



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 02:17 PM UTC

PDB ID : 3JAB / pdb_00003jab
EMDB ID : EMD-6258
Title : Domain organization and conformational plasticity of the G protein effector, PDE6
Authors : Zhang, Z.; He, F.; Constantine, R.; Baker, M.L.; Baehr, W.; Schmid, M.F.; Wensel, T.G.; Agosto, M.A.
Deposited on : 2015-05-26
Resolution : 11.00 Å(reported)
Based on initial models : 3DBA, 3JWR, 3IBJ, 12E8

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

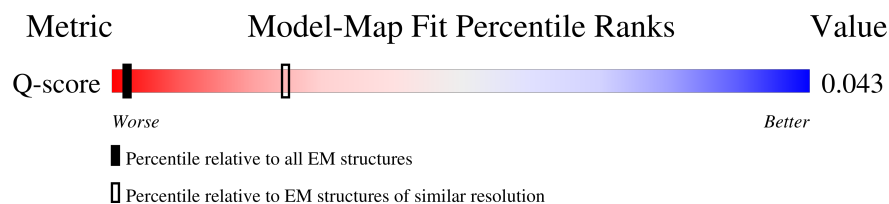
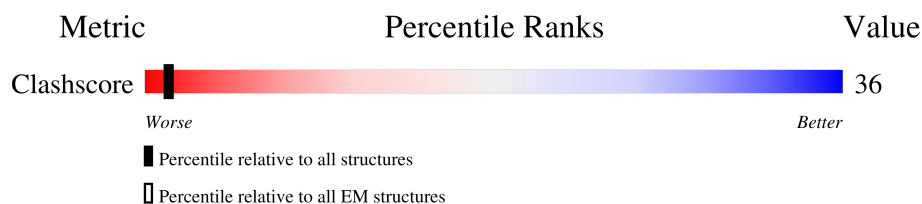
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

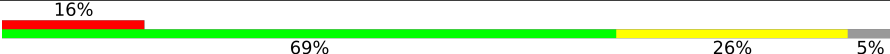
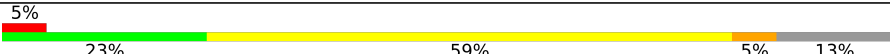
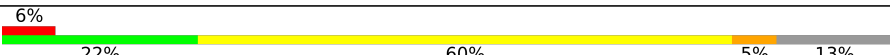
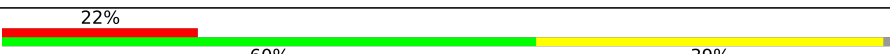
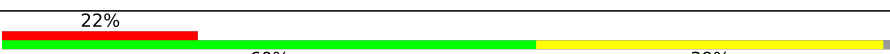
The reported resolution of this entry is 11.00 Å.

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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Q-score	-	25397	97 (10.50 - 11.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	180	 17% 68% 27% 5%
1	M	180	 16% 69% 26% 5%
2	B	185	 5% 23% 59% 5% 13%
2	N	185	 6% 22% 60% 5% 13%
3	C	330	 22% 60% 39% 5% 13%
3	O	330	 22% 60% 39% 5% 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	18	
4	P	18	
5	L	214	
5	R	214	
6	H	221	
6	Q	221	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17620 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 GafA domain of cone phosphodiesterase 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	171	Total	C	N	O	S	0	0
			1368	874	230	256	8		
1	M	171	Total	C	N	O	S	0	0
			1368	874	230	256	8		

- Molecule 2 is a protein called GafB domain of phosphodiesterase 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	161	Total	C	N	O	S	0	0
			1267	805	215	240	7		
2	N	161	Total	C	N	O	S	0	0
			1267	805	215	240	7		

- Molecule 3 is a protein called phosphodiesterase 5/6 chimera catalytic domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	328	Total	C	N	O	S	0	0
			2671	1700	465	487	19		
3	O	328	Total	C	N	O	S	0	0
			2671	1700	465	487	19		

- Molecule 4 is a protein called phosphodiesterase 6 gamma subunit inhibitory peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	17	Total	C	N	O	0	0
			141	92	23	26		
4	P	17	Total	C	N	O	0	0
			141	92	23	26		

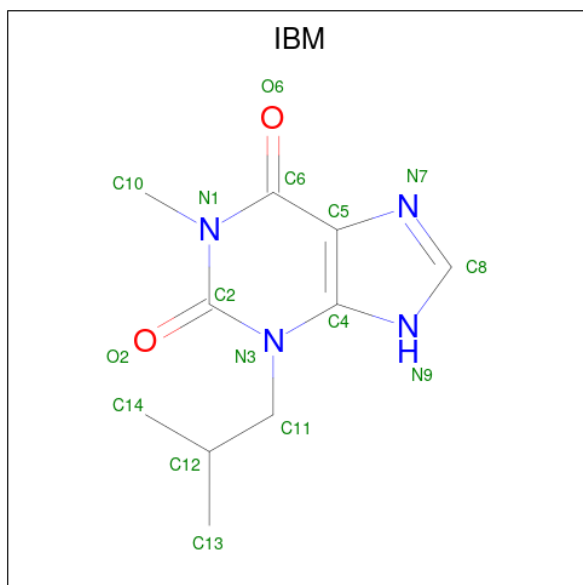
- Molecule 5 is a protein called IgG1-kappa 2E8 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	214	Total	C	N	O	S	0	0
			1649	1020	277	342	10		
5	R	214	Total	C	N	O	S	0	0
			1649	1020	277	342	10		

- Molecule 6 is a protein called IgG1-kappa 2E8 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	221	Total	C	N	O	S	0	0
			1682	1064	276	336	6		
6	Q	221	Total	C	N	O	S	0	0
			1682	1064	276	336	6		

- Molecule 7 is 3-ISOBUTYL-1-METHYLNANTHINE (CCD ID: IBM) (formula: C₁₀H₁₄N₄O₂).

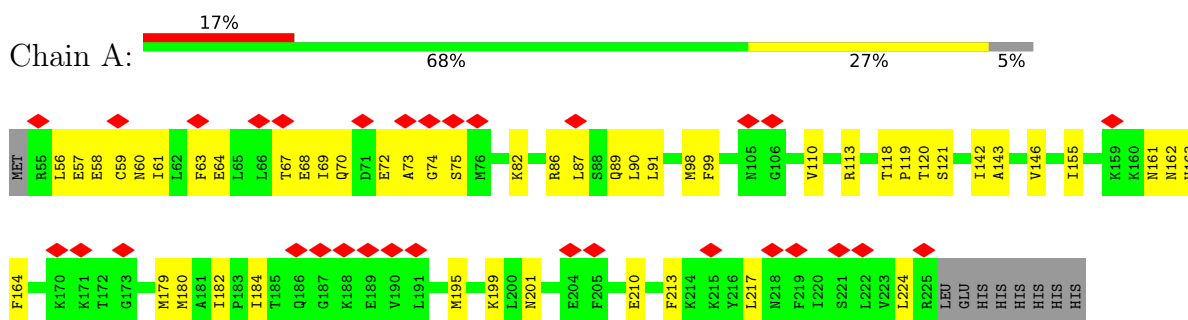


Mol	Chain	Residues	Atoms				AltConf
7	C	1	Total	C	N	O	0
			16	10	4	2	
7	C	1	Total	C	N	O	0
			16	10	4	2	
7	O	1	Total	C	N	O	0
			16	10	4	2	
7	O	1	Total	C	N	O	0
			16	10	4	2	

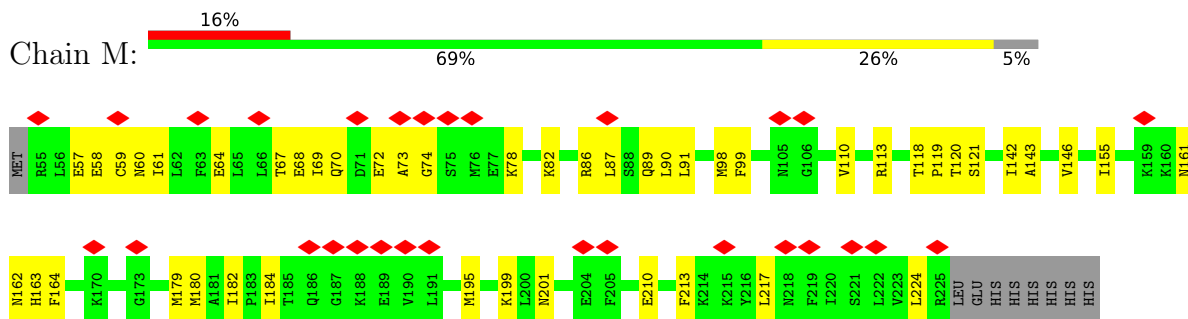
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

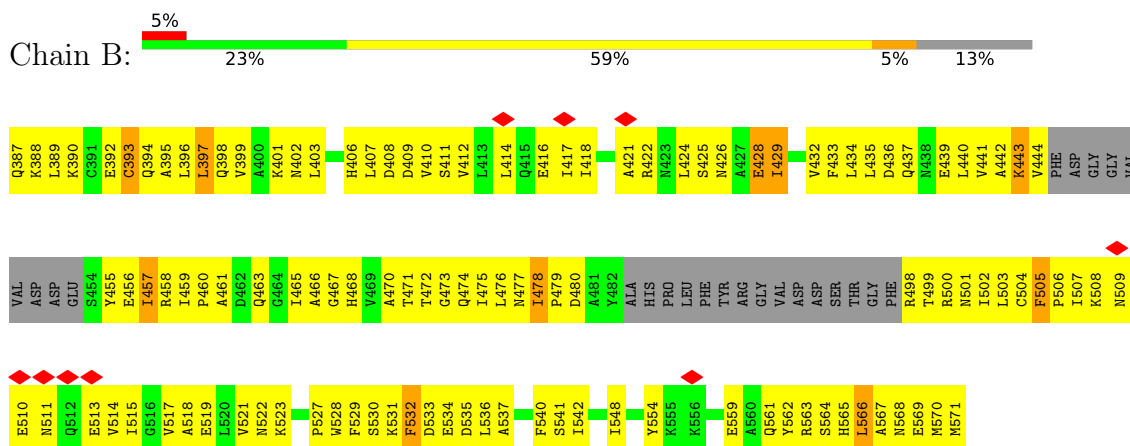
- Molecule 1: GafA domain of cone phosphodiesterase 6C



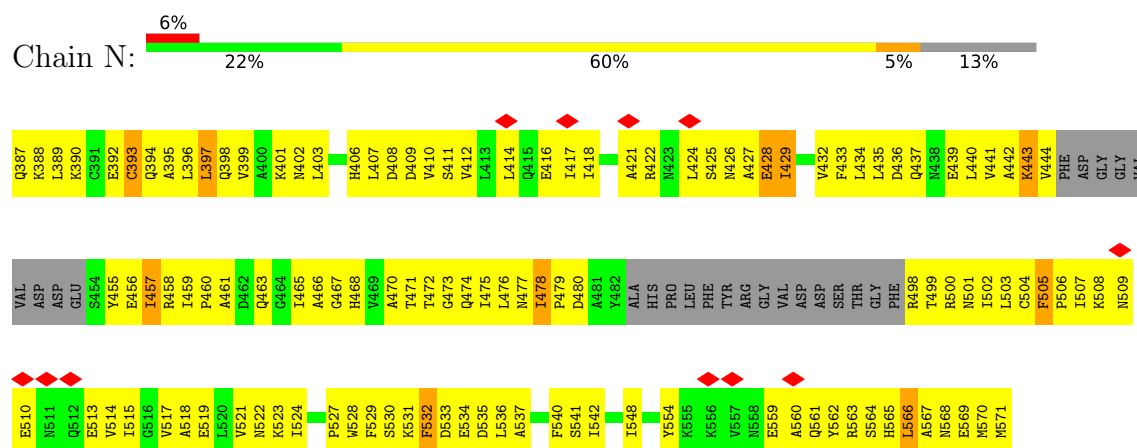
- Molecule 1: GafA domain of cone phosphodiesterase 6C



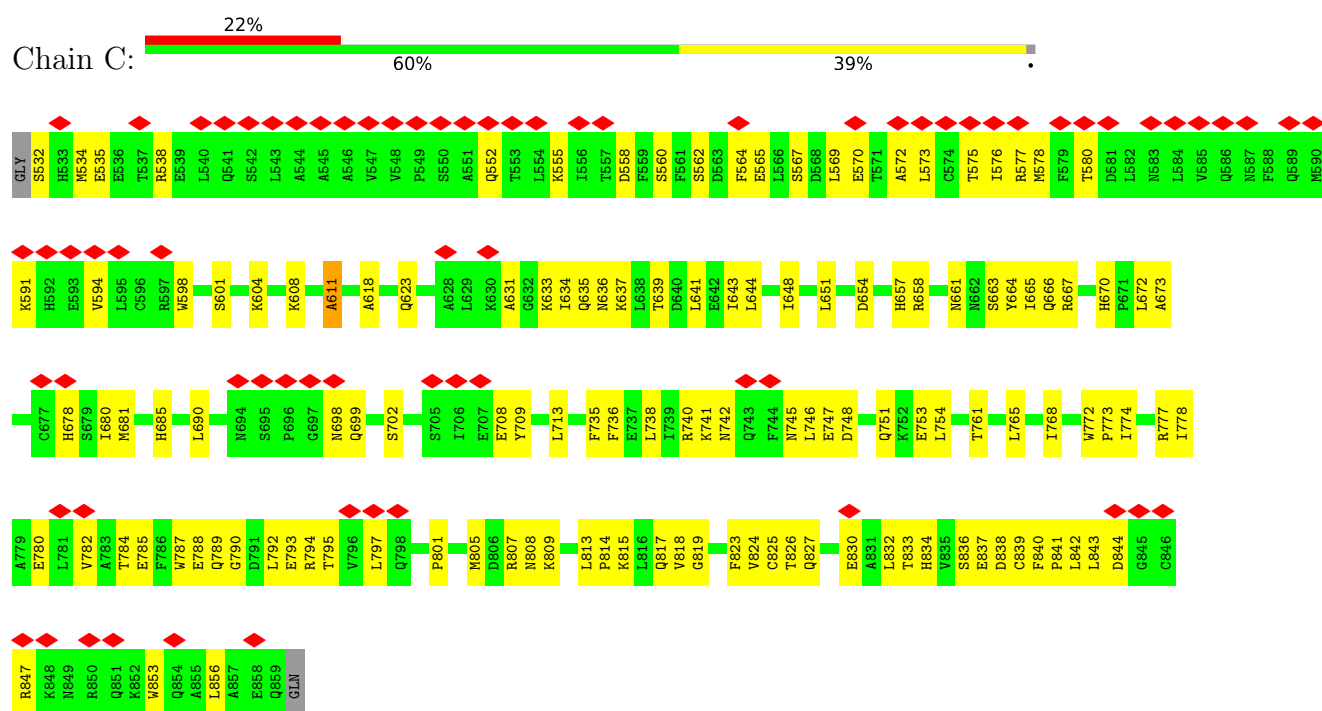
- Molecule 2: GafB domain of phosphodiesterase 2A



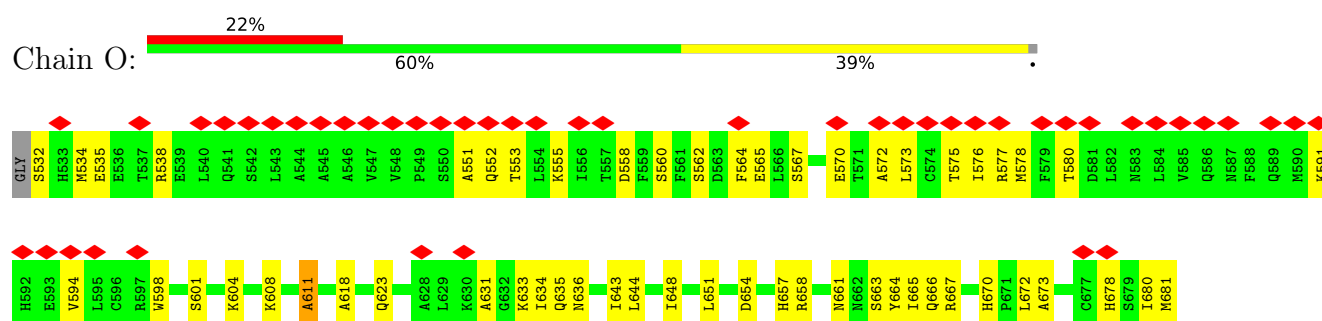
- Molecule 2: GafB domain of phosphodiesterase 2A

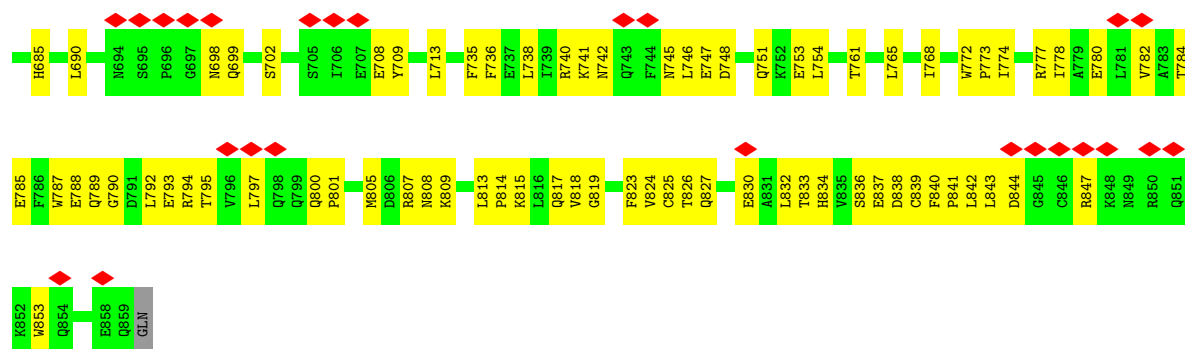


- Molecule 3: phosphodiesterase 5/6 chimera catalytic domain

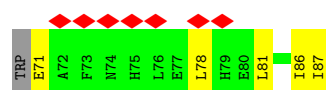


- Molecule 3: phosphodiesterase 5/6 chimera catalytic domain

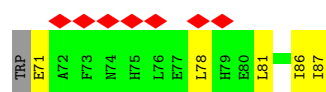
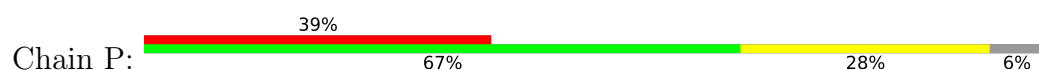




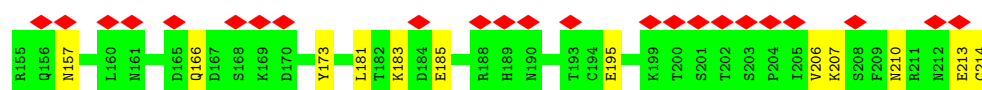
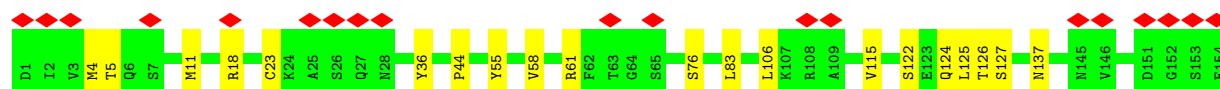
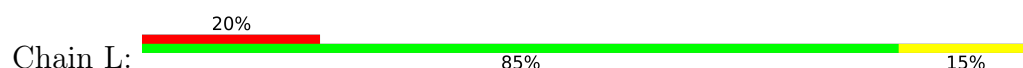
- Molecule 4: phosphodiesterase 6 gamma subunit inhibitory peptide



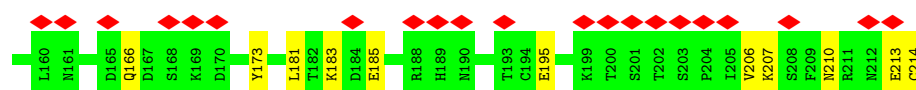
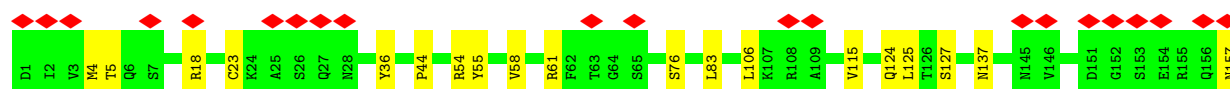
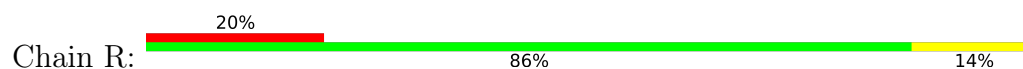
- Molecule 4: phosphodiesterase 6 gamma subunit inhibitory peptide



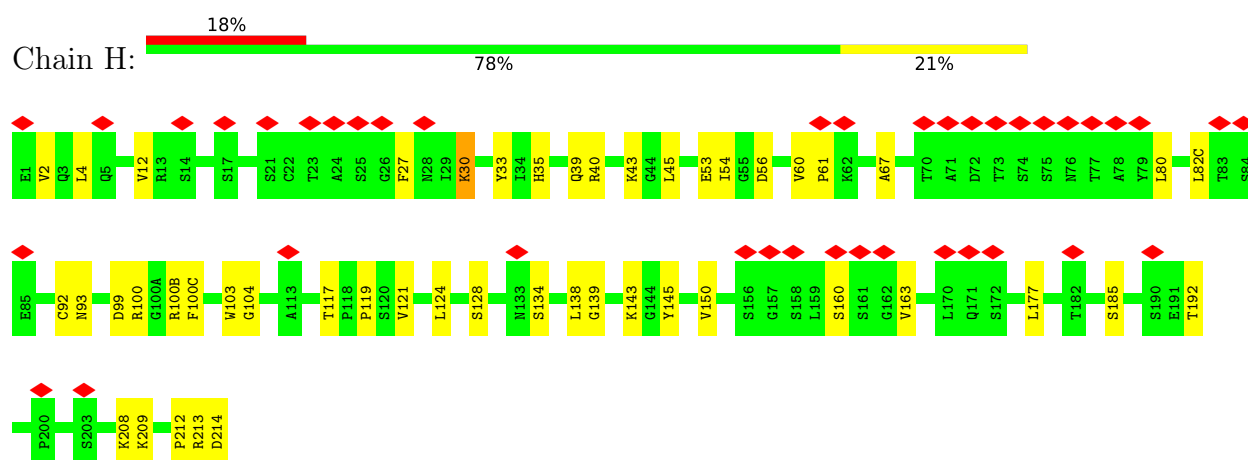
- Molecule 5: IgG1-kappa 2E8 light chain



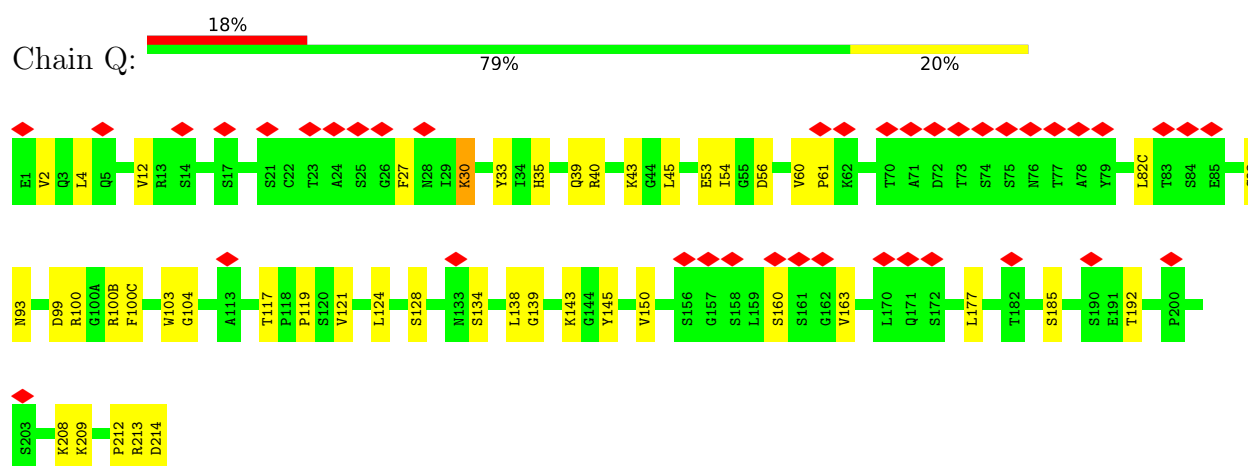
- Molecule 5: IgG1-kappa 2E8 light chain



- Molecule 6: IgG1-kappa 2E8 heavy chain



• Molecule 6: IgG1-kappa 2E8 heavy chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	12373	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	EMAN ctf	Depositor
Microscope	JEOL 2010F	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	60000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	1.835	Depositor
Minimum map value	-0.758	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.104	Depositor
Recommended contour level	1	Depositor
Map size ($\text{\AA}$)	434.4, 434.4, 434.4	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.81, 1.81, 1.81	Depositor

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: IBM

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	0.57	0/1391	0.77	0/1877
1	M	0.57	0/1391	0.77	0/1877
2	B	0.82	1/1285 (0.1%)	1.33	17/1738 (1.0%)
2	N	0.82	1/1285 (0.1%)	1.33	17/1738 (1.0%)
3	C	0.51	0/2726	0.83	1/3685 (0.0%)
3	O	0.51	0/2726	0.83	1/3685 (0.0%)
4	D	0.49	0/144	0.86	0/194
4	P	0.49	0/144	0.86	0/194
5	L	0.63	0/1682	0.98	4/2278 (0.2%)
5	R	0.63	0/1682	0.98	4/2278 (0.2%)
6	H	0.63	0/1728	1.02	9/2366 (0.4%)
6	Q	0.63	0/1728	1.02	9/2366 (0.4%)
All	All	0.62	2/17912 (0.0%)	0.98	62/24276 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	393	CYS	CA-C	-5.38	1.47	1.52
2	N	393	CYS	CA-C	-5.32	1.47	1.52

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	478	ILE	CA-C-N	9.84	132.13	119.84
2	N	478	ILE	C-N-CA	9.84	132.13	119.84
2	B	478	ILE	CA-C-N	9.78	132.06	119.84
2	B	478	ILE	C-N-CA	9.78	132.06	119.84
2	B	505	PHE	CA-C-N	7.94	127.83	120.21
2	B	505	PHE	C-N-CA	7.94	127.83	120.21
2	N	505	PHE	CA-C-N	7.93	127.82	120.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	505	PHE	C-N-CA	7.93	127.82	120.21
2	N	532	PHE	N-CA-C	-7.84	103.84	113.41
2	B	532	PHE	N-CA-C	-7.80	103.90	113.41
2	B	397	LEU	N-CA-C	-7.46	103.09	111.07
2	N	397	LEU	N-CA-C	-7.44	103.11	111.07
2	B	393	CYS	N-CA-C	-7.15	103.57	112.72
2	N	393	CYS	N-CA-C	-7.13	103.59	112.72
2	B	566	LEU	N-CA-C	-6.95	102.92	111.33
2	N	566	LEU	N-CA-C	-6.95	102.92	111.33
6	H	92	CYS	N-CA-C	-6.24	100.03	109.95
6	Q	92	CYS	N-CA-C	-6.24	100.03	109.95
5	L	137	ASN	N-CA-C	6.17	120.10	110.17
5	R	137	ASN	N-CA-C	6.17	120.10	110.17
2	B	542	ILE	N-CA-C	-6.08	104.37	111.00
2	B	429	ILE	N-CA-C	6.06	115.82	108.06
2	N	408	ASP	CB-CA-C	-6.05	101.12	110.81
2	N	542	ILE	N-CA-C	-6.04	104.42	111.00
2	N	429	ILE	N-CA-C	6.04	115.79	108.06
6	H	33	TYR	N-CA-C	-6.03	99.36	109.07
6	Q	33	TYR	N-CA-C	-6.03	99.36	109.07
6	H	143	LYS	N-CA-C	5.92	118.85	109.50
6	Q	143	LYS	N-CA-C	5.92	118.85	109.50
2	N	457	ILE	N-CA-C	5.77	115.90	106.72
2	B	457	ILE	N-CA-C	5.76	115.88	106.72
2	B	408	ASP	CB-CA-C	-5.63	101.11	110.68
6	H	150	VAL	N-CA-C	-5.62	99.69	108.86
6	Q	150	VAL	N-CA-C	-5.62	99.69	108.86
6	H	117	THR	CA-C-N	5.60	123.69	119.66
6	H	117	THR	C-N-CA	5.60	123.69	119.66
6	Q	117	THR	CA-C-N	5.60	123.69	119.66
6	Q	117	THR	C-N-CA	5.60	123.69	119.66
2	B	407	LEU	CA-C-N	5.43	127.82	120.38
2	B	407	LEU	C-N-CA	5.43	127.82	120.38
2	N	407	LEU	CA-C-N	5.42	127.85	120.54
2	N	407	LEU	C-N-CA	5.42	127.85	120.54
5	L	157	ASN	N-CA-C	5.37	118.69	110.20
5	R	157	ASN	N-CA-C	5.37	118.69	110.20
3	C	611	ALA	N-CA-C	5.37	116.82	110.97
3	O	611	ALA	N-CA-C	5.37	116.82	110.97
6	H	104	GLY	N-CA-C	-5.17	104.53	112.85
6	Q	104	GLY	N-CA-C	-5.17	104.53	112.85
5	L	5	THR	N-CA-C	5.16	117.14	108.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	5	THR	N-CA-C	5.16	117.14	108.73
6	H	100	ARG	N-CA-C	5.15	117.63	111.71
6	Q	100	ARG	N-CA-C	5.15	117.63	111.71
2	N	443	LYS	N-CA-C	-5.12	105.70	111.28
2	N	428	GLU	N-CA-C	-5.10	105.80	111.36
2	B	428	GLU	N-CA-C	-5.09	105.81	111.36
2	B	443	LYS	N-CA-C	-5.08	105.74	111.28
6	H	30	LYS	N-CA-C	5.08	117.48	111.33
6	Q	30	LYS	N-CA-C	5.08	117.48	111.33
2	N	394	GLN	N-CA-C	-5.06	105.27	111.75
5	L	18	ARG	N-CA-C	-5.06	100.48	108.73
5	R	18	ARG	N-CA-C	-5.06	100.48	108.73
2	B	394	GLN	N-CA-C	-5.05	105.28	111.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1368	0	1390	274	0
1	M	1368	0	1393	276	0
2	B	1267	0	1270	279	0
2	N	1267	0	1272	310	0
3	C	2671	0	2668	265	0
3	O	2671	0	2668	263	0
4	D	141	0	131	7	0
4	P	141	0	131	7	0
5	L	1649	0	1578	17	0
5	R	1649	0	1578	16	0
6	H	1682	0	1625	60	0
6	Q	1682	0	1625	57	0
7	C	32	0	28	4	0
7	O	32	0	28	4	0
All	All	17620	0	17385	1264	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 36.

All (1264) 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)
3:C:633:LYS:HB2	3:O:840:PHE:CE2	1.21	1.69
3:C:840:PHE:CE2	3:O:633:LYS:HB2	1.21	1.63
2:B:554:TYR:HE1	2:N:554:TYR:CE1	1.04	1.62
2:B:554:TYR:CE1	2:N:554:TYR:HE1	1.05	1.61
3:C:633:LYS:CB	3:O:840:PHE:HE2	1.10	1.60
3:C:840:PHE:HE2	3:O:633:LYS:CB	1.10	1.59
1:A:57:GLU:CB	1:M:118:THR:CG2	1.81	1.57
2:B:563:ARG:HB3	3:C:555:LYS:CE	1.18	1.57
1:A:120:THR:HA	1:M:60:ASN:C	1.31	1.55
2:N:563:ARG:C	3:O:555:LYS:HD2	1.20	1.54
3:O:794:ARG:HD2	6:Q:54:ILE:CG2	1.11	1.54
1:A:118:THR:CG2	1:M:57:GLU:CB	1.81	1.53
1:A:60:ASN:C	1:M:120:THR:HA	1.31	1.52
2:B:563:ARG:CB	3:C:555:LYS:NZ	1.72	1.52
3:C:794:ARG:HD2	6:H:54:ILE:CG2	1.11	1.52
2:N:563:ARG:HB3	3:O:555:LYS:CE	1.36	1.51
3:C:794:ARG:CD	6:H:54:ILE:HG21	1.40	1.51
1:A:120:THR:CA	1:M:61:ILE:N	1.72	1.51
2:B:563:ARG:CA	3:C:555:LYS:NZ	1.68	1.51
1:A:72:GLU:HB2	2:B:389:LEU:CD2	1.36	1.49
3:O:794:ARG:CD	6:Q:54:ILE:CG2	1.89	1.49
1:M:78:LYS:NZ	2:N:388:LYS:HZ1	1.01	1.48
1:A:61:ILE:N	1:M:120:THR:CA	1.72	1.48
1:M:64:GLU:HA	2:B:387:GLN:NE2	1.21	1.48
3:C:794:ARG:CD	6:H:54:ILE:CG2	1.89	1.47
1:A:118:THR:HG23	1:M:57:GLU:CB	1.37	1.46
1:A:118:THR:CG2	1:M:57:GLU:HB3	1.01	1.46
1:A:57:GLU:CB	1:M:118:THR:HG23	1.37	1.45
1:A:57:GLU:HB3	1:M:118:THR:CG2	1.01	1.45
2:N:563:ARG:HA	3:O:555:LYS:NZ	1.13	1.45
2:N:563:ARG:CA	3:O:555:LYS:NZ	1.80	1.44
3:O:794:ARG:CD	6:Q:54:ILE:HG21	1.40	1.43
1:A:61:ILE:CG1	1:M:119:PRO:C	1.92	1.42
1:A:61:ILE:N	1:M:120:THR:HA	1.19	1.42
1:A:89:GLN:CB	1:M:89:GLN:CB	1.96	1.42
1:A:89:GLN:NE2	1:M:86:ARG:HD2	1.33	1.42
1:A:70:GLN:O	2:B:389:LEU:CD1	1.65	1.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:795:THR:CG2	6:H:53:GLU:OE2	1.68	1.41
1:A:119:PRO:C	1:M:61:ILE:CG1	1.92	1.40
1:A:120:THR:HA	1:M:61:ILE:N	1.19	1.40
1:A:86:ARG:HD2	1:M:89:GLN:NE2	1.33	1.39
3:O:795:THR:CG2	6:Q:53:GLU:OE2	1.68	1.38
1:A:120:THR:HB	1:M:60:ASN:N	1.03	1.36
1:M:78:LYS:HZ1	2:N:388:LYS:NZ	0.91	1.35
1:A:60:ASN:N	1:M:120:THR:HB	1.03	1.35
2:N:563:ARG:O	3:O:555:LYS:CD	1.74	1.34
1:M:72:GLU:HB2	2:N:389:LEU:CD2	1.58	1.33
1:A:61:ILE:HG13	1:M:119:PRO:C	1.35	1.33
1:A:120:THR:CB	1:M:61:ILE:N	1.91	1.33
1:A:119:PRO:C	1:M:61:ILE:HG13	1.35	1.33
2:B:568:ASN:HD21	2:N:567:ALA:CB	1.41	1.33
1:A:64:GLU:HA	2:N:387:GLN:NE2	1.44	1.31
1:M:64:GLU:CA	2:B:387:GLN:HE22	1.42	1.31
1:A:120:THR:HG21	1:M:58:GLU:C	1.55	1.31
1:M:70:GLN:O	2:N:389:LEU:CD1	1.77	1.31
2:B:568:ASN:ND2	2:N:567:ALA:HB3	1.44	1.31
1:A:89:GLN:CB	1:M:89:GLN:HB3	1.58	1.30
1:A:61:ILE:N	1:M:120:THR:CB	1.91	1.30
1:A:67:THR:CB	2:N:390:LYS:HE2	1.60	1.30
2:N:563:ARG:CB	3:O:555:LYS:CE	2.08	1.30
1:A:58:GLU:C	1:M:120:THR:HG21	1.55	1.29
2:B:554:TYR:CE1	2:N:554:TYR:CE1	1.90	1.29
2:B:571:MET:O	3:O:631:ALA:HB2	1.14	1.28
1:A:60:ASN:N	1:M:120:THR:CB	1.96	1.28
1:A:120:THR:CB	1:M:60:ASN:N	1.96	1.28
1:A:57:GLU:C	1:M:120:THR:OG1	1.70	1.27
3:O:794:ARG:NE	6:Q:54:ILE:HG21	1.47	1.27
3:C:794:ARG:NE	6:H:54:ILE:HG21	1.47	1.27
1:A:70:GLN:O	2:B:389:LEU:HD13	1.09	1.27
1:A:120:THR:CA	1:M:60:ASN:C	2.00	1.26
1:A:89:GLN:HB2	1:M:89:GLN:CB	1.59	1.26
2:N:571:MET:O	3:C:631:ALA:HB2	1.22	1.26
1:A:61:ILE:N	1:M:120:THR:CG2	1.99	1.26
1:A:120:THR:CG2	1:M:61:ILE:N	1.99	1.26
2:B:563:ARG:C	3:C:555:LYS:HD2	1.59	1.25
2:B:567:ALA:CB	2:N:568:ASN:HD21	1.49	1.25
1:A:89:GLN:HB3	1:M:89:GLN:CB	1.58	1.25
2:N:563:ARG:O	3:O:555:LYS:HD2	1.09	1.24

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:THR:HB	2:N:390:LYS:CE	1.67	1.23
1:A:120:THR:HB	1:M:60:ASN:CA	1.68	1.23
2:B:567:ALA:HB3	2:N:568:ASN:ND2	1.51	1.23
1:A:58:GLU:CA	1:M:120:THR:HG21	1.66	1.22
1:A:120:THR:HG22	1:M:61:ILE:N	1.52	1.22
1:A:60:ASN:CA	1:M:120:THR:HB	1.68	1.21
1:A:89:GLN:CB	1:M:89:GLN:HB2	1.59	1.21
1:A:60:ASN:CA	1:M:120:THR:CA	2.19	1.21
1:A:120:THR:CA	1:M:60:ASN:CA	2.19	1.20
3:C:795:THR:CG2	6:H:53:GLU:CD	2.13	1.19
2:B:563:ARG:CB	3:C:555:LYS:CE	2.10	1.19
3:O:795:THR:CG2	6:Q:53:GLU:CD	2.13	1.19
2:B:567:ALA:CB	3:C:558:ASP:OD2	1.89	1.19
1:A:120:THR:HG21	1:M:58:GLU:CA	1.66	1.18
1:A:120:THR:OG1	1:M:57:GLU:CA	1.92	1.18
1:A:120:THR:CA	1:M:60:ASN:HB2	1.29	1.18
3:C:837:GLU:N	3:O:833:THR:CG2	2.07	1.18
2:N:563:ARG:CB	3:O:555:LYS:HE2	1.70	1.17
3:C:840:PHE:CB	3:O:838:ASP:H	1.58	1.17
1:A:70:GLN:O	2:B:389:LEU:CG	1.89	1.17
1:A:89:GLN:HE22	1:M:86:ARG:CD	1.58	1.17
1:M:78:LYS:NZ	2:N:388:LYS:CE	2.07	1.16
3:C:795:THR:HG21	6:H:53:GLU:OE2	1.39	1.16
1:A:60:ASN:ND2	1:M:121:SER:HA	1.61	1.16
1:A:61:ILE:N	1:M:120:THR:HG22	1.52	1.16
2:B:568:ASN:ND2	2:N:567:ALA:CB	2.03	1.16
1:A:57:GLU:CA	1:M:120:THR:OG1	1.92	1.16
1:A:121:SER:HA	1:M:60:ASN:ND2	1.61	1.16
3:C:833:THR:CG2	3:O:837:GLU:N	2.07	1.15
1:A:86:ARG:CD	1:M:89:GLN:HE22	1.58	1.15
1:M:70:GLN:O	2:N:389:LEU:HD13	0.98	1.15
3:C:795:THR:HG22	6:H:53:GLU:CG	1.76	1.15
3:C:838:ASP:H	3:O:840:PHE:CB	1.58	1.15
3:O:795:THR:HG22	6:Q:53:GLU:CG	1.76	1.15
1:A:57:GLU:HB2	1:M:118:THR:HG23	1.29	1.14
1:A:120:THR:CB	1:M:60:ASN:CA	2.26	1.13
2:N:569:GLU:CG	3:C:552:GLN:HB2	1.78	1.13
3:C:633:LYS:CB	3:O:840:PHE:CE2	1.97	1.13
3:O:795:THR:HG22	6:Q:53:GLU:HG3	1.18	1.13
1:A:60:ASN:C	1:M:120:THR:CA	2.00	1.13
1:A:60:ASN:CA	1:M:120:THR:CB	2.26	1.13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:GLN:HG3	2:B:388:LYS:O	1.41	1.13
3:C:795:THR:HG21	6:H:53:GLU:CD	1.71	1.13
3:C:795:THR:HG22	6:H:53:GLU:HG3	1.18	1.13
3:O:795:THR:CG2	6:Q:53:GLU:CG	2.26	1.13
3:O:795:THR:HG23	6:Q:53:GLU:OE2	1.36	1.13
1:A:120:THR:N	1:M:61:ILE:HG13	1.62	1.13
1:A:60:ASN:HB2	1:M:120:THR:CA	1.29	1.12
2:N:499:THR:HG22	2:N:500:ARG:H	1.11	1.12
2:N:563:ARG:C	3:O:555:LYS:CD	2.15	1.12
2:N:567:ALA:HA	3:O:558:ASP:OD2	1.44	1.12
3:C:840:PHE:CE2	3:O:633:LYS:CB	1.97	1.12
2:N:563:ARG:CB	3:O:555:LYS:NZ	2.13	1.12
1:A:120:THR:OG1	1:M:57:GLU:C	1.70	1.11
3:C:795:THR:CG2	6:H:53:GLU:CG	2.26	1.11
1:A:72:GLU:CB	2:B:389:LEU:CD2	2.28	1.11
2:B:563:ARG:HA	3:C:555:LYS:NZ	1.38	1.11
1:A:61:ILE:HG13	1:M:120:THR:N	1.62	1.11
2:B:568:ASN:HD21	2:N:567:ALA:HB1	1.14	1.11
2:B:567:ALA:HB1	3:C:558:ASP:OD2	1.45	1.11
2:N:571:MET:O	3:C:631:ALA:CB	1.97	1.11
1:A:61:ILE:HA	1:M:119:PRO:O	1.50	1.10
3:O:795:THR:HG21	6:Q:53:GLU:CD	1.71	1.10
2:B:460:PRO:HG2	2:B:463:GLN:HB3	1.30	1.09
2:B:569:GLU:CG	3:O:552:GLN:HB2	1.81	1.09
1:A:69:ILE:CG2	2:B:389:LEU:HD12	1.81	1.09
1:M:73:ALA:HB1	1:M:74:GLY:HA3	1.27	1.09
2:B:568:ASN:CB	2:N:568:ASN:HB2	1.82	1.08
2:B:568:ASN:HB2	2:N:568:ASN:CB	1.83	1.08
3:C:795:THR:HG23	6:H:53:GLU:OE2	1.36	1.08
1:A:73:ALA:HB1	1:A:74:GLY:HA3	1.27	1.08
1:A:119:PRO:O	1:M:61:ILE:HA	1.50	1.08
3:O:795:THR:HG21	6:Q:53:GLU:OE2	1.39	1.08
2:B:567:ALA:CB	2:N:568:ASN:ND2	2.09	1.08
1:A:120:THR:OG1	1:M:57:GLU:HA	1.52	1.08
2:N:563:ARG:CA	3:O:555:LYS:HZ2	1.50	1.08
2:B:499:THR:HG22	2:B:500:ARG:H	1.11	1.07
2:B:569:GLU:HG2	3:O:552:GLN:HB2	1.30	1.07
3:C:833:THR:HG21	3:O:837:GLU:H	1.19	1.07
2:B:563:ARG:O	3:C:555:LYS:HD2	1.54	1.06
2:B:567:ALA:HB1	2:N:568:ASN:HD21	1.17	1.06
3:C:840:PHE:CD2	3:O:633:LYS:HB2	1.91	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:THR:HG23	1:M:57:GLU:HB2	1.29	1.06
3:C:633:LYS:HB2	3:O:840:PHE:CD2	1.91	1.05
1:A:57:GLU:HA	1:M:120:THR:OG1	1.52	1.04
2:N:563:ARG:O	3:O:555:LYS:CG	2.04	1.04
2:N:567:ALA:CA	3:O:558:ASP:OD2	2.05	1.04
3:C:837:GLU:H	3:O:833:THR:HG21	1.19	1.04
2:N:563:ARG:CB	3:O:555:LYS:HZ3	1.70	1.04
3:C:840:PHE:HE2	3:O:633:LYS:HB3	1.20	1.04
1:M:72:GLU:OE1	2:N:389:LEU:HD23	1.56	1.04
2:N:460:PRO:HG2	2:N:463:GLN:HB3	1.30	1.04
1:A:69:ILE:HG22	2:B:389:LEU:HD12	1.39	1.03
2:B:571:MET:O	3:O:631:ALA:CB	2.04	1.03
1:A:72:GLU:CB	2:B:389:LEU:HD21	1.89	1.02
2:N:567:ALA:CB	3:O:558:ASP:OD2	2.08	1.02
3:C:633:LYS:HB3	3:O:840:PHE:HE2	1.20	1.02
1:M:72:GLU:HB2	2:N:389:LEU:HD21	1.03	1.02
1:A:70:GLN:O	2:B:389:LEU:CD2	2.07	1.02
2:B:570:MET:HG2	3:C:560:SER:OG	1.55	1.02
2:N:563:ARG:HB3	3:O:555:LYS:CD	1.88	1.01
3:C:794:ARG:HD2	6:H:54:ILE:HG22	1.03	1.01
1:A:60:ASN:HB2	1:M:120:THR:CB	1.90	1.00
3:O:794:ARG:HD2	6:Q:54:ILE:HG22	1.03	1.00
1:A:120:THR:HG22	1:M:61:ILE:CA	1.91	1.00
1:M:78:LYS:HZ3	2:N:388:LYS:CE	1.70	1.00
3:C:840:PHE:HB3	3:O:838:ASP:H	1.11	1.00
4:D:86:ILE:O	4:D:87:ILE:HG12	1.62	1.00
3:C:838:ASP:N	3:O:840:PHE:HB3	1.76	0.99
1:A:120:THR:CB	1:M:60:ASN:HB2	1.90	0.99
1:A:61:ILE:CA	1:M:120:THR:HG22	1.91	0.99
2:B:563:ARG:O	3:C:555:LYS:CD	2.11	0.98
3:C:840:PHE:HB3	3:O:838:ASP:N	1.76	0.98
1:A:60:ASN:H	1:M:120:THR:CB	1.67	0.98
1:A:57:GLU:CB	1:M:118:THR:HG21	1.64	0.97
1:A:86:ARG:CD	1:M:89:GLN:NE2	2.20	0.97
1:A:89:GLN:HB3	1:M:89:GLN:HB2	0.98	0.97
2:B:563:ARG:CA	3:C:555:LYS:HZ2	1.68	0.97
3:C:633:LYS:HD3	3:O:844:ASP:OD1	1.64	0.97
4:P:86:ILE:O	4:P:87:ILE:HG12	1.62	0.97
1:M:72:GLU:CB	2:N:389:LEU:CD2	2.42	0.97
3:C:794:ARG:HD2	6:H:54:ILE:CB	1.95	0.97
3:O:794:ARG:HD2	6:Q:54:ILE:CB	1.95	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:563:ARG:HB3	3:C:555:LYS:NZ	1.47	0.96
3:C:844:ASP:OD1	3:O:633:LYS:HD3	1.64	0.96
1:M:72:GLU:CB	2:N:389:LEU:HD21	1.96	0.95
1:M:70:GLN:C	2:N:389:LEU:HD13	1.89	0.95
1:A:89:GLN:HB2	1:M:89:GLN:HB3	0.98	0.94
2:B:563:ARG:HB3	3:C:555:LYS:HE2	0.97	0.94
1:A:64:GLU:HA	2:N:387:GLN:HE22	1.15	0.94
1:A:61:ILE:HG12	1:M:119:PRO:C	1.78	0.94
1:A:60:ASN:CB	1:M:120:THR:CB	2.45	0.94
1:A:61:ILE:HB	1:M:120:THR:HG22	1.49	0.94
1:A:120:THR:CB	1:M:60:ASN:H	1.67	0.94
1:A:120:THR:CG2	1:M:61:ILE:HB	1.97	0.94
3:C:794:ARG:CD	6:H:54:ILE:HG22	1.71	0.94
1:A:120:THR:HG22	1:M:61:ILE:HB	1.49	0.94
1:M:73:ALA:CB	1:M:74:GLY:HA3	1.96	0.94
3:O:794:ARG:CD	6:Q:54:ILE:HG22	1.71	0.94
1:A:67:THR:CG2	2:N:387:GLN:HE21	1.81	0.94
2:N:569:GLU:HG3	3:C:552:GLN:HB2	1.48	0.94
1:A:72:GLU:HB2	2:B:389:LEU:HD21	0.95	0.93
1:A:61:ILE:CB	1:M:120:THR:HG22	1.98	0.93
1:A:61:ILE:HB	1:M:120:THR:CG2	1.97	0.93
2:B:563:ARG:CB	3:C:555:LYS:HE2	1.87	0.93
2:B:568:ASN:HB2	2:N:568:ASN:HB2	0.93	0.93
3:C:740:ARG:O	3:O:742:ASN:HB2	1.69	0.93
3:C:837:GLU:H	3:O:833:THR:CG2	1.74	0.93
1:A:73:ALA:CB	1:A:74:GLY:HA3	1.96	0.93
3:C:742:ASN:HB2	3:O:740:ARG:O	1.69	0.93
1:A:58:GLU:C	1:M:120:THR:CG2	2.42	0.92
1:A:119:PRO:C	1:M:61:ILE:HG12	1.78	0.92
3:O:795:THR:CG2	6:Q:53:GLU:HG3	1.94	0.92
1:A:70:GLN:O	2:B:389:LEU:HD22	1.68	0.92
1:M:67:THR:HB	2:B:390:LYS:HE2	1.52	0.92
1:A:89:GLN:NE2	1:M:86:ARG:CD	2.20	0.91
1:A:120:THR:HG22	1:M:61:ILE:CB	1.98	0.91
2:B:570:MET:CG	3:C:560:SER:OG	2.13	0.91
1:A:120:THR:CG2	1:M:58:GLU:C	2.42	0.91
3:C:795:THR:CG2	6:H:53:GLU:HG3	1.94	0.91
1:A:142:ILE:HD13	1:A:155:ILE:HD13	1.54	0.90
1:A:120:THR:CB	1:M:60:ASN:CB	2.45	0.90
3:O:808:ASN:ND2	6:Q:56:ASP:OD2	2.04	0.90
3:C:808:ASN:ND2	6:H:56:ASP:OD2	2.04	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:838:ASP:N	3:O:840:PHE:CB	2.34	0.90
2:N:563:ARG:HB3	3:O:555:LYS:HE2	0.91	0.90
2:B:563:ARG:C	3:C:555:LYS:CD	2.43	0.89
3:O:794:ARG:CG	6:Q:54:ILE:HG22	2.01	0.89
1:M:64:GLU:CA	2:B:387:GLN:NE2	2.16	0.89
2:N:563:ARG:CA	3:O:555:LYS:HZ3	1.59	0.89
1:M:78:LYS:CE	2:N:388:LYS:HE2	2.02	0.89
1:A:118:THR:HG21	1:M:57:GLU:CB	1.64	0.89
3:C:840:PHE:CB	3:O:838:ASP:N	2.34	0.89
1:M:142:ILE:HD13	1:M:155:ILE:HD13	1.54	0.88
2:N:563:ARG:CG	3:O:555:LYS:HZ3	1.85	0.88
3:C:838:ASP:H	3:O:840:PHE:HB3	1.11	0.88
3:C:794:ARG:CG	6:H:54:ILE:HG22	2.01	0.88
2:N:460:PRO:HG2	2:N:463:GLN:CB	2.04	0.88
1:A:58:GLU:HA	1:M:120:THR:HG21	1.55	0.88
1:A:67:THR:HB	2:N:390:LYS:HE2	0.88	0.88
1:A:57:GLU:HB3	1:M:118:THR:HG21	0.88	0.87
1:M:78:LYS:HE2	2:N:388:LYS:HE2	1.53	0.87
2:N:567:ALA:HB2	3:O:555:LYS:HG3	1.54	0.87
1:A:64:GLU:CA	2:N:387:GLN:HE22	1.87	0.87
2:N:563:ARG:CA	3:O:555:LYS:CE	2.49	0.86
1:A:60:ASN:H	1:M:120:THR:HB	1.03	0.86
2:B:460:PRO:HG2	2:B:463:GLN:CB	2.04	0.86
1:A:118:THR:HG21	1:M:57:GLU:HB3	0.88	0.86
1:A:120:THR:HG21	1:M:58:GLU:HA	1.55	0.86
1:A:118:THR:HG23	1:M:57:GLU:HB3	0.94	0.85
1:A:121:SER:HA	1:M:60:ASN:CG	2.01	0.85
1:A:120:THR:CG2	1:M:61:ILE:CB	2.55	0.85
1:A:73:ALA:CB	1:A:74:GLY:CA	2.54	0.85
1:A:121:SER:CA	1:M:60:ASN:ND2	2.40	0.85
1:M:67:THR:CB	2:B:390:LYS:HE2	2.08	0.84
1:M:73:ALA:CB	1:M:74:GLY:CA	2.54	0.84
1:M:78:LYS:NZ	2:N:388:LYS:HE2	1.92	0.84
1:A:69:ILE:HG23	2:B:389:LEU:HD12	1.57	0.84
2:N:563:ARG:CA	3:O:555:LYS:HD2	2.07	0.84
6:Q:39:GLN:HB2	6:Q:45:LEU:HD23	1.58	0.84
1:A:60:ASN:ND2	1:M:121:SER:CA	2.40	0.84
1:A:119:PRO:O	1:M:61:ILE:CA	2.26	0.84
1:A:61:ILE:CB	1:M:120:THR:CG2	2.55	0.84
2:N:499:THR:CG2	2:N:500:ARG:H	1.90	0.84
6:H:39:GLN:HB2	6:H:45:LEU:HD23	1.58	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:563:ARG:HA	3:O:555:LYS:HZ3	1.13	0.84
1:A:89:GLN:O	1:M:90:LEU:CA	2.26	0.83
2:N:567:ALA:HB2	3:O:555:LYS:CG	2.08	0.83
2:N:499:THR:HG22	2:N:500:ARG:N	1.93	0.83
2:N:570:MET:HE1	3:O:560:SER:C	1.83	0.83
1:A:89:GLN:HA	1:M:90:LEU:HD23	1.60	0.83
1:A:90:LEU:HD23	1:M:89:GLN:HA	1.60	0.83
2:B:499:THR:HG22	2:B:500:ARG:N	1.93	0.83
1:A:61:ILE:CA	1:M:119:PRO:O	2.26	0.83
3:C:636:ASN:ND2	3:O:844:ASP:OD2	2.12	0.83
1:A:120:THR:HB	1:M:60:ASN:H	1.03	0.82
2:B:499:THR:CG2	2:B:500:ARG:H	1.90	0.82
3:C:838:ASP:H	3:O:840:PHE:HB2	1.43	0.82
1:A:89:GLN:O	1:M:90:LEU:HA	1.80	0.82
3:C:844:ASP:OD2	3:O:636:ASN:ND2	2.12	0.82
1:A:90:LEU:HA	1:M:89:GLN:O	1.80	0.82
1:M:78:LYS:NZ	2:N:388:LYS:NZ	1.69	0.82
1:A:60:ASN:CG	1:M:121:SER:HA	2.01	0.82
1:A:120:THR:CB	1:M:60:ASN:C	2.43	0.82
2:N:507:ILE:HG22	2:N:515:ILE:HG22	1.61	0.82
1:M:67:THR:HB	2:B:390:LYS:CE	2.10	0.82
1:A:70:GLN:C	2:B:389:LEU:HD22	2.04	0.82
1:A:57:GLU:CA	1:M:118:THR:CG2	2.58	0.82
1:A:64:GLU:HG2	2:N:387:GLN:HB2	1.62	0.82
3:C:840:PHE:HB2	3:O:838:ASP:H	1.43	0.82
1:A:61:ILE:CG1	1:M:119:PRO:O	2.27	0.81
1:A:72:GLU:HB2	2:B:389:LEU:HD22	1.56	0.81
3:C:532:SER:HA	3:C:535:GLU:OE1	1.80	0.81
1:A:119:PRO:O	1:M:61:ILE:CG1	2.27	0.81
1:A:118:THR:HG21	1:M:57:GLU:CA	2.10	0.81
2:B:432:VAL:HG12	2:B:518:ALA:HB2	1.62	0.81
1:A:86:ARG:HD2	1:M:89:GLN:HE22	0.99	0.81
2:N:432:VAL:HG12	2:N:518:ALA:HB2	1.62	0.81
1:A:57:GLU:CA	1:M:118:THR:HG21	2.10	0.81
2:B:563:ARG:C	3:C:555:LYS:NZ	2.38	0.81
2:B:507:ILE:HG22	2:B:515:ILE:HG22	1.61	0.81
2:N:569:GLU:HG2	3:C:552:GLN:HB2	1.62	0.81
3:C:833:THR:CG2	3:O:837:GLU:H	1.74	0.81
1:A:69:ILE:HG22	2:B:389:LEU:CD1	2.11	0.81
1:M:69:ILE:CG2	2:N:389:LEU:HD12	2.11	0.81
1:M:142:ILE:HG21	1:M:179:MET:HE1	1.63	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:563:ARG:HA	3:C:555:LYS:HZ2	1.25	0.80
1:A:90:LEU:CA	1:M:89:GLN:O	2.26	0.80
1:A:59:CYS:C	1:M:120:THR:HB	2.04	0.80
1:M:72:GLU:HB2	2:N:389:LEU:HD22	1.61	0.80
3:C:794:ARG:HD2	6:H:54:ILE:HG21	1.07	0.80
1:A:118:THR:CG2	1:M:57:GLU:CA	2.58	0.80
1:A:142:ILE:HG21	1:A:179:MET:HE1	1.63	0.80
3:O:809:LYS:HA	3:O:809:LYS:HE3	1.63	0.80
1:A:75:SER:HB3	2:B:389:LEU:HD11	1.63	0.80
1:A:86:ARG:NH2	1:M:86:ARG:NH2	2.29	0.80
3:C:838:ASP:HA	3:O:838:ASP:HA	1.62	0.80
3:O:532:SER:HA	3:O:535:GLU:OE1	1.80	0.80
2:B:563:ARG:HB3	3:C:555:LYS:CD	2.09	0.79
1:A:89:GLN:HE22	1:M:86:ARG:HD2	0.99	0.79
3:C:809:LYS:HE3	3:C:809:LYS:HA	1.63	0.79
1:A:142:ILE:HG21	1:A:179:MET:CE	2.13	0.79
1:A:60:ASN:C	1:M:120:THR:CB	2.43	0.79
2:B:396:LEU:HA	2:B:399:VAL:HG13	1.65	0.79
2:B:569:GLU:HG2	3:O:552:GLN:CB	2.11	0.79
1:A:120:THR:HB	1:M:59:CYS:C	2.04	0.79
2:N:396:LEU:HA	2:N:399:VAL:HG13	1.65	0.79
2:N:563:ARG:HA	3:O:555:LYS:HZ2	0.78	0.78
2:N:570:MET:HE1	3:O:560:SER:O	1.82	0.78
1:A:64:GLU:CA	2:N:387:GLN:NE2	2.37	0.78
2:B:554:TYR:CE1	2:N:554:TYR:CD1	2.71	0.78
3:C:735:PHE:HB2	3:C:754:LEU:HD21	1.64	0.78
1:A:70:GLN:C	2:B:389:LEU:HD13	2.06	0.78
2:B:399:VAL:HG21	2:B:540:PHE:HE1	1.48	0.78
2:B:568:ASN:CG	2:N:567:ALA:HB3	2.08	0.78
3:O:735:PHE:HB2	3:O:754:LEU:HD21	1.64	0.78
3:O:761:THR:O	3:O:765:LEU:HD22	1.84	0.78
1:A:58:GLU:CA	1:M:120:THR:CG2	2.58	0.78
1:A:120:THR:HG21	1:M:58:GLU:O	1.84	0.77
3:C:795:THR:HB	6:H:30:LYS:NZ	1.99	0.77
3:O:794:ARG:CG	6:Q:54:ILE:CG2	2.60	0.77
3:O:795:THR:HB	6:Q:30:LYS:NZ	1.99	0.77
1:M:142:ILE:HG21	1:M:179:MET:CE	2.13	0.77
1:A:73:ALA:HB1	1:A:74:GLY:CA	2.10	0.77
2:N:479:PRO:HG3	2:N:528:TRP:CZ3	2.19	0.77
2:B:563:ARG:O	3:C:555:LYS:CG	2.32	0.77
1:A:119:PRO:HG2	1:M:90:LEU:HD21	1.66	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:399:VAL:HG21	2:N:540:PHE:HE1	1.48	0.77
1:M:69:ILE:HG23	2:N:389:LEU:HD12	1.67	0.77
2:B:567:ALA:HB2	3:C:555:LYS:CG	2.14	0.77
3:O:794:ARG:CZ	6:Q:54:ILE:HD13	2.14	0.77
3:C:794:ARG:CZ	6:H:54:ILE:HD13	2.14	0.77
3:C:761:THR:O	3:C:765:LEU:HD22	1.84	0.77
2:B:479:PRO:HG3	2:B:528:TRP:CZ3	2.19	0.76
1:A:57:GLU:HB3	1:M:118:THR:HG23	0.94	0.76
1:A:120:THR:CG2	1:M:58:GLU:CA	2.58	0.76
1:A:58:GLU:O	1:M:120:THR:HG21	1.84	0.76
2:N:508:LYS:HA	2:N:513:GLU:O	1.86	0.76
3:C:794:ARG:CG	6:H:54:ILE:CG2	2.60	0.76
2:B:508:LYS:HA	2:B:513:GLU:O	1.86	0.76
1:M:73:ALA:HB1	1:M:74:GLY:CA	2.10	0.76
2:B:561:GLN:HE21	2:B:561:GLN:HA	1.51	0.76
3:O:611:ALA:HB3	3:O:785:GLU:HB2	1.68	0.76
1:A:70:GLN:HB2	2:B:389:LEU:CD2	2.06	0.75
2:B:500:ARG:HG2	2:B:522:ASN:OD1	1.87	0.75
2:B:567:ALA:HB3	2:N:568:ASN:CG	2.11	0.75
3:C:611:ALA:HB3	3:C:785:GLU:HB2	1.68	0.75
1:A:184:ILE:HD13	1:A:224:LEU:HD12	1.68	0.75
2:N:500:ARG:HG2	2:N:522:ASN:OD1	1.87	0.75
2:B:563:ARG:CG	3:C:555:LYS:NZ	2.49	0.74
1:A:90:LEU:HD21	1:M:119:PRO:HG2	1.66	0.74
1:A:119:PRO:O	1:M:61:ILE:HG12	1.86	0.74
3:O:736:PHE:CE1	3:O:827:GLN:HG3	2.22	0.74
1:M:184:ILE:HD13	1:M:224:LEU:HD12	1.68	0.74
1:A:61:ILE:HG12	1:M:119:PRO:O	1.86	0.74
3:C:608:LYS:CD	3:C:608:LYS:H	2.01	0.74
2:B:563:ARG:C	3:C:555:LYS:HZ2	1.96	0.74
2:B:570:MET:HG2	3:C:560:SER:HG	1.53	0.74
3:C:736:PHE:CE1	3:C:827:GLN:HG3	2.22	0.74
5:R:55:TYR:O	5:R:58:VAL:HG13	1.88	0.73
2:N:561:GLN:HA	2:N:561:GLN:HE21	1.51	0.73
5:L:55:TYR:O	5:L:58:VAL:HG13	1.88	0.73
1:M:70:GLN:OE1	2:N:393:CYS:SG	2.46	0.73
2:N:563:ARG:CA	3:O:555:LYS:CD	2.67	0.73
3:C:780:GLU:O	3:C:784:THR:HG23	1.89	0.73
3:O:608:LYS:CD	3:O:608:LYS:H	2.01	0.73
2:N:569:GLU:HG2	3:C:552:GLN:CB	2.18	0.73
1:M:70:GLN:O	2:N:389:LEU:CG	2.36	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:213:PHE:O	1:M:217:LEU:HD12	1.89	0.73
2:B:443:LYS:HD2	2:B:456:GLU:CB	2.19	0.73
2:N:440:LEU:HG	2:N:461:ALA:HA	1.71	0.73
2:B:567:ALA:CA	3:C:558:ASP:OD2	2.38	0.72
1:A:73:ALA:HB3	1:A:74:GLY:C	2.15	0.72
1:M:73:ALA:HB3	1:M:74:GLY:C	2.15	0.72
2:B:554:TYR:CD1	2:N:554:TYR:CE1	2.72	0.72
6:Q:2:VAL:HG13	6:Q:27:PHE:CD1	2.24	0.72
6:H:2:VAL:HG13	6:H:27:PHE:CD1	2.24	0.72
1:M:99:PHE:CE1	1:M:195:MET:HE3	2.25	0.72
2:B:569:GLU:HG3	3:O:552:GLN:HB2	1.72	0.72
2:N:562:TYR:CZ	2:N:566:LEU:HD21	2.25	0.72
1:M:64:GLU:HG2	2:B:387:GLN:CD	2.15	0.72
2:N:443:LYS:HD2	2:N:456:GLU:CB	2.19	0.72
2:N:569:GLU:CG	3:C:552:GLN:CB	2.63	0.72
3:C:844:ASP:CB	3:O:633:LYS:HD3	2.20	0.72
2:N:563:ARG:CB	3:O:555:LYS:CD	2.59	0.72
1:A:67:THR:CG2	2:N:387:GLN:NE2	2.52	0.71
3:O:738:LEU:HD13	3:O:751:GLN:HE21	1.55	0.71
1:A:99:PHE:CE1	1:A:195:MET:HE3	2.25	0.71
2:N:567:ALA:CB	3:O:555:LYS:HG3	2.21	0.71
2:B:468:HIS:O	2:B:472:THR:HG23	1.90	0.71
2:N:563:ARG:HG2	3:O:555:LYS:HZ3	1.54	0.71
3:O:780:GLU:O	3:O:784:THR:HG23	1.89	0.71
2:B:562:TYR:CZ	2:B:566:LEU:HD21	2.25	0.71
3:C:633:LYS:HD3	3:O:844:ASP:CB	2.20	0.71
3:C:813:LEU:HB3	3:C:814:PRO:HD3	1.72	0.71
2:N:468:HIS:O	2:N:472:THR:HG23	1.90	0.71
2:B:440:LEU:HG	2:B:461:ALA:HA	1.71	0.71
1:A:61:ILE:CA	1:M:120:THR:HA	2.20	0.71
1:A:67:THR:CB	2:N:390:LYS:CE	2.46	0.71
3:C:837:GLU:N	3:O:833:THR:HG21	1.85	0.71
2:N:563:ARG:CG	3:O:555:LYS:HE2	2.21	0.71
2:B:567:ALA:HB1	3:C:558:ASP:CG	2.16	0.70
1:A:213:PHE:O	1:A:217:LEU:HD12	1.89	0.70
3:C:738:LEU:HD13	3:C:751:GLN:HE21	1.55	0.70
1:A:180:MET:HE2	1:A:210:GLU:HG2	1.73	0.70
3:O:813:LEU:HB3	3:O:814:PRO:HD3	1.72	0.70
3:C:633:LYS:HD3	3:O:844:ASP:CG	2.17	0.70
1:A:60:ASN:C	1:M:120:THR:HB	2.15	0.69
2:B:433:PHE:CD2	2:B:442:ALA:HB2	2.27	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:PRO:HD2	1:M:57:GLU:HB2	1.75	0.69
3:O:748:ASP:HB3	3:O:751:GLN:HB2	1.74	0.69
1:M:180:MET:HE2	1:M:210:GLU:HG2	1.73	0.69
2:B:500:ARG:HG2	2:B:522:ASN:CG	2.18	0.69
2:N:433:PHE:CD2	2:N:442:ALA:HB2	2.27	0.69
3:C:844:ASP:CG	3:O:633:LYS:HD3	2.17	0.69
2:B:567:ALA:CB	2:N:568:ASN:CG	2.64	0.69
3:O:567:SER:OG	3:O:570:GLU:HG3	1.93	0.69
3:C:567:SER:OG	3:C:570:GLU:HG3	1.93	0.69
1:A:57:GLU:HB2	1:M:119:PRO:HD2	1.75	0.68
2:B:461:ALA:O	2:B:467:GLY:HA2	1.94	0.68
1:M:142:ILE:CG2	1:M:179:MET:HE1	2.23	0.68
2:B:443:LYS:HD2	2:B:456:GLU:CG	2.23	0.68
3:C:838:ASP:HA	3:O:838:ASP:CA	2.23	0.68
3:C:838:ASP:CA	3:O:838:ASP:HA	2.23	0.68
2:N:443:LYS:HD2	2:N:456:GLU:CG	2.24	0.68
2:N:461:ALA:O	2:N:467:GLY:HA2	1.94	0.68
1:A:72:GLU:HB2	2:B:389:LEU:HD23	1.64	0.68
1:A:142:ILE:CG2	1:A:179:MET:HE1	2.23	0.68
2:B:523:LYS:NZ	2:B:533:ASP:OD2	2.26	0.68
2:N:500:ARG:HG2	2:N:522:ASN:CG	2.18	0.68
2:N:523:LYS:NZ	2:N:533:ASP:OD2	2.26	0.68
1:A:120:THR:HB	1:M:60:ASN:C	2.15	0.68
1:M:70:GLN:HG3	2:N:388:LYS:O	1.90	0.68
3:C:840:PHE:CE2	3:O:633:LYS:HB3	2.05	0.68
2:N:399:VAL:HG21	2:N:540:PHE:CE1	2.29	0.68
2:B:399:VAL:HG21	2:B:540:PHE:CE1	2.29	0.67
3:C:748:ASP:HB3	3:C:751:GLN:HB2	1.74	0.67
2:B:507:ILE:CG2	2:B:515:ILE:HG22	2.24	0.67
1:A:120:THR:HA	1:M:61:ILE:CA	2.20	0.67
1:A:60:ASN:CG	1:M:121:SER:CA	2.67	0.67
2:N:507:ILE:CG2	2:N:515:ILE:HG22	2.24	0.67
3:C:787:TRP:CD1	3:C:807:ARG:HA	2.30	0.67
2:B:479:PRO:HG3	2:B:528:TRP:HZ3	1.58	0.67
2:N:479:PRO:HG3	2:N:528:TRP:HZ3	1.58	0.67
2:B:439:GLU:HB2	2:B:459:ILE:O	1.95	0.66
2:B:530:SER:O	2:B:533:ASP:N	2.28	0.66
2:B:418:ILE:HD11	2:B:432:VAL:CG2	2.26	0.66
2:N:470:ALA:HB2	2:N:517:VAL:HG21	1.78	0.66
2:N:439:GLU:HB2	2:N:459:ILE:O	1.96	0.66
2:N:530:SER:O	2:N:533:ASP:N	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLU:O	1:M:120:THR:CG2	2.43	0.66
3:O:787:TRP:CD1	3:O:807:ARG:HA	2.30	0.66
2:N:535:ASP:OD1	2:N:535:ASP:N	2.27	0.66
2:B:567:ALA:HB2	3:C:558:ASP:OD2	1.91	0.66
2:B:498:ARG:O	2:B:522:ASN:ND2	2.29	0.65
2:N:418:ILE:HD11	2:N:432:VAL:CG2	2.26	0.65
6:H:212:PRO:O	6:H:213:ARG:HB2	1.95	0.65
6:Q:212:PRO:O	6:Q:213:ARG:HB2	1.95	0.65
1:A:67:THR:HG21	2:N:387:GLN:HE21	1.58	0.65
2:N:443:LYS:HD2	2:N:456:GLU:HG2	1.78	0.65
3:O:644:LEU:O	3:O:648:ILE:HG13	1.96	0.65
2:B:528:TRP:N	2:B:528:TRP:CD1	2.64	0.65
2:B:568:ASN:CB	2:N:568:ASN:CB	2.57	0.65
2:N:567:ALA:HB1	3:O:558:ASP:OD2	1.94	0.65
1:A:72:GLU:OE1	2:B:389:LEU:HD23	1.95	0.65
2:B:443:LYS:HD2	2:B:456:GLU:HG2	1.78	0.65
2:N:530:SER:C	2:N:532:PHE:H	2.04	0.65
3:C:644:LEU:O	3:C:648:ILE:HG13	1.96	0.65
2:B:530:SER:C	2:B:532:PHE:H	2.04	0.65
2:N:498:ARG:O	2:N:522:ASN:ND2	2.29	0.65
2:B:527:PRO:HG2	2:B:528:TRP:CD1	2.32	0.64
1:M:78:LYS:HZ3	2:N:388:LYS:HE3	1.57	0.64
1:M:78:LYS:CE	2:N:388:LYS:CE	2.71	0.64
2:B:470:ALA:HB2	2:B:517:VAL:HG21	1.78	0.64
2:N:434:LEU:HD21	2:N:548:ILE:HG21	1.80	0.64
2:N:527:PRO:HG2	2:N:528:TRP:CD1	2.32	0.64
2:N:528:TRP:CD1	2:N:528:TRP:N	2.64	0.64
3:C:833:THR:HG21	3:O:837:GLU:N	1.85	0.64
1:A:60:ASN:HB3	1:M:121:SER:N	1.48	0.64
3:O:794:ARG:CZ	6:Q:54:ILE:CD1	2.76	0.64
3:C:794:ARG:CZ	6:H:54:ILE:CD1	2.76	0.64
2:B:570:MET:HE1	3:C:560:SER:O	1.95	0.63
1:M:64:GLU:HG2	2:B:387:GLN:HB2	1.78	0.63
2:N:531:LYS:HA	2:N:534:GLU:OE1	1.98	0.63
2:B:434:LEU:HD21	2:B:548:ILE:HG21	1.80	0.63
3:C:843:LEU:O	3:C:847:ARG:HG2	1.98	0.63
3:O:843:LEU:O	3:O:847:ARG:HG2	1.98	0.63
1:A:120:THR:CG2	1:M:58:GLU:O	2.43	0.63
1:A:120:THR:HG1	1:M:57:GLU:C	2.00	0.63
1:A:64:GLU:HA	2:N:387:GLN:CD	2.21	0.63
1:M:64:GLU:HA	2:B:387:GLN:CD	2.15	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:417:ILE:HD13	2:N:548:ILE:HD11	1.81	0.62
2:B:433:PHE:CG	2:B:442:ALA:HB2	2.33	0.62
2:N:510:GLU:HA	2:N:510:GLU:OE1	2.00	0.62
2:B:527:PRO:HB2	2:B:528:TRP:CD1	2.35	0.62
3:C:608:LYS:H	3:C:608:LYS:HE3	1.65	0.62
2:N:458:ARG:HH11	2:N:458:ARG:CG	2.12	0.62
2:N:460:PRO:CG	2:N:463:GLN:HB3	2.20	0.62
2:N:570:MET:HE2	3:O:560:SER:H	1.63	0.62
1:A:118:THR:HG22	1:A:120:THR:H	1.64	0.62
2:B:458:ARG:HH11	2:B:458:ARG:CG	2.12	0.62
3:C:837:GLU:N	3:O:840:PHE:HB2	2.14	0.62
3:O:608:LYS:H	3:O:608:LYS:CE	2.13	0.62
2:B:531:LYS:HA	2:B:534:GLU:OE1	1.98	0.62
2:N:527:PRO:HB2	2:N:528:TRP:CD1	2.35	0.62
1:M:72:GLU:OE1	2:N:389:LEU:CD2	2.40	0.62
2:B:561:GLN:O	2:N:561:GLN:OE1	2.07	0.62
3:O:665:ILE:HD11	3:O:680:ILE:HG21	1.82	0.62
2:N:410:VAL:O	2:N:414:LEU:HB2	2.00	0.62
2:N:433:PHE:CG	2:N:442:ALA:HB2	2.33	0.62
3:O:814:PRO:HD2	3:O:815:LYS:HE3	1.82	0.62
1:A:67:THR:HG21	2:N:387:GLN:NE2	2.15	0.62
3:O:608:LYS:H	3:O:608:LYS:HE3	1.65	0.62
1:A:61:ILE:CB	1:M:120:THR:HG23	2.30	0.61
1:A:67:THR:HG23	2:N:387:GLN:HE21	1.64	0.61
1:M:72:GLU:CG	2:N:389:LEU:CD2	2.77	0.61
2:B:458:ARG:HH11	2:B:458:ARG:HG2	1.65	0.61
3:O:608:LYS:H	3:O:608:LYS:HD3	1.64	0.61
2:B:410:VAL:O	2:B:414:LEU:HB2	2.00	0.61
3:C:608:LYS:H	3:C:608:LYS:HD3	1.64	0.61
3:C:665:ILE:HD11	3:C:680:ILE:HG21	1.82	0.61
2:B:527:PRO:HG2	2:B:528:TRP:HD1	1.65	0.61
3:C:840:PHE:HB2	3:O:837:GLU:N	2.14	0.61
2:B:440:LEU:HD13	2:B:466:ALA:HB1	1.83	0.61
2:N:440:LEU:HD13	2:N:466:ALA:HB1	1.83	0.61
1:A:120:THR:HG23	1:M:61:ILE:CB	2.30	0.61
2:B:435:LEU:HD11	2:B:437:GLN:O	2.01	0.61
3:C:788:GLU:O	3:C:792:LEU:HD13	2.01	0.61
2:N:561:GLN:HE21	2:N:561:GLN:CA	2.10	0.61
1:A:67:THR:CA	2:N:390:LYS:CE	2.75	0.61
3:C:814:PRO:HD2	3:C:815:LYS:HE3	1.82	0.61
1:M:118:THR:HG22	1:M:120:THR:H	1.64	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:475:ILE:HD13	2:B:506:PRO:CD	2.31	0.61
2:B:535:ASP:OD1	2:B:535:ASP:N	2.27	0.61
2:N:458:ARG:HH11	2:N:458:ARG:HG2	1.65	0.61
3:C:838:ASP:C	3:O:838:ASP:HA	2.26	0.61
5:L:125:LEU:HD22	5:L:183:LYS:HG3	1.81	0.61
1:A:118:THR:HG21	1:M:57:GLU:HA	1.83	0.61
2:B:561:GLN:OE1	2:N:561:GLN:O	2.09	0.61
5:R:125:LEU:HD22	5:R:183:LYS:HG3	1.81	0.61
2:B:441:VAL:HG21	2:B:458:ARG:CZ	2.31	0.60
2:N:475:ILE:HD13	2:N:506:PRO:HD3	1.83	0.60
3:C:633:LYS:HB3	3:O:840:PHE:CE2	2.05	0.60
3:O:788:GLU:O	3:O:792:LEU:HD13	2.01	0.60
1:A:61:ILE:CG1	1:M:120:THR:HG23	2.32	0.60
2:B:417:ILE:HD13	2:B:548:ILE:HD11	1.81	0.60
3:C:740:ARG:NH1	3:C:741:LYS:HE2	2.16	0.60
3:C:608:LYS:H	3:C:608:LYS:CE	2.13	0.60
2:B:475:ILE:HD13	2:B:506:PRO:HD3	1.83	0.60
2:B:505:PHE:HD1	2:B:541:SER:HG	1.46	0.60
1:A:121:SER:CA	1:M:60:ASN:CG	2.67	0.60
2:N:570:MET:HE2	3:O:560:SER:N	1.80	0.60
2:B:399:VAL:HG11	2:B:424:LEU:HD11	1.84	0.60
2:B:510:GLU:HA	2:B:510:GLU:OE1	2.00	0.60
2:N:475:ILE:HD13	2:N:506:PRO:CD	2.31	0.60
3:O:740:ARG:NH1	3:O:741:LYS:HE2	2.16	0.60
1:A:57:GLU:HA	1:M:118:THR:CG2	2.31	0.60
1:M:69:ILE:HG22	2:N:389:LEU:HD12	1.83	0.60
1:M:184:ILE:CD1	1:M:224:LEU:HD12	2.31	0.60
2:B:443:LYS:HD2	2:B:456:GLU:HB3	1.83	0.60
2:N:435:LEU:HD11	2:N:437:GLN:O	2.01	0.60
2:N:441:VAL:HG21	2:N:458:ARG:CZ	2.31	0.60
1:A:118:THR:CG2	1:M:57:GLU:HA	2.31	0.60
1:A:118:THR:HB	1:A:121:SER:HB2	1.82	0.60
1:A:120:THR:HG23	1:M:61:ILE:CG1	2.32	0.60
1:M:118:THR:HB	1:M:121:SER:HB2	1.82	0.60
2:N:459:ILE:HG13	2:N:463:GLN:OE1	2.02	0.60
6:Q:128:SER:H	6:Q:213:ARG:HH21	1.50	0.59
1:M:70:GLN:O	2:N:389:LEU:CD2	2.50	0.59
1:M:70:GLN:C	2:N:389:LEU:HD22	2.28	0.59
2:B:459:ILE:HG13	2:B:463:GLN:OE1	2.02	0.59
3:C:838:ASP:HA	3:O:838:ASP:C	2.26	0.59
1:A:184:ILE:CD1	1:A:224:LEU:HD12	2.31	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:4:MET:HE3	5:R:23:CYS:SG	2.42	0.59
2:N:443:LYS:HD2	2:N:456:GLU:HB3	1.83	0.59
3:O:702:SER:HA	7:O:902:IBM:O6	2.03	0.59
5:L:4:MET:HE3	5:L:23:CYS:SG	2.42	0.59
2:N:527:PRO:HG2	2:N:528:TRP:HD1	1.65	0.59
3:C:702:SER:HA	7:C:902:IBM:O6	2.03	0.59
3:C:840:PHE:CE2	3:O:633:LYS:CG	2.85	0.59
1:A:57:GLU:HA	1:M:118:THR:HG21	1.83	0.59
2:N:399:VAL:HG11	2:N:424:LEU:HD11	1.84	0.59
2:N:563:ARG:C	3:O:555:LYS:HZ2	2.11	0.59
2:B:432:VAL:CG1	2:B:518:ALA:HB2	2.33	0.59
2:B:509:ASN:OD1	2:B:513:GLU:HG3	2.03	0.59
3:O:664:TYR:HB2	3:O:789:GLN:NE2	2.18	0.58
3:C:564:PHE:HD1	3:C:777:ARG:CZ	2.17	0.58
3:C:664:TYR:HB2	3:C:789:GLN:NE2	2.18	0.58
6:H:128:SER:H	6:H:213:ARG:HH21	1.50	0.58
1:M:72:GLU:CB	2:N:389:LEU:HD22	2.27	0.58
2:B:471:THR:HG22	2:B:472:THR:N	2.19	0.58
2:B:476:LEU:HD23	2:B:478:ILE:HD12	1.85	0.58
1:A:67:THR:HG23	2:N:387:GLN:NE2	2.17	0.58
2:B:567:ALA:HB2	3:C:555:LYS:HG2	1.85	0.58
2:B:567:ALA:HB2	3:C:555:LYS:HG3	1.84	0.58
2:N:476:LEU:HD23	2:N:478:ILE:HD12	1.85	0.58
3:C:837:GLU:CB	3:O:836:SER:O	2.52	0.58
1:A:118:THR:OG1	1:M:57:GLU:OE2	2.20	0.57
2:B:530:SER:C	2:B:532:PHE:N	2.62	0.57
2:N:398:GLN:HE22	2:N:401:LYS:HD3	1.69	0.57
2:B:443:LYS:HA	2:B:456:GLU:HA	1.85	0.57
2:B:475:ILE:HG23	2:B:505:PHE:HB3	1.85	0.57
2:B:564:SER:N	3:C:555:LYS:HD2	2.17	0.57
3:C:795:THR:HB	6:H:30:LYS:HZ2	1.68	0.57
2:B:460:PRO:CG	2:B:463:GLN:HB3	2.20	0.57
2:N:443:LYS:HA	2:N:456:GLU:HA	1.85	0.57
3:C:807:ARG:HG3	3:C:807:ARG:HH11	1.69	0.57
2:N:471:THR:HG22	2:N:472:THR:N	2.19	0.57
2:N:509:ASN:OD1	2:N:513:GLU:HG3	2.04	0.57
2:N:530:SER:C	2:N:532:PHE:N	2.62	0.57
1:A:120:THR:CG2	1:M:58:GLU:HA	2.29	0.57
2:N:475:ILE:HG23	2:N:505:PHE:HB3	1.85	0.57
3:O:564:PHE:HD1	3:O:777:ARG:CZ	2.17	0.57
3:O:807:ARG:HG3	3:O:807:ARG:HH11	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:563:ARG:HG2	3:O:555:LYS:NZ	2.18	0.57
2:N:500:ARG:NE	2:N:522:ASN:HB3	2.20	0.57
3:O:808:ASN:HD21	6:Q:56:ASP:CB	2.18	0.57
1:A:61:ILE:HB	1:M:120:THR:HG23	1.82	0.57
2:N:502:ILE:HG21	2:N:519:GLU:OE1	2.05	0.57
6:H:60:VAL:HG22	6:H:61:PRO:HD2	1.87	0.57
2:B:567:ALA:HA	3:C:558:ASP:OD2	2.03	0.57
2:B:403:LEU:HD22	2:B:417:ILE:HG13	1.87	0.56
2:B:528:TRP:N	2:B:528:TRP:HD1	2.03	0.56
3:C:836:SER:O	3:O:837:GLU:CB	2.52	0.56
6:H:54:ILE:HG13	6:H:56:ASP:H	1.70	0.56
2:B:471:THR:HG22	2:B:472:THR:HG22	1.88	0.56
2:B:459:ILE:HD12	2:B:460:PRO:CD	2.35	0.56
6:Q:60:VAL:HG22	6:Q:61:PRO:HD2	1.87	0.56
1:A:58:GLU:HA	1:M:120:THR:CG2	2.29	0.56
2:B:398:GLN:HE22	2:B:401:LYS:HD3	1.69	0.56
2:N:528:TRP:N	2:N:528:TRP:HD1	2.03	0.56
6:Q:54:ILE:HG13	6:Q:56:ASP:H	1.70	0.56
3:C:808:ASN:HD21	6:H:56:ASP:CB	2.18	0.56
2:N:432:VAL:CG1	2:N:518:ALA:HB2	2.33	0.56
1:A:72:GLU:CB	2:B:389:LEU:HD22	2.21	0.56
2:N:459:ILE:HD12	2:N:460:PRO:CD	2.35	0.56
3:O:608:LYS:CD	3:O:608:LYS:N	2.69	0.56
3:C:690:LEU:O	3:C:690:LEU:HD23	2.05	0.56
2:N:471:THR:HG22	2:N:472:THR:CG2	2.36	0.56
2:N:563:ARG:CG	3:O:555:LYS:CE	2.81	0.56
3:C:608:LYS:HD3	3:C:608:LYS:N	2.21	0.56
6:Q:12:VAL:HG21	6:Q:82(C):LEU:HD13	1.88	0.56
2:B:506:PRO:O	2:B:507:ILE:HD12	2.06	0.56
2:N:403:LEU:HD22	2:N:417:ILE:HG13	1.87	0.56
6:H:134:SER:O	6:H:185:SER:HB2	2.06	0.56
1:A:64:GLU:OE2	1:M:82:LYS:NZ	2.38	0.55
2:B:500:ARG:NE	2:B:522:ASN:HB3	2.20	0.55
2:B:502:ILE:HG21	2:B:519:GLU:OE1	2.05	0.55
2:B:439:GLU:HA	2:B:461:ALA:HB2	1.88	0.55
3:O:690:LEU:O	3:O:690:LEU:HD23	2.05	0.55
5:L:36:TYR:HE1	6:H:100(C):PHE:O	1.90	0.55
2:B:530:SER:O	2:B:533:ASP:HB2	2.07	0.55
2:N:506:PRO:O	2:N:507:ILE:HD12	2.06	0.55
3:O:709:TYR:CZ	3:O:713:LEU:HD11	2.42	0.55
3:O:809:LYS:HA	3:O:809:LYS:CE	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:36:TYR:HE1	6:Q:100(C):PHE:O	1.90	0.55
2:N:505:PHE:HB2	2:N:506:PRO:HD2	1.88	0.55
3:C:794:ARG:HG3	6:H:54:ILE:HG22	1.85	0.55
6:H:12:VAL:HG21	6:H:82(C):LEU:HD13	1.88	0.55
1:M:70:GLN:O	2:N:389:LEU:HD22	2.06	0.55
2:B:471:THR:HG22	2:B:472:THR:CG2	2.36	0.55
2:B:500:ARG:NH2	2:B:523:LYS:O	2.40	0.55
2:N:439:GLU:HA	2:N:461:ALA:HB2	1.88	0.55
2:N:530:SER:O	2:N:533:ASP:HB2	2.07	0.55
3:O:608:LYS:HD3	3:O:608:LYS:N	2.21	0.55
6:Q:134:SER:O	6:Q:185:SER:HB2	2.06	0.55
2:B:418:ILE:CD1	2:B:444:VAL:HG21	2.37	0.55
2:B:563:ARG:O	3:C:555:LYS:HG2	2.04	0.55
2:B:568:ASN:ND2	2:N:567:ALA:HB1	1.91	0.55
2:N:471:THR:HG22	2:N:472:THR:HG22	1.88	0.55
3:O:794:ARG:HG3	6:Q:54:ILE:HG22	1.85	0.55
1:A:90:LEU:N	1:M:89:GLN:HB3	2.22	0.55
2:B:505:PHE:HB2	2:B:506:PRO:HD2	1.88	0.55
3:C:709:TYR:CZ	3:C:713:LEU:HD11	2.42	0.55
1:A:89:GLN:HB3	1:M:90:LEU:N	2.22	0.54
3:O:736:PHE:CZ	3:O:827:GLN:HG3	2.42	0.54
3:C:608:LYS:CD	3:C:608:LYS:N	2.69	0.54
3:O:572:ALA:O	3:O:576:ILE:HG13	2.08	0.54
2:B:505:PHE:HB2	2:B:506:PRO:CD	2.37	0.54
2:N:500:ARG:NH2	2:N:523:LYS:O	2.39	0.54
3:O:830:GLU:HA	3:O:843:LEU:HD22	1.90	0.54
1:A:72:GLU:CG	2:B:389:LEU:CD2	2.84	0.54
2:B:439:GLU:CA	2:B:461:ALA:HB2	2.38	0.54
2:N:457:ILE:HG22	2:N:457:ILE:O	2.07	0.54
3:C:633:LYS:CG	3:O:840:PHE:CE2	2.85	0.54
3:C:736:PHE:CZ	3:C:827:GLN:HG3	2.42	0.54
3:C:841:PRO:HA	3:O:633:LYS:HD2	1.89	0.54
3:O:795:THR:CB	6:Q:30:LYS:NZ	2.70	0.54
2:N:567:ALA:HB1	3:O:558:ASP:CG	2.33	0.54
3:C:834:HIS:HA	3:O:834:HIS:HA	1.89	0.54
1:A:56:LEU:O	1:M:120:THR:OG1	2.26	0.54
2:N:418:ILE:CD1	2:N:444:VAL:HG21	2.37	0.54
2:N:443:LYS:CD	2:N:456:GLU:HB3	2.38	0.54
3:C:815:LYS:H	3:C:815:LYS:CE	2.20	0.54
3:C:840:PHE:N	3:O:837:GLU:CB	2.71	0.54
1:A:75:SER:CB	2:B:389:LEU:HD11	2.35	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:THR:HG23	1:M:61:ILE:HB	1.82	0.54
3:C:838:ASP:N	3:O:840:PHE:H	2.06	0.54
3:O:772:TRP:HB3	3:O:773:PRO:HD3	1.90	0.54
6:H:119:PRO:HB3	6:H:145:TYR:HB3	1.90	0.54
2:B:499:THR:O	2:B:500:ARG:HD3	2.08	0.54
2:N:505:PHE:HB2	2:N:506:PRO:CD	2.37	0.54
6:H:39:GLN:HB2	6:H:45:LEU:CD2	2.36	0.54
2:B:561:GLN:HE21	2:B:561:GLN:CA	2.10	0.54
2:N:455:TYR:CD2	2:N:455:TYR:N	2.76	0.54
3:C:572:ALA:O	3:C:576:ILE:HG13	2.08	0.54
3:C:633:LYS:HD2	3:O:841:PRO:HA	1.89	0.54
3:O:793:GLU:O	3:O:797:LEU:HB2	2.08	0.53
1:A:161:ASN:OD1	1:A:162:ASN:O	2.27	0.53
2:B:567:ALA:HB1	2:N:568:ASN:ND2	1.94	0.53
6:Q:119:PRO:HB3	6:Q:145:TYR:HB3	1.90	0.53
2:N:439:GLU:CA	2:N:461:ALA:HB2	2.38	0.53
3:C:836:SER:O	3:O:837:GLU:HB3	2.09	0.53
3:O:815:LYS:H	3:O:815:LYS:CE	2.20	0.53
1:M:180:MET:HE1	1:M:210:GLU:N	2.23	0.53
2:B:444:VAL:O	2:B:444:VAL:HG13	2.08	0.53
3:C:793:GLU:O	3:C:797:LEU:HB2	2.08	0.53
6:H:40:ARG:HD3	6:H:43:LYS:HD2	1.90	0.53
2:B:521:VAL:HG12	2:B:522:ASN:OD1	2.08	0.53
3:C:837:GLU:CB	3:O:840:PHE:N	2.71	0.53
1:M:161:ASN:OD1	1:M:162:ASN:O	2.27	0.53
2:B:398:GLN:OE1	2:B:398:GLN:HA	2.06	0.53
2:N:499:THR:O	2:N:500:ARG:HD3	2.08	0.53
3:C:830:GLU:HA	3:C:843:LEU:HD22	1.90	0.53
1:A:89:GLN:HB3	1:M:89:GLN:C	2.34	0.53
1:M:69:ILE:HG22	2:N:389:LEU:CD1	2.39	0.53
2:B:443:LYS:CD	2:B:456:GLU:HB3	2.38	0.53
2:N:521:VAL:HG12	2:N:522:ASN:OD1	2.08	0.53
3:C:670:HIS:ND1	3:C:672:LEU:HB2	2.24	0.53
6:Q:39:GLN:HB2	6:Q:45:LEU:CD2	2.36	0.53
1:A:180:MET:HE1	1:A:210:GLU:N	2.23	0.53
2:B:567:ALA:CB	3:C:555:LYS:HG3	2.39	0.53
6:Q:40:ARG:HD3	6:Q:43:LYS:HD2	1.90	0.53
2:N:501:ASN:C	2:N:502:ILE:HG13	2.34	0.52
3:C:772:TRP:HB3	3:C:773:PRO:HD3	1.90	0.52
3:O:670:HIS:ND1	3:O:672:LEU:HB2	2.24	0.52
1:A:70:GLN:C	2:B:389:LEU:CD1	2.68	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:479:PRO:HB3	2:B:528:TRP:CE3	2.45	0.52
2:N:458:ARG:O	2:N:459:ILE:HB	2.09	0.52
2:N:563:ARG:O	3:O:555:LYS:HG3	2.05	0.52
3:C:840:PHE:H	3:O:838:ASP:N	2.06	0.52
2:B:457:ILE:O	2:B:457:ILE:HG22	2.07	0.52
2:N:479:PRO:HB3	2:N:528:TRP:CE3	2.45	0.52
3:O:795:THR:HB	6:Q:30:LYS:HZ2	1.73	0.52
2:B:421:ALA:HB2	2:B:540:PHE:CE2	2.45	0.52
2:N:435:LEU:HD13	2:N:436:ASP:N	2.24	0.52
1:A:89:GLN:HB3	1:M:89:GLN:CA	2.36	0.52
2:B:435:LEU:HD13	2:B:436:ASP:N	2.24	0.52
2:N:444:VAL:HG13	2:N:444:VAL:O	2.08	0.52
3:C:663:SER:O	3:C:667:ARG:HD3	2.10	0.52
3:C:808:ASN:HD21	6:H:56:ASP:HB3	1.75	0.52
3:O:745:ASN:OD1	3:O:747:GLU:HG2	2.09	0.52
5:L:83:LEU:HD11	5:L:106:LEU:HD13	1.92	0.52
1:M:72:GLU:CG	2:N:389:LEU:HD22	2.40	0.52
3:C:745:ASN:OD1	3:C:747:GLU:HG2	2.09	0.52
3:C:837:GLU:HB3	3:O:836:SER:O	2.09	0.52
3:O:794:ARG:HG3	6:Q:54:ILE:CG2	2.40	0.52
1:A:87:LEU:HD22	1:A:91:LEU:HD11	1.92	0.52
3:O:777:ARG:O	3:O:780:GLU:HB2	2.09	0.52
1:A:89:GLN:C	1:M:89:GLN:HB3	2.34	0.51
4:D:81:LEU:HB3	4:D:87:ILE:HD13	1.92	0.51
3:O:690:LEU:HD23	3:O:690:LEU:C	2.35	0.51
1:A:57:GLU:HA	1:M:120:THR:HG1	1.72	0.51
3:C:690:LEU:HD23	3:C:690:LEU:C	2.35	0.51
3:C:795:THR:CB	6:H:30:LYS:NZ	2.70	0.51
2:B:532:PHE:CD1	2:B:532:PHE:C	2.89	0.51
2:N:398:GLN:HA	2:N:398:GLN:OE1	2.06	0.51
3:O:663:SER:O	3:O:667:ARG:HD3	2.10	0.51
1:A:99:PHE:CE1	1:A:195:MET:CE	2.93	0.51
2:B:458:ARG:CG	2:B:458:ARG:NH1	2.73	0.51
2:N:563:ARG:O	3:O:555:LYS:HG2	2.05	0.51
5:R:124:GLN:O	5:R:127:SER:HB2	2.11	0.51
2:N:421:ALA:HB2	2:N:540:PHE:CE2	2.45	0.51
2:N:467:GLY:O	2:N:471:THR:HB	2.10	0.51
2:N:571:MET:O	3:C:631:ALA:HB1	2.05	0.51
5:R:83:LEU:HD11	5:R:106:LEU:HD13	1.92	0.51
2:B:477:ASN:OD1	2:B:478:ILE:N	2.44	0.51
2:N:477:ASN:OD1	2:N:478:ILE:N	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:901:IBM:H12	7:O:901:IBM:O2	2.11	0.51
1:A:61:ILE:CA	1:M:120:THR:CG2	2.69	0.51
2:B:455:TYR:CD2	2:B:455:TYR:N	2.76	0.51
2:B:458:ARG:O	2:B:459:ILE:HB	2.09	0.51
2:B:563:ARG:CA	3:C:555:LYS:CE	2.72	0.51
2:N:532:PHE:CD1	2:N:532:PHE:C	2.89	0.51
3:C:794:ARG:HG3	6:H:54:ILE:CG2	2.40	0.51
5:L:124:GLN:O	5:L:127:SER:HB2	2.11	0.51
5:L:195:GLU:HG2	5:L:206:VAL:HG22	1.93	0.51
3:C:777:ARG:O	3:C:780:GLU:HB2	2.09	0.51
3:O:808:ASN:HD21	6:Q:56:ASP:HB3	1.75	0.51
1:A:57:GLU:HB2	1:M:118:THR:CG2	2.03	0.51
2:N:441:VAL:HG11	2:N:443:LYS:HE3	1.93	0.51
3:O:794:ARG:NH1	6:Q:54:ILE:HD12	2.26	0.51
1:A:61:ILE:HG13	1:M:120:THR:HG23	1.93	0.51
1:M:72:GLU:CD	2:N:389:LEU:HD23	2.32	0.51
1:M:180:MET:HE2	1:M:210:GLU:CG	2.40	0.51
2:B:465:ILE:HG22	2:B:466:ALA:N	2.25	0.51
2:N:569:GLU:CD	3:C:552:GLN:HB2	2.35	0.51
3:C:562:SER:HB2	3:C:774:ILE:CD1	2.41	0.51
3:C:840:PHE:CE2	3:O:633:LYS:CD	2.94	0.51
2:B:501:ASN:C	2:B:502:ILE:HG13	2.35	0.50
3:O:562:SER:HB2	3:O:774:ILE:CD1	2.41	0.50
4:P:81:LEU:HB3	4:P:87:ILE:HD13	1.92	0.50
1:M:142:ILE:CB	1:M:179:MET:HE1	2.41	0.50
2:N:418:ILE:CG1	2:N:432:VAL:HG22	2.41	0.50
2:N:465:ILE:HG22	2:N:466:ALA:N	2.26	0.50
3:O:765:LEU:HD22	3:O:765:LEU:H	1.76	0.50
1:A:82:LYS:NZ	1:M:64:GLU:OE2	2.38	0.50
2:B:467:GLY:O	2:B:471:THR:HB	2.10	0.50
2:B:508:LYS:HA	2:B:513:GLU:C	2.37	0.50
3:C:740:ARG:HG2	3:O:742:ASN:HB3	1.94	0.50
3:C:823:PHE:HD2	3:C:824:VAL:HG23	1.76	0.50
3:O:658:ARG:HG2	3:O:681:MET:HE1	1.93	0.50
1:A:180:MET:HE2	1:A:210:GLU:CG	2.40	0.50
2:B:473:GLY:HA2	2:B:514:VAL:HG21	1.93	0.50
2:B:536:LEU:HD22	2:B:536:LEU:O	2.12	0.50
3:C:765:LEU:HD22	3:C:765:LEU:H	1.76	0.50
3:C:742:ASN:HB3	3:O:740:ARG:HG2	1.94	0.50
3:C:809:LYS:HD2	3:C:809:LYS:N	2.27	0.50
3:O:761:THR:O	3:O:765:LEU:CD2	2.58	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:809:LYS:HD2	3:O:809:LYS:N	2.27	0.50
1:A:120:THR:HG23	1:M:61:ILE:HG13	1.93	0.50
2:B:418:ILE:CG1	2:B:432:VAL:HG22	2.41	0.50
2:N:473:GLY:HA2	2:N:514:VAL:HG21	1.93	0.50
7:C:901:IBM:H12	7:C:901:IBM:O2	2.11	0.50
6:H:99:ASP:OD2	6:H:100(B):ARG:HD3	2.12	0.50
3:C:794:ARG:NH1	6:H:54:ILE:HD12	2.26	0.50
1:A:142:ILE:CB	1:A:179:MET:HE1	2.41	0.50
1:M:87:LEU:HD22	1:M:91:LEU:HD11	1.92	0.50
2:N:428:GLU:O	2:N:429:ILE:HG23	2.12	0.50
3:C:840:PHE:HB2	3:O:838:ASP:N	2.17	0.50
1:A:120:THR:OG1	1:M:60:ASN:HB2	2.12	0.50
2:N:507:ILE:O	2:N:508:LYS:O	2.30	0.50
3:O:823:PHE:HD2	3:O:824:VAL:HG23	1.76	0.50
5:R:195:GLU:HG2	5:R:206:VAL:HG22	1.93	0.50
3:C:658:ARG:HG2	3:C:681:MET:HE1	1.93	0.49
1:M:99:PHE:CE1	1:M:195:MET:CE	2.93	0.49
2:N:536:LEU:HD22	2:N:536:LEU:O	2.12	0.49
2:B:428:GLU:O	2:B:429:ILE:HG23	2.12	0.49
2:B:441:VAL:HG11	2:B:443:LYS:HE3	1.93	0.49
3:C:840:PHE:CA	3:O:837:GLU:HB2	2.43	0.49
2:B:433:PHE:CD2	2:B:442:ALA:CB	2.96	0.49
2:N:560:ALA:HB1	3:O:553:THR:HG23	1.95	0.49
3:C:740:ARG:HG2	3:O:742:ASN:CB	2.43	0.49
1:A:60:ASN:H	1:M:120:THR:HG1	1.58	0.49
2:B:441:VAL:HG22	2:B:458:ARG:HG3	1.94	0.49
3:C:562:SER:HB2	3:C:774:ILE:HD13	1.95	0.49
3:C:837:GLU:HB2	3:O:840:PHE:CA	2.43	0.49
1:A:89:GLN:HG2	1:M:90:LEU:HG	1.95	0.49
2:N:439:GLU:HA	2:N:461:ALA:N	2.27	0.49
2:N:508:LYS:HA	2:N:513:GLU:C	2.37	0.49
2:B:417:ILE:CD1	2:B:548:ILE:HD11	2.42	0.49
2:N:416:GLU:HA	2:N:416:GLU:OE1	2.12	0.49
2:N:417:ILE:HD13	2:N:548:ILE:CD1	2.43	0.49
3:O:795:THR:HG23	6:Q:53:GLU:CD	2.10	0.49
1:A:98:MET:HE3	1:A:113:ARG:HG2	1.94	0.49
1:A:121:SER:CA	1:M:60:ASN:HD22	2.21	0.49
1:A:199:LYS:HE2	1:A:201:ASN:OD1	2.12	0.49
2:N:441:VAL:HG22	2:N:458:ARG:HG3	1.94	0.49
6:Q:99:ASP:OD2	6:Q:100(B):ARG:HD3	2.12	0.49
1:M:98:MET:HE3	1:M:113:ARG:HG2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:118:THR:HG23	1:M:119:PRO:HD2	1.95	0.49
2:B:417:ILE:HD13	2:B:548:ILE:CD1	2.43	0.49
3:C:633:LYS:CD	3:O:840:PHE:CE2	2.94	0.49
7:C:902:IBM:HN9	7:C:902:IBM:H133	1.78	0.49
1:A:60:ASN:HB2	1:M:120:THR:OG1	2.12	0.49
1:M:199:LYS:HE2	1:M:201:ASN:OD1	2.12	0.49
2:B:568:ASN:CA	2:N:568:ASN:CB	2.91	0.49
2:N:433:PHE:CD2	2:N:442:ALA:CB	2.96	0.49
3:O:562:SER:HB2	3:O:774:ILE:HD13	1.95	0.49
2:B:507:ILE:O	2:B:508:LYS:O	2.30	0.48
7:O:902:IBM:H133	7:O:902:IBM:HN9	1.78	0.48
2:B:439:GLU:HA	2:B:461:ALA:N	2.27	0.48
2:B:479:PRO:CB	2:B:528:TRP:CE3	2.97	0.48
2:N:402:ASN:O	2:N:406:HIS:HD2	1.95	0.48
3:O:795:THR:HB	6:Q:30:LYS:HZ3	1.73	0.48
1:A:90:LEU:HG	1:M:89:GLN:HG2	1.95	0.48
2:B:402:ASN:O	2:B:406:HIS:HD2	1.95	0.48
1:A:119:PRO:C	1:M:61:ILE:CA	2.85	0.48
2:B:527:PRO:CB	2:B:528:TRP:CD1	2.97	0.48
2:N:417:ILE:CD1	2:N:548:ILE:HD11	2.42	0.48
3:C:742:ASN:CB	3:O:740:ARG:HG2	2.43	0.48
3:C:825:CYS:O	3:C:826:THR:C	2.57	0.48
5:R:44:PRO:HD2	6:Q:103:TRP:HB3	1.95	0.48
2:B:565:HIS:HB2	2:N:564:SER:HB3	1.95	0.48
2:B:416:GLU:HA	2:B:416:GLU:OE1	2.12	0.48
2:B:559:GLU:O	2:B:562:TYR:HB3	2.14	0.48
2:N:433:PHE:CE2	2:N:442:ALA:HB3	2.49	0.48
2:N:508:LYS:H	2:N:514:VAL:HA	1.79	0.48
1:M:72:GLU:OE2	2:N:392:GLU:CB	2.37	0.48
2:N:527:PRO:CB	2:N:528:TRP:CD1	2.97	0.48
3:C:601:SER:O	3:C:604:LYS:HG2	2.14	0.48
2:N:441:VAL:HG21	2:N:458:ARG:NH2	2.29	0.48
3:C:753:GLU:O	3:C:753:GLU:HG2	2.13	0.48
1:A:118:THR:HG23	1:A:119:PRO:HD2	1.95	0.47
2:B:478:ILE:HG23	2:B:480:ASP:O	2.14	0.47
2:B:563:ARG:HG2	3:C:555:LYS:NZ	2.27	0.47
2:B:433:PHE:CE2	2:B:442:ALA:HB3	2.49	0.47
2:B:568:ASN:CB	2:N:568:ASN:CA	2.91	0.47
3:C:765:LEU:O	3:C:768:ILE:HG22	2.14	0.47
3:O:765:LEU:O	3:O:768:ILE:HG22	2.14	0.47
2:B:460:PRO:HG2	2:B:463:GLN:CG	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:753:GLU:O	3:O:753:GLU:HG2	2.13	0.47
6:Q:60:VAL:HG22	6:Q:61:PRO:CD	2.44	0.47
2:B:567:ALA:O	2:B:570:MET:HB2	2.14	0.47
3:O:839:CYS:C	3:O:841:PRO:HD2	2.39	0.47
2:B:503:LEU:HD12	2:B:504:CYS:N	2.30	0.47
2:N:478:ILE:HG23	2:N:480:ASP:O	2.14	0.47
2:N:479:PRO:CB	2:N:528:TRP:CE3	2.97	0.47
3:O:793:GLU:OE2	3:O:801:PRO:HA	2.15	0.47
5:L:44:PRO:HD2	6:H:103:TRP:HB3	1.95	0.47
1:A:89:GLN:CA	1:M:89:GLN:HB3	2.36	0.47
2:B:441:VAL:HG21	2:B:458:ARG:NH2	2.29	0.47
2:N:567:ALA:O	2:N:570:MET:HB2	2.14	0.47
1:A:120:THR:HG1	1:M:60:ASN:H	1.60	0.47
2:N:567:ALA:HB2	3:O:558:ASP:OD2	2.05	0.47
3:C:840:PHE:N	3:O:837:GLU:HB2	2.29	0.47
3:O:601:SER:O	3:O:604:LYS:HG2	2.14	0.47
1:A:120:THR:CG2	1:M:61:ILE:CA	2.69	0.47
1:M:67:THR:CB	2:B:390:LYS:CE	2.81	0.47
3:C:795:THR:HB	6:H:30:LYS:HZ3	1.78	0.47
3:C:839:CYS:C	3:C:841:PRO:HD2	2.39	0.47
6:Q:35:HIS:HB2	6:Q:93:ASN:OD1	2.15	0.47
3:C:837:GLU:HB2	3:O:840:PHE:N	2.29	0.47
4:D:86:ILE:HG22	4:D:87:ILE:H	1.80	0.47
1:A:60:ASN:HD22	1:M:121:SER:CA	2.21	0.46
1:M:143:ALA:HB2	1:M:195:MET:HE1	1.97	0.46
3:C:813:LEU:HD22	3:C:853:TRP:CZ3	2.51	0.46
3:O:778:ILE:O	3:O:782:VAL:HG23	2.15	0.46
1:A:142:ILE:O	1:A:146:VAL:HG23	2.15	0.46
2:N:570:MET:CE	3:O:560:SER:C	2.49	0.46
3:C:778:ILE:O	3:C:782:VAL:HG23	2.15	0.46
1:A:143:ALA:HB2	1:A:195:MET:HE1	1.97	0.46
2:B:508:LYS:H	2:B:514:VAL:HA	1.79	0.46
2:B:563:ARG:C	3:C:555:LYS:CE	2.87	0.46
2:N:559:GLU:O	2:N:562:TYR:HB3	2.14	0.46
3:C:665:ILE:HD12	3:C:673:ALA:HB2	1.97	0.46
3:C:840:PHE:N	3:C:841:PRO:CD	2.78	0.46
3:O:790:GLY:HA3	3:O:805:MET:O	2.16	0.46
3:O:825:CYS:O	3:O:826:THR:C	2.57	0.46
2:B:460:PRO:CG	2:B:463:GLN:NE2	2.78	0.46
2:N:460:PRO:CG	2:N:463:GLN:NE2	2.78	0.46
3:C:641:LEU:HD23	3:C:641:LEU:HA	1.73	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:142:ILE:O	1:M:146:VAL:HG23	2.15	0.46
2:B:459:ILE:HD12	2:B:460:PRO:HD3	1.97	0.46
2:N:508:LYS:N	2:N:514:VAL:HA	2.31	0.46
3:C:793:GLU:OE2	3:C:801:PRO:HA	2.15	0.46
3:O:840:PHE:N	3:O:841:PRO:CD	2.78	0.46
2:N:459:ILE:HD12	2:N:460:PRO:HD3	1.97	0.46
2:N:460:PRO:HG2	2:N:463:GLN:CG	2.44	0.46
3:C:702:SER:C	7:C:902:IBM:H103	2.41	0.46
6:H:60:VAL:HG22	6:H:61:PRO:CD	2.44	0.46
1:A:61:ILE:CA	1:M:119:PRO:C	2.85	0.46
1:A:68:GLU:OE1	1:M:64:GLU:OE2	2.34	0.46
1:A:121:SER:N	1:M:60:ASN:HB3	1.48	0.46
2:N:503:LEU:HD12	2:N:504:CYS:N	2.30	0.46
3:C:618:ALA:HB1	3:C:651:LEU:O	2.16	0.46
1:M:78:LYS:CE	2:N:388:LYS:NZ	2.70	0.46
2:N:428:GLU:HB2	2:N:522:ASN:HB2	1.97	0.46
3:O:534:MET:HE3	3:O:538:ARG:NH1	2.31	0.46
3:O:570:GLU:HA	3:O:573:LEU:HD12	1.98	0.46
6:H:35:HIS:HB2	6:H:93:ASN:OD1	2.15	0.46
2:B:471:THR:CG2	2:B:472:THR:N	2.79	0.46
2:B:568:ASN:CG	2:N:567:ALA:CB	2.62	0.46
3:C:665:ILE:HG13	3:C:666:GLN:N	2.31	0.46
3:C:795:THR:HG23	6:H:53:GLU:CD	2.10	0.46
3:O:665:ILE:HD12	3:O:673:ALA:HB2	1.97	0.46
2:N:465:ILE:CD1	2:N:502:ILE:HD13	2.46	0.46
3:C:570:GLU:HA	3:C:573:LEU:HD12	1.98	0.46
1:M:162:ASN:O	1:M:163:HIS:HB2	2.16	0.45
2:B:508:LYS:N	2:B:514:VAL:HA	2.31	0.45
2:N:536:LEU:HA	2:N:536:LEU:HD23	1.71	0.45
3:C:813:LEU:HB3	3:C:814:PRO:CD	2.45	0.45
1:A:64:GLU:OE2	1:M:68:GLU:OE1	2.34	0.45
2:N:458:ARG:CG	2:N:458:ARG:NH1	2.73	0.45
2:N:471:THR:CG2	2:N:472:THR:N	2.79	0.45
3:C:809:LYS:HA	3:C:809:LYS:CE	2.36	0.45
3:O:702:SER:C	7:O:902:IBM:H103	2.41	0.45
6:H:192:THR:HG23	6:H:209:LYS:HE3	1.99	0.45
2:B:528:TRP:HB2	2:B:529:PHE:H	1.49	0.45
2:N:433:PHE:CE2	2:N:442:ALA:CB	2.99	0.45
3:C:790:GLY:HA3	3:C:805:MET:O	2.16	0.45
6:Q:192:THR:HG23	6:Q:209:LYS:HE3	1.99	0.45
2:B:433:PHE:CE2	2:B:442:ALA:CB	2.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:618:ALA:HB1	3:O:651:LEU:O	2.16	0.45
4:P:86:ILE:HG22	4:P:87:ILE:N	2.31	0.45
2:B:392:GLU:OE2	2:B:532:PHE:CE1	2.70	0.45
3:C:654:ASP:HA	3:C:685:HIS:CD2	2.51	0.45
3:O:813:LEU:HD22	3:O:853:TRP:CZ3	2.51	0.45
1:M:162:ASN:O	1:M:163:HIS:CB	2.65	0.45
3:C:534:MET:HE3	3:C:538:ARG:NH1	2.31	0.45
3:C:708:GLU:O	3:C:709:TYR:C	2.60	0.45
3:C:826:THR:O	3:C:827:GLN:C	2.60	0.45
1:M:142:ILE:HG21	1:M:155:ILE:CD1	2.47	0.45
2:N:393:CYS:O	2:N:397:LEU:N	2.35	0.45
3:C:633:LYS:CD	3:O:844:ASP:CB	2.92	0.45
4:D:78:LEU:HD23	4:D:78:LEU:HA	1.76	0.45
4:D:86:ILE:HG22	4:D:87:ILE:N	2.31	0.45
4:P:86:ILE:HG22	4:P:87:ILE:H	1.80	0.45
6:Q:177:LEU:C	6:Q:177:LEU:HD12	2.42	0.45
1:M:213:PHE:CE1	1:M:217:LEU:HD11	2.52	0.45
1:A:213:PHE:CE1	1:A:217:LEU:HD11	2.52	0.45
3:C:844:ASP:CB	3:O:633:LYS:CD	2.92	0.45
1:A:121:SER:CA	1:M:60:ASN:HB3	2.33	0.45
2:B:428:GLU:HB2	2:B:522:ASN:HB2	1.98	0.45
2:N:392:GLU:OE2	2:N:532:PHE:CE1	2.70	0.45
2:N:395:ALA:O	2:N:399:VAL:HG12	2.17	0.45
6:Q:160:SER:O	6:Q:163:VAL:HG13	2.17	0.45
1:A:162:ASN:O	1:A:163:HIS:CB	2.65	0.44
1:M:99:PHE:HD2	1:M:110:VAL:HG13	1.82	0.44
2:N:425:SER:O	2:N:426:ASN:HB2	2.17	0.44
3:O:654:ASP:HA	3:O:685:HIS:CD2	2.51	0.44
3:O:826:THR:O	3:O:827:GLN:C	2.60	0.44
6:H:177:LEU:C	6:H:177:LEU:HD12	2.42	0.44
1:A:63:PHE:C	2:N:387:GLN:HE22	2.26	0.44
2:N:459:ILE:CG1	2:N:460:PRO:HD2	2.48	0.44
3:C:807:ARG:HG3	3:C:807:ARG:NH1	2.32	0.44
2:B:465:ILE:CD1	2:B:502:ILE:HD13	2.46	0.44
3:C:856:LEU:HD23	3:C:856:LEU:HA	1.79	0.44
5:L:214:CYS:OXT	5:L:214:CYS:SG	2.76	0.44
6:H:124:LEU:HB2	6:H:139:GLY:C	2.43	0.44
1:A:89:GLN:CD	1:M:86:ARG:HD2	2.27	0.44
2:B:459:ILE:CG1	2:B:460:PRO:HD2	2.48	0.44
2:B:501:ASN:OD1	2:B:522:ASN:HA	2.18	0.44
2:N:528:TRP:HB2	2:N:529:PHE:H	1.49	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:665:ILE:CD1	3:O:673:ALA:HB2	2.48	0.44
6:Q:124:LEU:HB2	6:Q:139:GLY:C	2.43	0.44
1:A:70:GLN:OE1	2:B:393:CYS:SG	2.74	0.44
2:B:418:ILE:CG1	2:B:432:VAL:CG2	2.96	0.44
2:B:459:ILE:HG13	2:B:460:PRO:HD2	2.00	0.44
3:C:761:THR:O	3:C:765:LEU:CD2	2.58	0.44
3:C:842:LEU:HD23	3:C:842:LEU:HA	1.78	0.44
5:R:214:CYS:SG	5:R:214:CYS:OXT	2.76	0.44
2:N:472:THR:O	2:N:474:GLN:HG3	2.17	0.44
3:C:577:ARG:NH1	3:C:580:THR:HG21	2.32	0.44
3:C:746:LEU:HD13	3:C:746:LEU:HA	1.76	0.44
3:O:577:ARG:NH1	3:O:580:THR:HG21	2.32	0.44
3:O:736:PHE:CE1	3:O:827:GLN:CG	2.98	0.44
1:A:90:LEU:CD2	1:M:89:GLN:HA	2.41	0.44
2:B:478:ILE:HA	2:B:479:PRO:HD2	1.61	0.44
1:A:142:ILE:HG21	1:A:155:ILE:CD1	2.47	0.44
1:A:162:ASN:O	1:A:163:HIS:HB2	2.16	0.44
1:M:142:ILE:CG2	1:M:179:MET:CE	2.90	0.44
2:B:439:GLU:HA	2:B:461:ALA:H	1.83	0.44
2:B:472:THR:O	2:B:474:GLN:HG3	2.17	0.44
2:B:536:LEU:HD23	2:B:536:LEU:HA	1.71	0.44
3:C:672:LEU:HD12	3:C:672:LEU:HA	1.83	0.44
3:C:837:GLU:HB3	3:O:840:PHE:N	2.33	0.44
3:O:740:ARG:HH12	3:O:741:LYS:HE2	1.82	0.44
6:H:160:SER:O	6:H:163:VAL:HG13	2.17	0.44
2:B:527:PRO:CG	2:B:528:TRP:CD1	3.01	0.43
2:B:568:ASN:CB	2:N:564:SER:O	2.66	0.43
2:N:459:ILE:HG13	2:N:460:PRO:HD2	2.00	0.43
2:N:505:PHE:HE1	2:N:541:SER:HG	1.63	0.43
2:N:537:ALA:O	2:N:541:SER:HB2	2.18	0.43
3:O:665:ILE:HG13	3:O:666:GLN:N	2.31	0.43
3:O:708:GLU:O	3:O:709:TYR:C	2.60	0.43
5:R:61:ARG:HB2	5:R:76:SER:O	2.18	0.43
1:A:57:GLU:OE2	1:M:118:THR:OG1	2.20	0.43
2:B:395:ALA:O	2:B:399:VAL:HG12	2.17	0.43
2:N:418:ILE:CG1	2:N:432:VAL:CG2	2.96	0.43
2:N:443:LYS:O	2:N:455:TYR:O	2.36	0.43
2:N:508:LYS:CA	2:N:514:VAL:HA	2.48	0.43
3:C:836:SER:H	3:O:837:GLU:CD	2.25	0.43
3:O:807:ARG:HG3	3:O:807:ARG:NH1	2.32	0.43
1:A:64:GLU:N	2:N:387:GLN:HE22	2.16	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLN:HA	1:M:90:LEU:CD2	2.41	0.43
1:A:99:PHE:HD2	1:A:110:VAL:HG13	1.82	0.43
2:N:476:LEU:HD23	2:N:478:ILE:CD1	2.48	0.43
3:C:818:VAL:HG12	3:C:819:GLY:N	2.33	0.43
2:N:409:ASP:HB3	2:N:412:VAL:HB	2.00	0.43
2:N:501:ASN:OD1	2:N:522:ASN:HA	2.18	0.43
3:C:840:PHE:N	3:O:837:GLU:HB3	2.33	0.43
2:B:389:LEU:HD23	2:B:389:LEU:HA	1.60	0.43
2:B:508:LYS:CA	2:B:514:VAL:HA	2.48	0.43
3:C:808:ASN:ND2	6:H:56:ASP:CG	2.75	0.43
2:B:443:LYS:O	2:B:455:TYR:O	2.36	0.43
2:B:501:ASN:HB2	2:B:529:PHE:CE1	2.54	0.43
2:N:398:GLN:NE2	2:N:401:LYS:HD3	2.34	0.43
2:N:501:ASN:HB2	2:N:529:PHE:CE1	2.54	0.43
3:O:832:LEU:O	3:O:832:LEU:HG	2.18	0.43
2:B:417:ILE:CD1	2:B:548:ILE:CD1	2.97	0.43
2:B:425:SER:O	2:B:426:ASN:HB2	2.17	0.43
5:L:61:ARG:HB2	5:L:76:SER:O	2.18	0.43
6:H:213:ARG:HB3	6:H:214:ASP:H	1.64	0.43
2:B:537:ALA:O	2:B:541:SER:HB2	2.18	0.43
2:N:421:ALA:HB2	2:N:540:PHE:HE2	1.83	0.43
3:O:634:ILE:O	3:O:635:GLN:C	2.61	0.43
5:R:181:LEU:HD22	5:R:185:GLU:HG2	2.01	0.43
2:N:399:VAL:CG2	2:N:540:PHE:HE1	2.24	0.43
2:N:437:GLN:C	2:N:437:GLN:NE2	2.77	0.43
3:O:818:VAL:HG12	3:O:819:GLY:N	2.33	0.43
5:L:181:LEU:HD22	5:L:185:GLU:HG2	2.01	0.43
6:H:138:LEU:HD12	6:H:138:LEU:N	2.34	0.43
3:C:661:ASN:O	3:C:665:ILE:HG23	2.19	0.43
3:O:661:ASN:O	3:O:665:ILE:HG23	2.19	0.43
3:O:813:LEU:HB3	3:O:814:PRO:CD	2.45	0.43
2:B:409:ASP:HB3	2:B:412:VAL:HB	1.99	0.42
2:B:564:SER:HB3	2:N:565:HIS:HB2	2.00	0.42
2:N:504:CYS:SG	2:N:519:GLU:HB3	2.59	0.42
3:C:634:ILE:O	3:C:635:GLN:C	2.61	0.42
2:B:443:LYS:HA	2:B:457:ILE:H	1.84	0.42
2:N:417:ILE:CD1	2:N:548:ILE:CD1	2.97	0.42
2:N:439:GLU:N	2:N:461:ALA:HB2	2.35	0.42
3:C:665:ILE:CD1	3:C:673:ALA:HB2	2.48	0.42
3:C:699:GLN:HB3	3:C:702:SER:HB3	2.01	0.42
3:C:740:ARG:HH12	3:C:741:LYS:HE2	1.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:837:GLU:CD	3:O:836:SER:H	2.25	0.42
3:O:808:ASN:ND2	6:Q:56:ASP:CG	2.75	0.42
3:O:842:LEU:HD23	3:O:842:LEU:HA	1.78	0.42
2:B:476:LEU:CD2	2:B:478:ILE:CD1	2.98	0.42
3:O:746:LEU:O	3:O:747:GLU:C	2.62	0.42
2:N:476:LEU:CD2	2:N:478:ILE:CD1	2.98	0.42
2:N:422:ARG:HD3	2:N:429:ILE:HA	2.02	0.42
5:L:11:MET:HB3	5:L:11:MET:HE2	1.78	0.42
5:L:36:TYR:CZ	6:H:100(C):PHE:HB2	2.54	0.42
5:R:36:TYR:CZ	6:Q:100(C):PHE:HB2	2.54	0.42
5:R:210:ASN:HB2	5:R:213:GLU:HG2	2.02	0.42
2:B:398:GLN:NE2	2:B:401:LYS:HD3	2.34	0.42
2:B:439:GLU:N	2:B:461:ALA:HB2	2.35	0.42
2:N:397:LEU:HD12	2:N:397:LEU:HA	1.92	0.42
4:D:71:GLU:N	4:D:71:GLU:OE1	2.53	0.42
5:L:210:ASN:HB2	5:L:213:GLU:HG2	2.02	0.42
2:B:437:GLN:NE2	2:B:437:GLN:C	2.77	0.42
2:B:504:CYS:SG	2:B:519:GLU:HB3	2.59	0.42
2:N:439:GLU:HA	2:N:461:ALA:H	1.83	0.42
2:N:567:ALA:HB2	3:O:555:LYS:CB	2.50	0.42
3:C:768:ILE:HG13	3:C:768:ILE:O	2.19	0.42
3:O:768:ILE:O	3:O:768:ILE:HG13	2.19	0.42
3:O:815:LYS:HE3	3:O:815:LYS:H	1.85	0.42
2:B:563:ARG:CB	3:C:555:LYS:CD	2.84	0.42
3:C:654:ASP:O	3:C:657:HIS:HB2	2.20	0.42
3:C:814:PRO:HD2	3:C:815:LYS:CE	2.48	0.42
3:O:635:GLN:HG3	3:O:643:ILE:HD13	2.02	0.42
3:O:817:GLN:OE1	3:O:817:GLN:HA	2.20	0.42
4:P:71:GLU:N	4:P:71:GLU:OE1	2.53	0.42
5:L:115:VAL:O	5:L:207:LYS:HE3	2.20	0.42
3:O:654:ASP:O	3:O:657:HIS:HB2	2.20	0.42
3:O:699:GLN:HB3	3:O:702:SER:HB3	2.01	0.42
6:Q:4:LEU:HD12	6:Q:4:LEU:HA	1.89	0.42
2:B:421:ALA:HB2	2:B:540:PHE:HE2	1.83	0.42
3:C:591:LYS:HB2	3:C:594:VAL:HG23	2.02	0.42
3:C:746:LEU:O	3:C:747:GLU:C	2.62	0.42
3:O:591:LYS:HB2	3:O:594:VAL:HG23	2.02	0.42
6:H:121:VAL:HG12	6:H:208:LYS:HG3	2.02	0.42
1:A:72:GLU:OE1	2:B:388:LYS:HE3	2.19	0.41
1:M:67:THR:CG2	2:B:387:GLN:HE21	2.32	0.41
2:B:422:ARG:HD3	2:B:429:ILE:HA	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:78:LEU:HD23	4:P:78:LEU:HA	1.76	0.41
1:A:86:ARG:CZ	1:M:86:ARG:NH2	2.83	0.41
2:B:428:GLU:C	2:B:429:ILE:HG23	2.45	0.41
2:B:508:LYS:H	2:B:515:ILE:H	1.68	0.41
2:N:473:GLY:O	2:N:508:LYS:NZ	2.47	0.41
3:C:765:LEU:H	3:C:765:LEU:CD2	2.33	0.41
3:C:817:GLN:OE1	3:C:817:GLN:HA	2.20	0.41
3:O:598:TRP:HA	3:O:698:ASN:OD1	2.20	0.41
5:R:54:ARG:CG	5:R:58:VAL:HG22	2.50	0.41
2:N:409:ASP:C	2:N:411:SER:N	2.78	0.41
2:N:443:LYS:HA	2:N:457:ILE:H	1.84	0.41
3:C:565:GLU:CD	3:C:565:GLU:H	2.28	0.41
3:C:635:GLN:HG3	3:C:643:ILE:HD13	2.02	0.41
3:O:800:GLN:HA	3:O:801:PRO:HD3	1.82	0.41
5:R:115:VAL:O	5:R:207:LYS:HE3	2.20	0.41
6:Q:138:LEU:N	6:Q:138:LEU:HD12	2.34	0.41
1:A:142:ILE:HG13	1:A:164:PHE:HA	2.03	0.41
1:A:182:ILE:HG21	1:A:217:LEU:HD13	2.02	0.41
1:M:182:ILE:HG21	1:M:217:LEU:HD13	2.02	0.41
2:N:527:PRO:CG	2:N:528:TRP:CD1	3.01	0.41
1:A:86:ARG:CZ	1:M:86:ARG:CZ	2.99	0.41
1:M:70:GLN:C	2:N:389:LEU:CD1	2.67	0.41
1:M:72:GLU:HG3	2:N:389:LEU:HD22	2.02	0.41
1:M:142:ILE:HG13	1:M:164:PHE:HA	2.03	0.41
2:N:389:LEU:HD23	2:N:389:LEU:HA	1.60	0.41
2:N:508:LYS:H	2:N:515:ILE:H	1.68	0.41
3:C:658:ARG:HG2	3:C:658:ARG:H	1.54	0.41
3:C:772:TRP:N	3:C:773:PRO:CD	2.83	0.41
3:O:745:ASN:O	3:O:751:GLN:OE1	2.39	0.41
5:L:166:GLN:HB2	5:L:173:TYR:CE2	2.56	0.41
6:H:67:ALA:HB1	6:H:80:LEU:HD11	2.02	0.41
1:A:70:GLN:CB	2:B:389:LEU:CD2	2.81	0.41
1:M:72:GLU:CD	2:N:389:LEU:CD2	2.94	0.41
1:M:118:THR:HG23	1:M:119:PRO:CD	2.51	0.41
2:B:476:LEU:HD23	2:B:478:ILE:CD1	2.48	0.41
2:B:569:GLU:OE2	3:O:551:ALA:HB3	2.21	0.41
3:C:575:THR:O	3:C:578:MET:HB2	2.21	0.41
3:C:578:MET:HE1	3:C:623:GLN:HB2	2.01	0.41
6:Q:213:ARG:HB3	6:Q:214:ASP:H	1.64	0.41
1:A:118:THR:HG23	1:A:119:PRO:CD	2.51	0.41
3:C:740:ARG:HA	3:O:742:ASN:CG	2.46	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:742:ASN:CG	3:O:740:ARG:HA	2.46	0.41
3:C:815:LYS:HE3	3:C:815:LYS:H	1.85	0.41
3:O:578:MET:HE1	3:O:623:GLN:HB2	2.01	0.41
6:H:4:LEU:HD12	6:H:4:LEU:HA	1.89	0.41
2:B:409:ASP:C	2:B:411:SER:N	2.77	0.41
2:B:441:VAL:CG1	2:B:443:LYS:HD3	2.51	0.41
3:C:569:LEU:HD22	3:C:569:LEU:HA	1.81	0.41
3:O:575:THR:O	3:O:578:MET:HB2	2.21	0.41
3:O:765:LEU:H	3:O:765:LEU:CD2	2.33	0.41
6:Q:121:VAL:HG12	6:Q:208:LYS:HG3	2.02	0.41
2:N:428:GLU:C	2:N:429:ILE:HG23	2.45	0.41
3:O:565:GLU:CD	3:O:565:GLU:H	2.28	0.41
2:N:422:ARG:HG3	2:N:427:ALA:HB3	2.03	0.40
3:C:736:PHE:CE1	3:C:827:GLN:CG	2.98	0.40
3:C:836:SER:N	3:O:837:GLU:CD	2.77	0.40
1:A:213:PHE:CZ	1:A:217:LEU:HD11	2.56	0.40
2:B:459:ILE:HD12	2:B:460:PRO:HD2	2.03	0.40
2:N:478:ILE:HA	2:N:479:PRO:HD2	1.61	0.40
3:C:765:LEU:HD22	3:C:765:LEU:N	2.36	0.40
3:C:832:LEU:O	3:C:832:LEU:HG	2.18	0.40
5:L:122:SER:O	5:L:126:THR:HG23	2.21	0.40
6:H:128:SER:H	6:H:213:ARG:NH2	2.18	0.40
2:B:418:ILE:CD1	2:B:432:VAL:CG2	2.98	0.40
2:N:428:GLU:HA	2:N:524:ILE:HD11	2.04	0.40
2:N:441:VAL:CG1	2:N:443:LYS:HD3	2.51	0.40
3:C:598:TRP:HA	3:C:698:ASN:OD1	2.20	0.40
3:C:678:HIS:HD2	4:D:71:GLU:OE2	2.03	0.40
2:B:511:ASN:ND2	2:B:511:ASN:N	2.69	0.40
2:N:459:ILE:HD12	2:N:460:PRO:HD2	2.03	0.40
3:C:639:THR:O	3:C:643:ILE:HG13	2.21	0.40
3:O:678:HIS:HD2	4:P:71:GLU:OE2	2.03	0.40
3:O:746:LEU:HD13	3:O:746:LEU:HA	1.76	0.40
3:O:772:TRP:N	3:O:773:PRO:CD	2.83	0.40
5:R:166:GLN:HB2	5:R:173:TYR:CE2	2.56	0.40
1:A:142:ILE:HB	1:A:179:MET:HE1	2.03	0.40
2:B:393:CYS:O	2:B:397:LEU:N	2.34	0.40
3:C:635:GLN:C	3:C:637:LYS:H	2.30	0.40
3:O:673:ALA:HA	3:O:680:ILE:HD13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	IBM	O	901	-	17,17,17	1.52	5 (29%)	19,25,25	2.17	10 (52%)
7	IBM	O	902	-	17,17,17	1.35	3 (17%)	19,25,25	1.94	7 (36%)
7	IBM	C	901	-	17,17,17	1.52	5 (29%)	19,25,25	2.17	10 (52%)
7	IBM	C	902	-	17,17,17	1.35	3 (17%)	19,25,25	1.94	7 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	IBM	O	901	-	-	2/4/4/4	0/2/2/2
7	IBM	O	902	-	-	2/4/4/4	0/2/2/2
7	IBM	C	901	-	-	2/4/4/4	0/2/2/2
7	IBM	C	902	-	-	2/4/4/4	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	901	IBM	C4-N3	-3.03	1.33	1.38
7	O	901	IBM	C4-N3	-3.03	1.33	1.38
7	C	902	IBM	C6-N1	-2.49	1.35	1.40
7	O	902	IBM	C6-N1	-2.49	1.35	1.40
7	C	901	IBM	C6-N1	-2.46	1.35	1.40
7	O	901	IBM	C6-N1	-2.46	1.35	1.40
7	C	901	IBM	C5-N7	-2.30	1.34	1.39
7	O	901	IBM	C5-N7	-2.30	1.34	1.39
7	C	902	IBM	C2-N3	-2.22	1.35	1.38
7	O	902	IBM	C2-N3	-2.22	1.35	1.38
7	C	902	IBM	C2-N1	-2.19	1.34	1.39
7	O	902	IBM	C2-N1	-2.19	1.34	1.39
7	C	901	IBM	C2-N1	-2.05	1.35	1.39
7	O	901	IBM	C2-N1	-2.05	1.35	1.39
7	C	901	IBM	O2-C2	2.02	1.26	1.22
7	O	901	IBM	O2-C2	2.02	1.26	1.22

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	902	IBM	N3-C2-N1	4.13	121.82	116.72
7	O	902	IBM	N3-C2-N1	4.13	121.82	116.72
7	C	901	IBM	N3-C2-N1	3.60	121.16	116.72
7	O	901	IBM	N3-C2-N1	3.60	121.16	116.72
7	C	901	IBM	C12-C11-N3	-3.51	107.29	112.38
7	O	901	IBM	C12-C11-N3	-3.51	107.29	112.38
7	C	901	IBM	N9-C8-N7	-3.27	109.19	112.98
7	O	901	IBM	N9-C8-N7	-3.27	109.19	112.98
7	C	901	IBM	C6-C5-N7	3.07	136.17	129.36
7	O	901	IBM	C6-C5-N7	3.07	136.17	129.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	902	IBM	C6-C5-N7	2.76	135.50	129.36
7	O	902	IBM	C6-C5-N7	2.76	135.50	129.36
7	C	901	IBM	C6-N1-C2	-2.72	121.23	125.66
7	O	901	IBM	C6-N1-C2	-2.72	121.23	125.66
7	C	901	IBM	C8-N7-C5	2.70	108.03	104.38
7	O	901	IBM	C8-N7-C5	2.70	108.03	104.38
7	C	902	IBM	C6-N1-C2	-2.67	121.32	125.66
7	O	902	IBM	C6-N1-C2	-2.67	121.32	125.66
7	C	901	IBM	O2-C2-N1	-2.66	117.66	121.33
7	O	901	IBM	O2-C2-N1	-2.66	117.66	121.33
7	C	902	IBM	N9-C8-N7	-2.59	109.97	112.98
7	O	902	IBM	N9-C8-N7	-2.59	109.97	112.98
7	C	902	IBM	C12-C11-N3	-2.38	108.93	112.38
7	O	902	IBM	C12-C11-N3	-2.38	108.93	112.38
7	C	902	IBM	O6-C6-C5	-2.25	118.78	124.59
7	O	902	IBM	O6-C6-C5	-2.25	118.78	124.59
7	C	901	IBM	C10-N1-C6	2.16	120.99	117.64
7	O	901	IBM	C10-N1-C6	2.16	120.99	117.64
7	C	902	IBM	C10-N1-C6	2.09	120.89	117.64
7	O	902	IBM	C10-N1-C6	2.09	120.89	117.64
7	C	901	IBM	O6-C6-C5	-2.07	119.26	124.59
7	O	901	IBM	O6-C6-C5	-2.07	119.26	124.59
7	C	901	IBM	C11-N3-C2	2.02	121.77	117.67
7	O	901	IBM	C11-N3-C2	2.02	121.77	117.67

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	902	IBM	N3-C11-C12-C13
7	C	902	IBM	N3-C11-C12-C14
7	O	902	IBM	N3-C11-C12-C13
7	O	902	IBM	N3-C11-C12-C14
7	C	901	IBM	C12-C11-N3-C2
7	O	901	IBM	C12-C11-N3-C2
7	C	901	IBM	C12-C11-N3-C4
7	O	901	IBM	C12-C11-N3-C4

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	O	901	IBM	1	0
7	O	902	IBM	3	0
7	C	901	IBM	1	0
7	C	902	IBM	3	0

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.

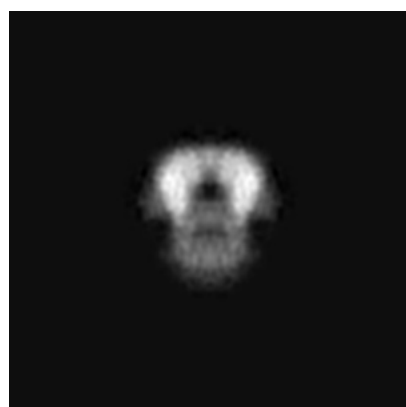
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6258. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

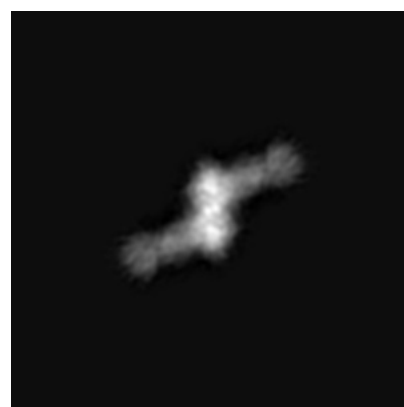
6.1.1 Primary map



X



Y



Z

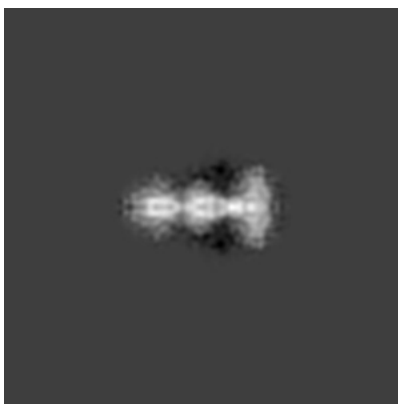
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 120



Y Index: 120



Z Index: 120

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 120



Y Index: 102

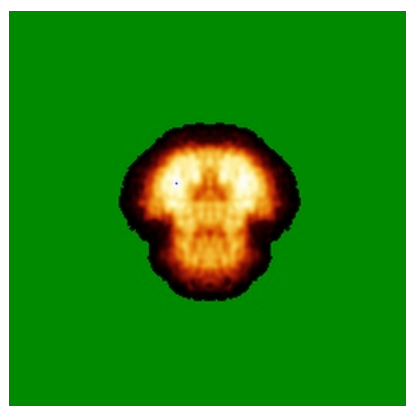


Z Index: 139

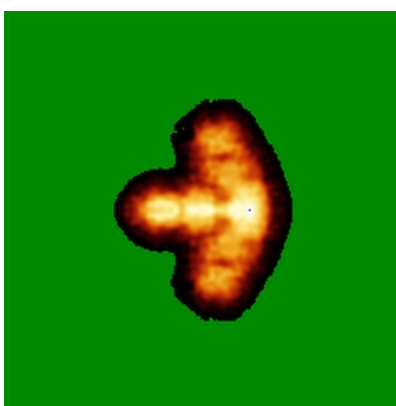
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

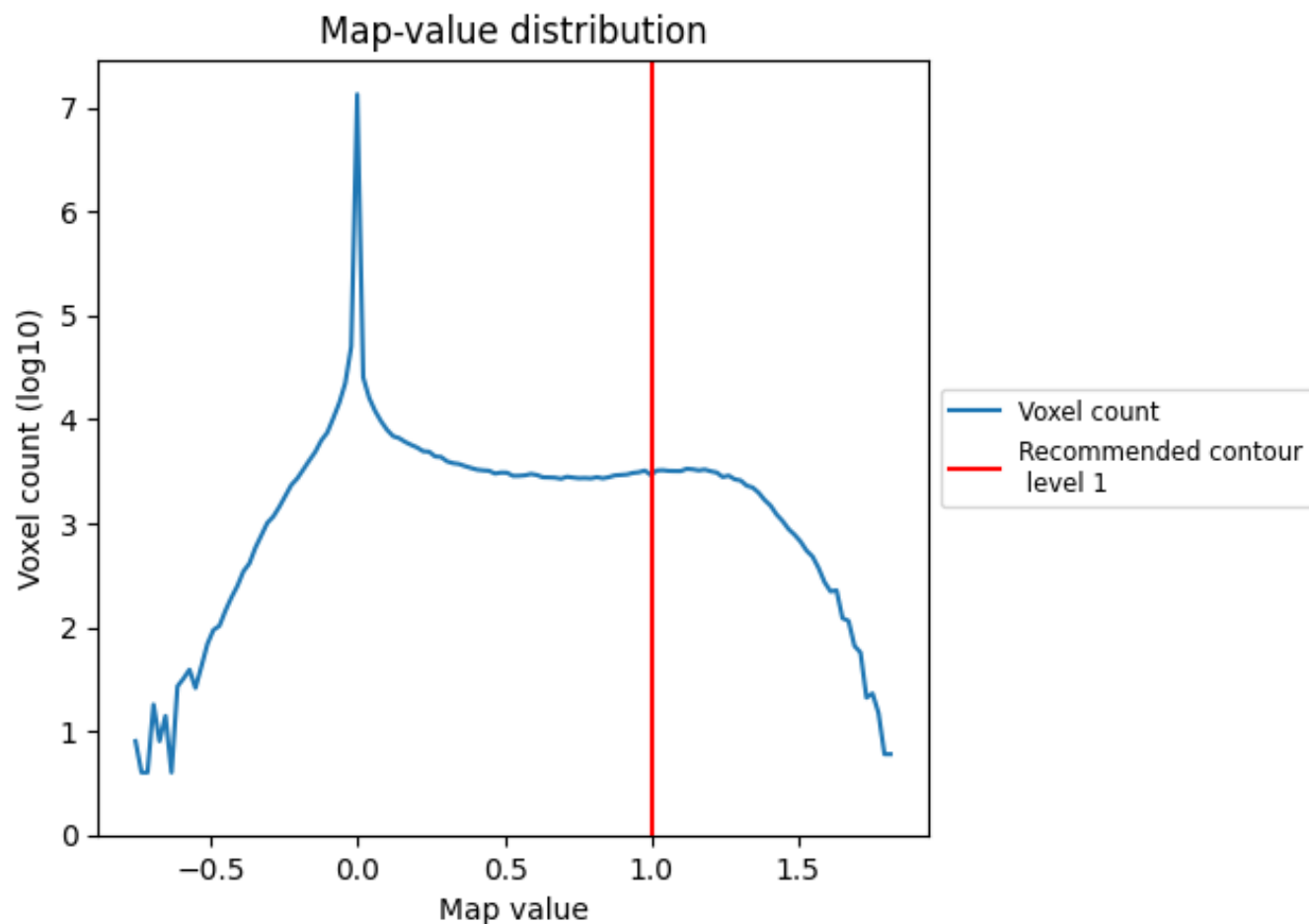
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

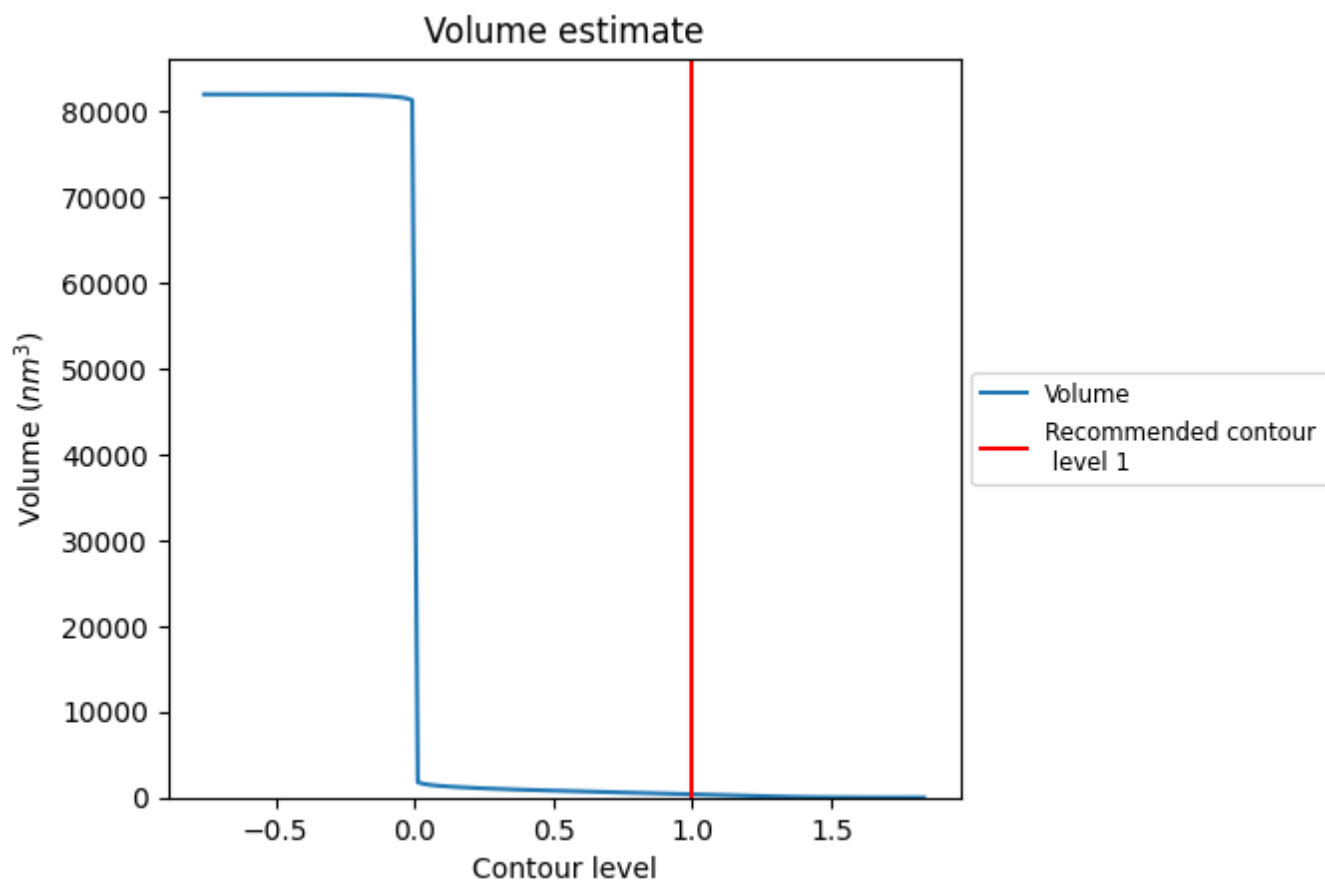
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

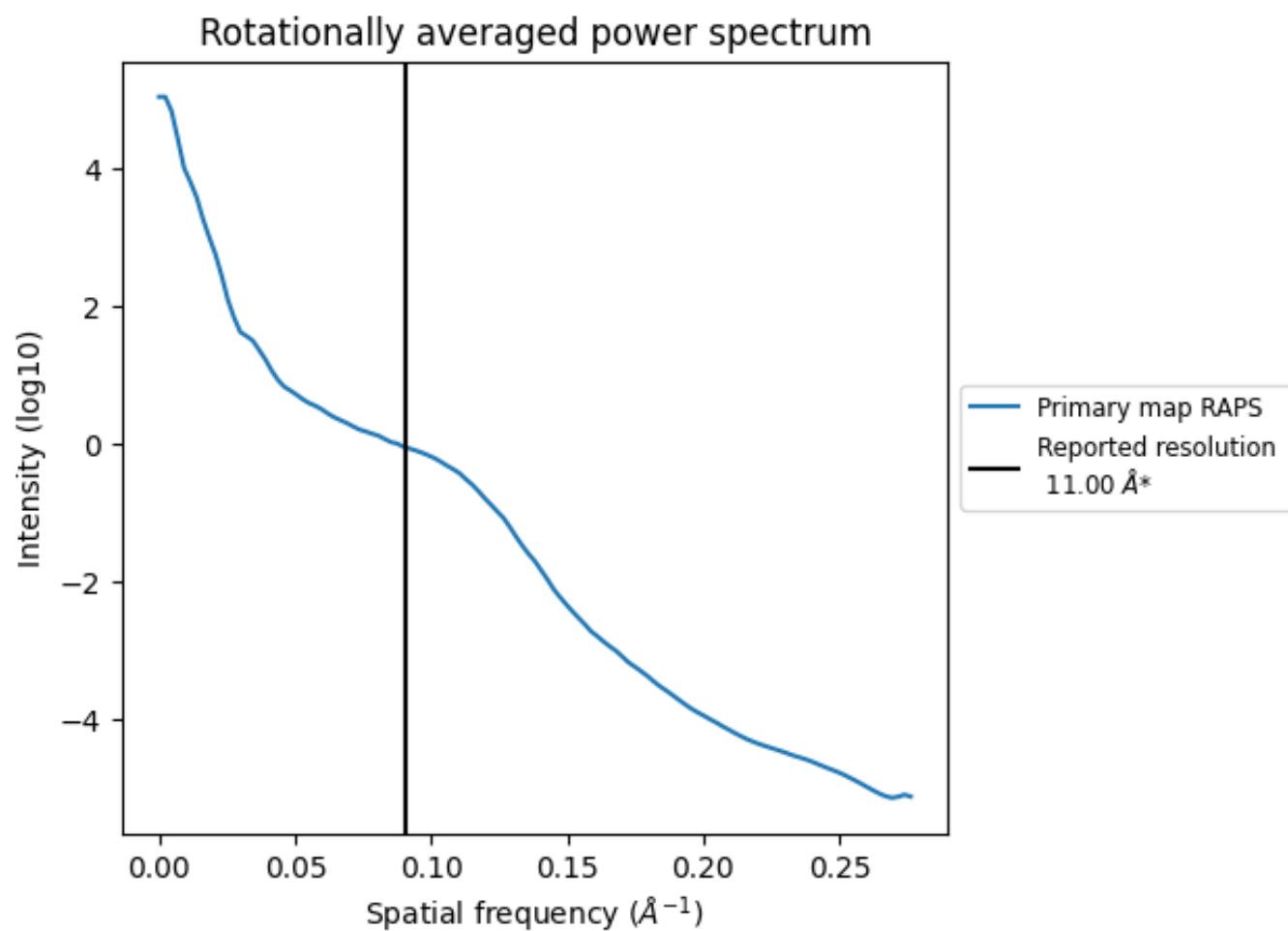
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 390 nm³; this corresponds to an approximate mass of 352 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.091 Å⁻¹

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

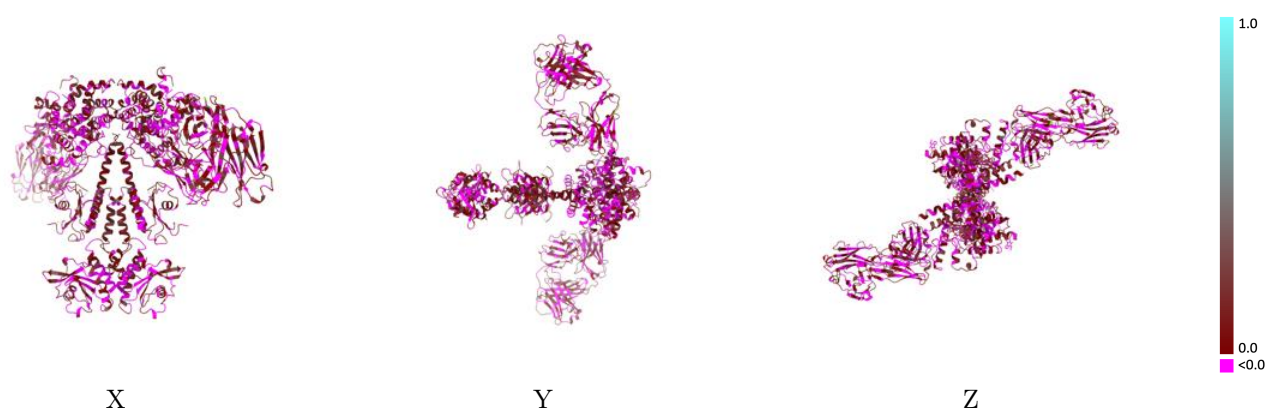
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6258 and PDB model 3JAB. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

This section was not generated.

9.2 Q-score mapped to coordinate model [i](#)

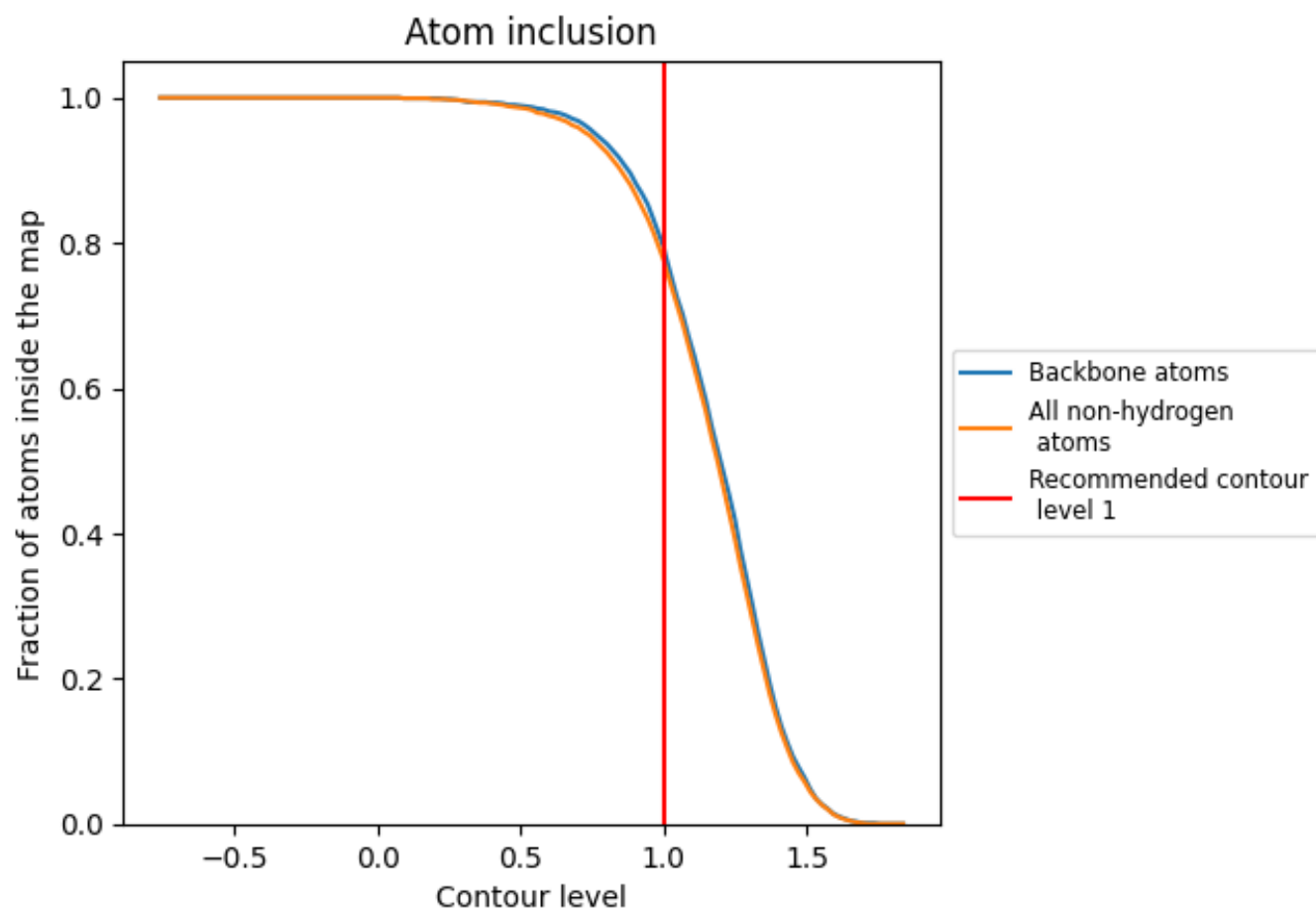


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7750	0.0430
A	0.7760	0.0250
B	0.9020	0.0870
C	0.7380	0.0240
D	0.5640	0.0160
H	0.7980	0.0550
L	0.7330	0.0450
M	0.7750	0.0260
N	0.8990	0.0820
O	0.7380	0.0250
P	0.5500	0.0160
Q	0.7970	0.0600
R	0.7350	0.0450

1.0

0.0

<0.0