	1.95	0.48
1:N:144:LYS:O	1:N:148:LYS:HG3	2.13	0.48
1:G:142:ALA:HB1	1:G:226:ASN:HB3	1.94	0.48
1:B:176:ASN:O	1:B:177:SER:OG	2.30	0.47
1:M:43:MSE:HG2	1:M:110:LEU:HD23	1.95	0.47
1:A:76:GLN:OE1	1:B:241:ARG:NH1	2.47	0.47
1:G:142:ALA:HB1	1:G:227:MSE:CE	2.43	0.47
1:M:227:MSE:HA	1:M:227:MSE:HE2	1.95	0.47
1:B:261:ASN:HD22	1:B:263:SER:N	2.12	0.47
1:B:297:MSE:HG2	1:B:299:TRP:CE2	2.49	0.47
1:G:37:ARG:O	1:G:40:ASN:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:197:LYS:HA	1:G:197:LYS:HD3	1.44	0.47
1:M:161:HIS:CE1	1:M:164:CYS:SG	3.06	0.47
1:M:257:ASN:C	1:M:257:ASN:ND2	2.72	0.47
1:G:216:VAL:O	1:G:220:THR:CG2	2.62	0.47
1:G:235:GLN:NE2	1:G:235:GLN:HA	2.30	0.47
1:H:85:GLY:C	1:H:88:MSE:HE2	2.39	0.47
1:B:85:GLY:CA	1:B:88:MSE:HE2	2.38	0.47
1:G:284:LEU:HD11	1:H:239:GLU:HG3	1.95	0.47
1:M:217:GLY:O	1:M:220:THR:HG22	2.14	0.47
1:H:191:LEU:O	1:H:195:VAL:HG23	2.14	0.47
1:A:180:GLU:HG2	1:A:183:VAL:HB	1.96	0.47
1:G:43:MSE:HE2	1:G:114:LYS:H	1.78	0.47
1:G:170:ALA:O	1:G:195:VAL:HG12	2.14	0.47
1:G:227:MSE:HE2	1:G:227:MSE:CA	2.40	0.47
1:G:304:GLU:C	1:G:306:ASN:O	2.57	0.47
1:M:167:GLU:CG	1:M:198:CYS:SG	2.97	0.47
1:N:142:ALA:HB1	1:N:226:ASN:HB3	1.96	0.47
1:B:142:ALA:C	1:B:227:MSE:HE3	2.39	0.47
1:M:157:LYS:HZ1	1:N:303:GLU:CB	2.26	0.47
1:N:123:LYS:HE2	1:N:123:LYS:HB3	1.55	0.47
1:A:302:PHE:C	1:A:302:PHE:HD2	2.23	0.46
1:G:253:LYS:NZ	1:H:272:GLU:HG3	2.29	0.46
1:N:140:ARG:HG3	1:N:141:LYS:N	2.30	0.46
1:A:222:GLN:HA	1:A:222:GLN:HE21	1.79	0.46
1:B:38:LEU:HD23	1:B:38:LEU:HA	1.74	0.46
1:H:162:LEU:O	1:H:166:GLU:HG2	2.14	0.46
1:M:25:TYR:CD2	1:M:139:PHE:HB3	2.50	0.46
1:N:142:ALA:HB3	1:N:227:MSE:HE3	1.96	0.46
1:H:54:LYS:HB2	1:H:102:LYS:CD	2.46	0.46
1:N:201:ASP:O	1:N:205:THR:OG1	2.22	0.46
1:A:144:LYS:HB3	1:A:145:PRO:HD3	1.97	0.46
1:G:281:GLN:H	1:G:281:GLN:NE2	2.14	0.46
1:H:40:ASN:HA	1:H:43:MSE:CE	2.44	0.46
1:H:267:VAL:HG22	1:H:268:TYR:CE2	2.51	0.46
1:B:122:HIS:HD2	1:B:131:GLU:OE2	1.98	0.46
1:H:261:ASN:HD22	1:H:262:SER:N	2.13	0.46
1:M:129:PHE:O	1:M:130:LYS:C	2.58	0.46
1:A:224:MSE:O	1:A:228:GLU:HB2	2.15	0.46
1:B:54:LYS:HB2	1:B:102:LYS:HD2	1.98	0.46
1:G:142:ALA:HB3	1:G:227:MSE:HE2	1.95	0.46
1:B:85:GLY:HA2	1:B:88:MSE:HE1	1.90	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:31:ARG:HH12	1:G:235:GLN:HE21	1.63	0.46
1:A:257:ASN:ND2	1:A:259:ALA:H	2.14	0.46
1:B:261:ASN:ND2	1:B:262:SER:N	2.62	0.46
1:G:174:GLU:HG2	1:G:191:LEU:HD11	1.96	0.46
1:G:90:GLU:OE2	1:H:49:ARG:NH2	2.48	0.46
1:A:224:MSE:HE3	1:B:299:TRP:CZ2	2.51	0.45
1:G:275:ILE:CG2	1:H:250:LEU:HD13	2.45	0.45
1:A:174:GLU:OE2	1:A:195:VAL:HG21	2.16	0.45
1:G:110:LEU:C	1:G:110:LEU:HD23	2.42	0.45
1:H:271:LEU:HD22	1:H:275:ILE:CD1	2.46	0.45
1:A:83:ALA:O	1:A:86:ALA:HB3	2.17	0.45
1:A:302:PHE:CD2	1:A:303:GLU:N	2.84	0.45
1:G:189:LYS:O	1:G:190:LYS:NZ	2.48	0.45
1:M:20:TRP:HB2	1:N:297:MSE:SE	2.67	0.45
1:M:196:ASP:OD1	1:M:196:ASP:N	2.48	0.45
1:N:244:PHE:O	1:N:248:VAL:HG23	2.16	0.45
1:N:258:LEU:O	1:N:261:ASN:HB3	2.17	0.45
1:H:31:ARG:HH22	1:H:235:GLN:NE2	2.15	0.45
1:N:38:LEU:HD13	1:N:241:ARG:NH1	2.31	0.45
1:A:70:LEU:HD23	1:A:70:LEU:HA	1.73	0.45
1:A:99:GLN:HE21	1:A:99:GLN:CA	2.25	0.45
1:M:258:LEU:HD23	1:M:258:LEU:HA	1.73	0.45
1:M:262:SER:O	1:M:266:HIS:CD2	2.69	0.45
1:G:71:ILE:CD1	1:G:88:MSE:HE1	2.46	0.45
1:A:224:MSE:HE3	1:B:299:TRP:HZ2	1.82	0.45
1:M:28:THR:O	1:M:32:ILE:HD12	2.15	0.45
1:G:175:MSE:O	1:G:176:ASN:CB	2.64	0.45
1:H:57:GLY:O	1:H:95:SER:OG	2.28	0.45
1:N:57:GLY:HA3	1:N:99:GLN:HE22	1.80	0.45
1:M:123:LYS:NZ	1:M:127:GLY:C	2.75	0.44
1:B:253:LYS:C	1:B:253:LYS:HE2	2.42	0.44
1:G:191:LEU:HD13	1:G:191:LEU:O	2.17	0.44
1:G:227:MSE:CE	1:G:227:MSE:CA	2.95	0.44
1:G:303:GLU:O	1:G:304:GLU:C	2.56	0.44
1:M:25:TYR:CE2	1:M:139:PHE:HB3	2.52	0.44
1:B:104:ASN:HB3	1:B:255:HIS:CG	2.53	0.44
1:A:56:TYR:CD1	1:B:56:TYR:HB2	2.52	0.44
1:B:51:LYS:HE3	1:M:127:GLY:H	1.82	0.44
1:N:77:TYR:N	1:N:77:TYR:CD1	2.85	0.44
1:N:141:LYS:HG3	1:N:142:ALA:N	2.32	0.44
1:A:232:GLU:O	1:A:236:GLN:HG2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:169:LEU:CD2	1:H:170:ALA:HA	2.46	0.44
1:A:31:ARG:HH21	1:A:235:GLN:NE2	2.15	0.44
1:G:85:GLY:HA2	1:G:88:MSE:HE1	1.92	0.44
1:M:31:ARG:NH2	1:M:235:GLN:NE2	2.65	0.44
1:A:160:TYR:HA	1:A:205:THR:HG21	1.97	0.44
1:G:289:SER:O	1:G:289:SER:OG	2.32	0.44
1:H:49:ARG:HD2	1:H:53:GLU:OE2	2.18	0.44
1:H:261:ASN:ND2	1:H:261:ASN:C	2.74	0.44
1:M:157:LYS:HZ2	1:N:303:GLU:CB	2.31	0.44
1:N:61:THR:HG22	1:N:95:SER:OG	2.18	0.44
1:B:279:ASP:OD2	1:B:282:GLU:HB2	2.18	0.43
1:G:110:LEU:HD23	1:G:110:LEU:O	2.18	0.43
1:G:174:GLU:HG2	1:G:191:LEU:CD1	2.48	0.43
1:A:261:ASN:ND2	1:A:263:SER:HB2	2.33	0.43
1:G:160:TYR:HA	1:G:205:THR:CG2	2.48	0.43
1:H:18:SER:O	1:H:24:ASN:ND2	2.50	0.43
1:G:38:LEU:HD23	1:G:38:LEU:HA	1.76	0.43
1:H:169:LEU:HD22	1:H:170:ALA:N	2.28	0.43
1:M:104:ASN:O	1:M:105:LEU:C	2.59	0.43
1:H:144:LYS:HB3	1:H:145:PRO:HD3	2.01	0.43
1:N:199:LYS:O	1:N:202:VAL:HG22	2.18	0.43
1:A:220:THR:N	1:A:221:PRO:CD	2.82	0.43
1:B:167:GLU:OE2	1:B:199:LYS:HD2	2.19	0.43
1:A:271:LEU:O	1:A:272:GLU:C	2.58	0.43
1:G:291:SER:HB3	1:H:27:ARG:HD2	2.00	0.43
1:H:85:GLY:O	1:H:88:MSE:HE2	2.18	0.43
1:A:174:GLU:CD	1:A:191:LEU:HD21	2.42	0.43
1:B:187:GLN:O	1:B:190:LYS:N	2.48	0.43
1:M:144:LYS:N	1:M:145:PRO:HD2	2.34	0.43
1:N:43:MSE:CE	1:N:114:LYS:HA	2.26	0.43
1:B:220:THR:O	1:B:224:MSE:HG3	2.18	0.43
1:N:23:GLY:HA2	1:N:25:TYR:CE2	2.53	0.43
1:G:128:GLY:HA3	1:G:133:LYS:NZ	2.26	0.43
1:G:264:TYR:O	1:G:267:VAL:HG13	2.18	0.43
1:H:248:VAL:O	1:H:251:ASP:HB2	2.19	0.43
1:N:261:ASN:HD22	1:N:261:ASN:HA	1.44	0.43
1:M:142:ALA:HB3	1:M:227:MSE:CE	2.49	0.42
1:A:33:ASP:O	1:A:34:ASP:C	2.62	0.42
1:M:224:MSE:HE2	1:N:299:TRP:CZ2	2.54	0.42
1:M:257:ASN:C	1:M:257:ASN:HD22	2.27	0.42
1:N:216:VAL:CG2	1:N:217:GLY:N	2.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ARG:CD	1:B:291:SER:HB3	2.43	0.42
1:A:106:LEU:HA	1:A:106:LEU:HD23	1.71	0.42
1:B:144:LYS:HB3	1:B:145:PRO:HD3	2.00	0.42
1:G:160:TYR:CD2	1:G:160:TYR:C	2.97	0.42
1:M:144:LYS:O	1:M:145:PRO:C	2.62	0.42
1:H:40:ASN:HA	1:H:43:MSE:HE3	2.02	0.42
1:H:139:PHE:CE2	1:H:230:VAL:HG23	2.54	0.42
1:B:288:ARG:O	1:B:289:SER:C	2.59	0.42
1:M:23:GLY:HA2	1:M:25:TYR:CE1	2.54	0.42
1:N:117:GLN:HE21	1:N:117:GLN:HB3	1.64	0.42
1:N:144:LYS:N	1:N:145:PRO:HD2	2.35	0.42
1:N:202:VAL:HG22	1:N:203:GLN:H	1.79	0.42
1:B:80:LEU:HD13	1:B:80:LEU:HA	1.89	0.42
1:M:23:GLY:HA2	1:M:25:TYR:HE1	1.85	0.42
1:M:163:ALA:O	1:M:164:CYS:C	2.61	0.42
1:G:23:GLY:O	1:G:26:LYS:HG2	2.20	0.42
1:G:71:ILE:HD12	1:G:88:MSE:HE1	2.01	0.42
1:M:130:LYS:O	1:M:134:GLU:HB2	2.20	0.42
1:M:244:PHE:O	1:M:248:VAL:HG23	2.20	0.42
1:M:297:MSE:HG2	1:M:299:TRP:CE2	2.55	0.42
1:N:131:GLU:H	1:N:131:GLU:CD	2.28	0.42
1:B:27:ARG:HA	1:B:30:LYS:HD2	2.02	0.42
1:M:125:ILE:C	1:M:126:MSE:O	2.54	0.42
1:M:137:ASP:O	1:M:138:GLY:C	2.63	0.42
1:A:179:THR:HA	1:A:180:GLU:HA	1.80	0.42
1:B:142:ALA:CB	1:B:226:ASN:HB3	2.43	0.42
1:G:304:GLU:C	1:G:306:ASN:N	2.70	0.42
1:M:287:PHE:CD2	1:N:31:ARG:NH2	2.87	0.42
1:A:306:ASN:HA	1:A:307:PRO:HD3	1.70	0.41
1:B:57:GLY:O	1:B:58:GLN:C	2.61	0.41
1:M:155:ALA:O	1:M:158:LYS:CG	2.57	0.41
1:B:67:TRP:O	1:B:71:ILE:HG13	2.20	0.41
1:M:293:PRO:HD2	1:N:231:PHE:CE2	2.55	0.41
1:N:220:THR:HB	1:N:221:PRO:HD3	2.01	0.41
1:G:174:GLU:HA	1:G:175:MSE:HA	1.69	0.41
1:B:160:TYR:CE2	1:B:206:GLN:HG3	2.55	0.41
1:G:307:PRO:HG2	1:H:165:LYS:HG2	2.02	0.41
1:M:264:TYR:HA	1:M:267:VAL:CG1	2.50	0.41
1:B:43:MSE:HE3	1:B:113:VAL:C	2.40	0.41
1:B:54:LYS:HB2	1:B:102:LYS:CD	2.51	0.41
1:G:187:GLN:O	1:G:187:GLN:CD	2.62	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:22:VAL:HG13	1:N:143:GLN:OE1	2.19	0.41
1:M:43:MSE:HE2	1:M:110:LEU:HD23	2.03	0.41
1:B:208:LYS:HA	1:B:208:LYS:HD2	1.86	0.41
1:G:173:ARG:O	1:G:191:LEU:CD2	2.69	0.41
1:H:80:LEU:HD13	1:H:80:LEU:HA	1.91	0.41
1:A:64:ALA:HA	1:A:88:MSE:HE2	2.02	0.41
1:A:80:LEU:HD13	1:A:80:LEU:HA	1.95	0.41
1:B:235:GLN:NE2	1:B:235:GLN:HA	2.34	0.41
1:B:250:LEU:HD12	1:B:250:LEU:HA	1.83	0.41
1:B:295:MSE:HA	1:B:296:PRO:HD3	1.97	0.41
1:G:250:LEU:HD12	1:G:250:LEU:HA	1.93	0.41
1:H:24:ASN:C	1:H:26:LYS:H	2.29	0.41
1:H:217:GLY:HA2	1:H:220:THR:CG2	2.51	0.41
1:H:261:ASN:ND2	1:H:263:SER:N	2.57	0.41
1:M:246:LYS:NZ	1:N:278:ALA:O	2.54	0.41
1:N:125:ILE:H	1:N:125:ILE:HD12	1.86	0.41
1:G:160:TYR:HA	1:G:205:THR:HG23	2.02	0.41
1:N:144:LYS:O	1:N:145:PRO:C	2.63	0.41
1:B:31:ARG:HH12	1:B:235:GLN:NE2	2.19	0.40
1:A:40:ASN:HA	1:A:43:MSE:HE3	2.03	0.40
1:A:238:GLU:O	1:A:238:GLU:HG3	2.20	0.40
1:B:26:LYS:HG2	1:B:27:ARG:N	2.36	0.40
1:B:158:LYS:O	1:B:159:ALA:C	2.63	0.40
1:M:47:GLN:HE21	1:M:47:GLN:HB2	1.60	0.40
1:N:216:VAL:HG23	1:N:217:GLY:N	2.37	0.40
1:A:273:GLN:O	1:A:274:ALA:C	2.64	0.40
1:A:291:SER:HB3	1:B:27:ARG:HD2	2.03	0.40
1:N:43:MSE:HG2	1:N:110:LEU:HG	2.03	0.40
1:N:222:GLN:NE2	1:N:226:ASN:HD21	2.20	0.40
1:N:239:GLU:O	1:N:240:LYS:C	2.64	0.40
1:A:157:LYS:NZ	1:B:303:GLU:OE1	2.49	0.40
1:G:57:GLY:O	1:G:58:GLN:C	2.62	0.40
1:G:190:LYS:CA	1:G:190:LYS:CE	3.00	0.40
1:H:163:ALA:HB3	1:H:205:THR:HG21	2.04	0.40
1:H:302:PHE:CE1	1:H:304:GLU:OE1	2.71	0.40
1:H:186:GLU:OE1	1:H:187:GLN:HG2	2.21	0.40
1:M:87:ILE:HB	1:M:88:MSE:HE2	2.04	0.40
1:M:96:GLU:O	1:M:100:GLU:HG3	2.22	0.40
1:N:216:VAL:O	1:N:219:THR:N	2.54	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:125:ILE:O	1:H:134:GLU:OE1[3_445]	1.89	0.31
1:A:210:GLU:OE2	1:B:265:ILE:CD1[4_546]	2.01	0.19

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	277/295 (94%)	272 (98%)	5 (2%)	0	100	100
1	B	280/295 (95%)	274 (98%)	6 (2%)	0	100	100
1	G	283/295 (96%)	279 (99%)	4 (1%)	0	100	100
1	H	284/295 (96%)	281 (99%)	3 (1%)	0	100	100
1	M	266/295 (90%)	260 (98%)	6 (2%)	0	100	100
1	N	262/295 (89%)	249 (95%)	13 (5%)	0	100	100
All	All	1652/1770 (93%)	1615 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	246/253 (97%)	206 (84%)	40 (16%)	2	8
1	B	247/253 (98%)	211 (85%)	36 (15%)	3	11
1	G	244/253 (96%)	206 (84%)	38 (16%)	2	9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	248/253 (98%)	205 (83%)	43 (17%)	2	7
1	M	232/253 (92%)	194 (84%)	38 (16%)	2	8
1	N	228/253 (90%)	191 (84%)	37 (16%)	2	8
All	All	1445/1518 (95%)	1213 (84%)	232 (16%)	2	8

All (232) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	THR
1	A	21	GLU
1	A	31	ARG
1	A	37	ARG
1	A	61	THR
1	A	69	GLN
1	A	72	GLU
1	A	88	MSE
1	A	90	GLU
1	A	110	LEU
1	A	114	LYS
1	A	118	LYS
1	A	125	ILE
1	A	126	MSE
1	A	133	LYS
1	A	140	ARG
1	A	150	MSE
1	A	162	LEU
1	A	169	LEU
1	A	173	ARG
1	A	174	GLU
1	A	180	GLU
1	A	183	VAL
1	A	191	LEU
1	A	205	THR
1	A	207	GLU
1	A	208	LYS
1	A	213	LEU
1	A	218	LYS
1	A	220	THR
1	A	222	GLN
1	A	236	GLN
1	A	250	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	261	ASN
1	A	267	VAL
1	A	269	ARG
1	A	281	GLN
1	A	285	ARG
1	A	290	THR
1	A	302	PHE
1	B	26	LYS
1	B	30	LYS
1	B	31	ARG
1	B	42	LEU
1	B	61	THR
1	B	96	GLU
1	B	99	GLN
1	B	110	LEU
1	B	126	MSE
1	B	144	LYS
1	B	149	LYS
1	B	150	MSE
1	B	158	LYS
1	B	166	GLU
1	B	168	LYS
1	B	169	LEU
1	B	171	MSE
1	B	172	THR
1	B	175	MSE
1	B	186	GLU
1	B	187	GLN
1	B	188	GLN
1	B	204	LYS
1	B	213	LEU
1	B	216	VAL
1	B	241	ARG
1	B	245	LEU
1	B	250	LEU
1	B	253	LYS
1	B	261	ASN
1	B	267	VAL
1	B	269	ARG
1	B	271	LEU
1	B	281	GLN
1	B	289	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	290	THR
1	G	22	VAL
1	G	31	ARG
1	G	66	ARG
1	G	69	GLN
1	G	80	LEU
1	G	110	LEU
1	G	113	VAL
1	G	118	LYS
1	G	124	GLN
1	G	131	GLU
1	G	133	LYS
1	G	150	MSE
1	G	166	GLU
1	G	168	LYS
1	G	172	THR
1	G	174	GLU
1	G	187	GLN
1	G	188	GLN
1	G	190	LYS
1	G	191	LEU
1	G	193	ASP
1	G	195	VAL
1	G	199	LYS
1	G	204	LYS
1	G	205	THR
1	G	220	THR
1	G	227	MSE
1	G	229	GLN
1	G	239	GLU
1	G	250	LEU
1	G	265	ILE
1	G	267	VAL
1	G	273	GLN
1	G	289	SER
1	G	290	THR
1	G	291	SER
1	G	295	MSE
1	G	301	GLN
1	H	16	THR
1	H	21	GLU
1	H	30	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	31	ARG
1	H	37	ARG
1	H	42	LEU
1	H	49	ARG
1	H	61	THR
1	H	99	GLN
1	H	123	LYS
1	H	134	GLU
1	H	140	ARG
1	H	148	LYS
1	H	149	LYS
1	H	150	MSE
1	H	153	LEU
1	H	157	LYS
1	H	162	LEU
1	H	169	LEU
1	H	171	MSE
1	H	186	GLU
1	H	187	GLN
1	H	188	GLN
1	H	193	ASP
1	H	202	VAL
1	H	204	LYS
1	H	205	THR
1	H	211	LYS
1	H	215	ASP
1	H	216	VAL
1	H	218	LYS
1	H	220	THR
1	H	229	GLN
1	H	236	GLN
1	H	245	LEU
1	H	250	LEU
1	H	261	ASN
1	H	267	VAL
1	H	269	ARG
1	H	271	LEU
1	H	272	GLU
1	H	290	THR
1	H	306	ASN
1	M	15	THR
1	M	16	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	26	LYS
1	M	29	VAL
1	M	30	LYS
1	M	31	ARG
1	M	37	ARG
1	M	66	ARG
1	M	80	LEU
1	M	88	MSE
1	M	102	LYS
1	M	110	LEU
1	M	113	VAL
1	M	123	LYS
1	M	125	ILE
1	M	126	MSE
1	M	134	GLU
1	M	150	MSE
1	M	153	LEU
1	M	162	LEU
1	M	168	LYS
1	M	169	LEU
1	M	193	ASP
1	M	194	LYS
1	M	200	GLN
1	M	203	GLN
1	M	208	LYS
1	M	212	VAL
1	M	213	LEU
1	M	214	GLU
1	M	215	ASP
1	M	226	ASN
1	M	227	MSE
1	M	239	GLU
1	M	240	LYS
1	M	263	SER
1	M	267	VAL
1	M	290	THR
1	N	15	THR
1	N	16	THR
1	N	17	ASP
1	N	26	LYS
1	N	31	ARG
1	N	37	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	42	LEU
1	N	53	GLU
1	N	61	THR
1	N	65	LYS
1	N	80	LEU
1	N	99	GLN
1	N	123	LYS
1	N	149	LYS
1	N	150	MSE
1	N	153	LEU
1	N	161	HIS
1	N	166	GLU
1	N	194	LYS
1	N	195	VAL
1	N	198	CYS
1	N	202	VAL
1	N	205	THR
1	N	207	GLU
1	N	212	VAL
1	N	214	GLU
1	N	216	VAL
1	N	233	GLN
1	N	239	GLU
1	N	243	VAL
1	N	245	LEU
1	N	250	LEU
1	N	262	SER
1	N	265	ILE
1	N	267	VAL
1	N	271	LEU
1	N	281	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	44	ASN
1	A	99	GLN
1	A	107	ASN
1	A	117	GLN
1	A	222	GLN
1	A	226	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	229	GLN
1	A	235	GLN
1	A	236	GLN
1	A	257	ASN
1	A	261	ASN
1	A	281	GLN
1	A	298	ASN
1	B	47	GLN
1	B	58	GLN
1	B	69	GLN
1	B	103	ASN
1	B	104	ASN
1	B	117	GLN
1	B	122	HIS
1	B	124	GLN
1	B	161	HIS
1	B	188	GLN
1	B	192	GLN
1	B	206	GLN
1	B	226	ASN
1	B	233	GLN
1	B	235	GLN
1	B	236	GLN
1	B	261	ASN
1	B	281	GLN
1	G	24	ASN
1	G	44	ASN
1	G	69	GLN
1	G	99	GLN
1	G	103	ASN
1	G	107	ASN
1	G	122	HIS
1	G	124	GLN
1	G	161	HIS
1	G	187	GLN
1	G	188	GLN
1	G	200	GLN
1	G	203	GLN
1	G	206	GLN
1	G	226	ASN
1	G	235	GLN
1	G	257	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	301	GLN
1	H	58	GLN
1	H	69	GLN
1	H	104	ASN
1	H	122	HIS
1	H	188	GLN
1	H	192	GLN
1	H	222	GLN
1	H	226	ASN
1	H	235	GLN
1	H	236	GLN
1	H	261	ASN
1	H	281	GLN
1	M	36	HIS
1	M	44	ASN
1	M	47	GLN
1	M	69	GLN
1	M	76	GLN
1	M	99	GLN
1	M	107	ASN
1	M	161	HIS
1	M	222	GLN
1	M	226	ASN
1	M	235	GLN
1	M	257	ASN
1	M	261	ASN
1	M	266	HIS
1	M	273	GLN
1	M	281	GLN
1	N	69	GLN
1	N	76	GLN
1	N	99	GLN
1	N	103	ASN
1	N	104	ASN
1	N	117	GLN
1	N	122	HIS
1	N	200	GLN
1	N	203	GLN
1	N	222	GLN
1	N	226	ASN
1	N	235	GLN
1	N	236	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	261	ASN
1	N	273	GLN
1	N	281	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	275/295 (93%)	-1.46	0 100 100	25, 44, 101, 123	0
1	B	275/295 (93%)	-1.47	0 100 100	25, 45, 95, 115	0
1	G	277/295 (93%)	-1.47	0 100 100	25, 43, 106, 114	0
1	H	278/295 (94%)	-1.44	0 100 100	23, 44, 111, 132	0
1	M	263/295 (89%)	-1.34	0 100 100	34, 58, 115, 121	0
1	N	264/295 (89%)	-1.38	0 100 100	36, 58, 105, 125	0
All	All	1632/1770 (92%)	-1.43	0 100 100	23, 48, 106, 132	0

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	B	400	1/1	0.97	0.05	87,87,87,87	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	N	400	1/1	0.97	0.07	92,92,92,92	0
2	CA	G	400	1/1	0.98	0.09	91,91,91,91	0
2	CA	M	400	1/1	0.99	0.03	85,85,85,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.