



Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 05:03 PM UTC

PDB ID : 4BZK / pdb_00004bzk
EMDB ID : EMD-2431
Title : The structure of the COPII coat assembled on membranes
Authors : Zanetti, G.; Prinz, S.; Daum, S.; Meister, A.; Schekman, R.; Bacia, K.; Briggs, J.A.G.
Deposited on : 2013-07-26
Resolution : 40.00 Å(reported)
Based on initial models : 2PM6, 2PM9

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:

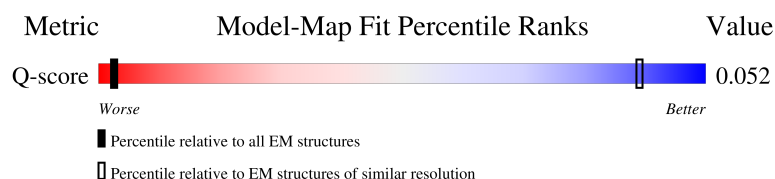
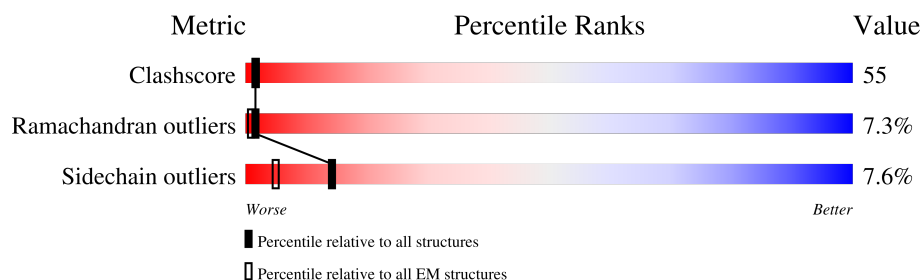
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 40.00 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	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	18 (40.00 - 40.00)

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	1273	 5% 19% 28% 7% 46%
1	C	1273	 20% 27% 7% 46%
2	B	297	 9% 40% 52% 6% 6%
3	F	297	 10% 23% 56% 15% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15423 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 Protein transport protein SEC31.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	691	Total	C	N	O	S	0	0
			5410	3406	908	1084	12		
1	C	693	Total	C	N	O	S	0	0
			5427	3417	911	1087	12		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	367	SER	THR	conflict	UNP P38968
C	367	SER	THR	conflict	UNP P38968

- Molecule 2 is a protein called Protein transport protein SEC13.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	279	Total	C	N	O	S	0	0
			2196	1403	375	415	3		

- Molecule 3 is a protein called Protein transport protein SEC13.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	280	Total	C	N	O	S	0	0
			2205	1402	376	418	9		

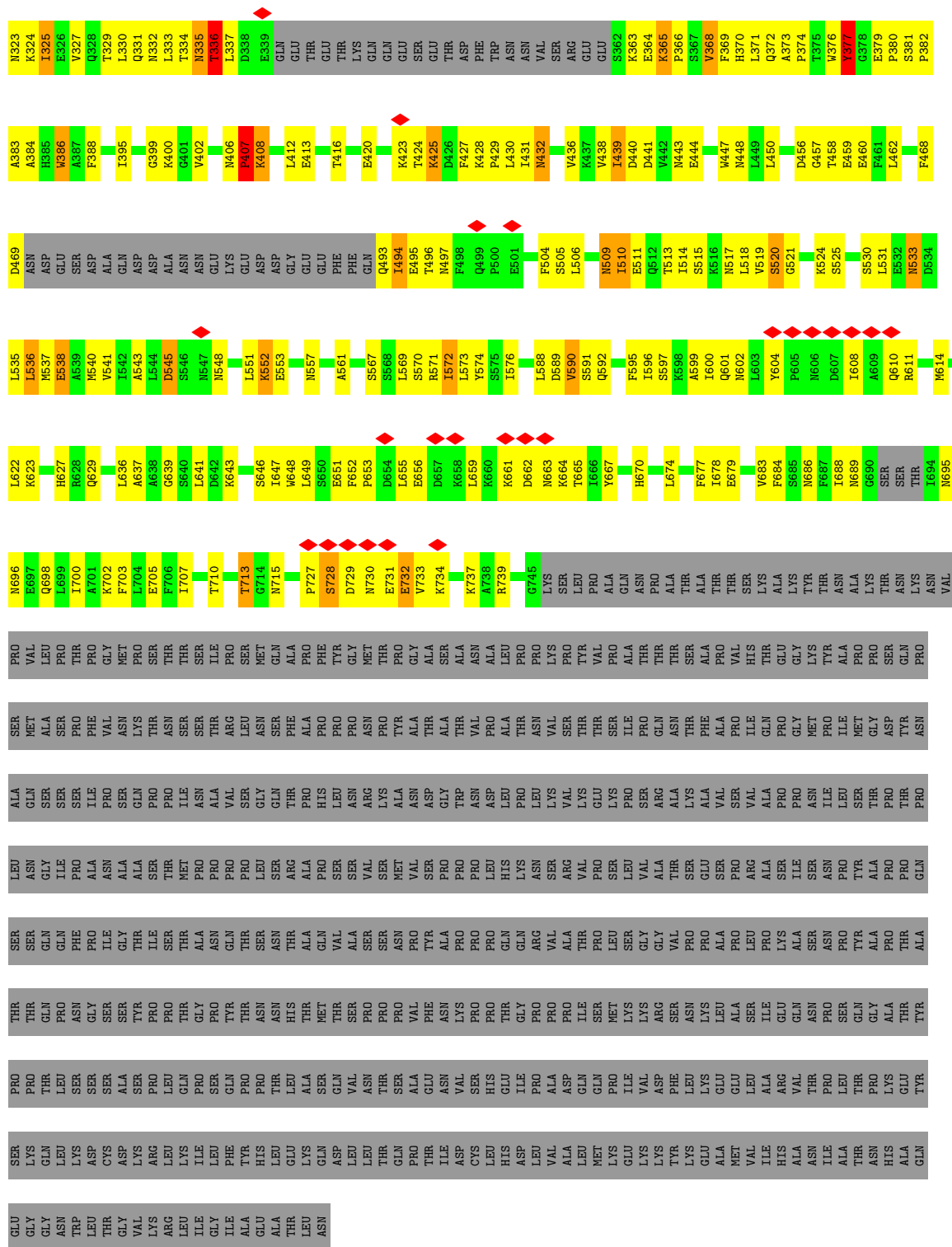
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	11	MET	LEU	conflict	UNP Q04491
F	17	MET	LEU	conflict	UNP Q04491
F	24	MET	LEU	conflict	UNP Q04491
F	80	MET	LEU	conflict	UNP Q04491
F	115	MET	LEU	conflict	UNP Q04491
F	222	MET	LEU	conflict	UNP Q04491

- Molecule 4 is water.

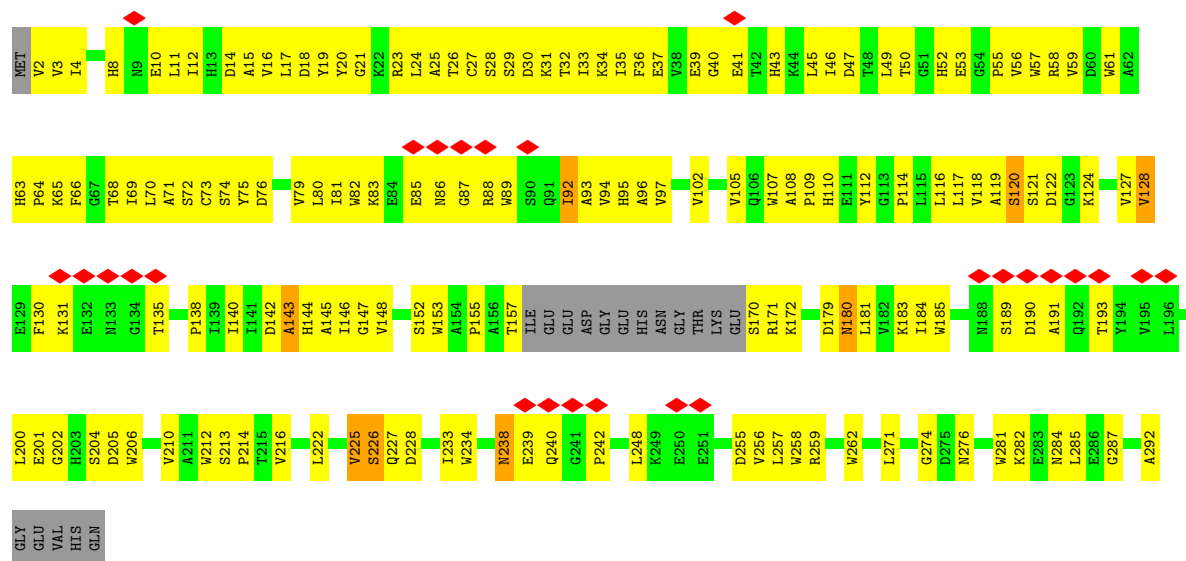
Mol	Chain	Residues	Atoms		AltConf
4	A	45	Total 45	O 45	0
4	B	61	Total 61	O 61	0
4	C	68	Total 68	O 68	0
4	F	11	Total 11	O 11	0



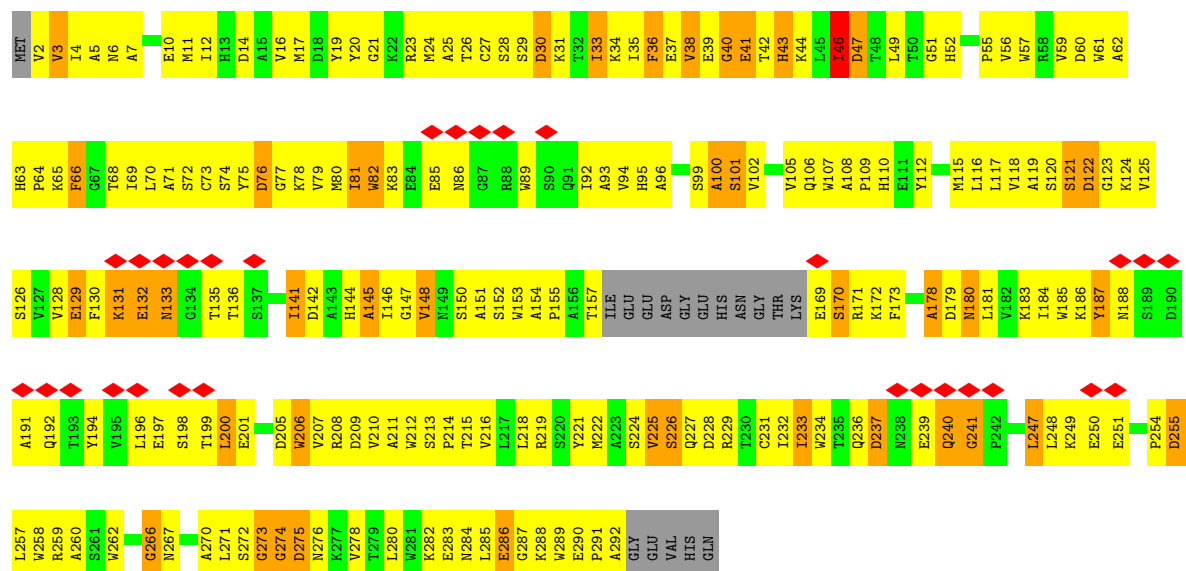


- Molecule 2: Protein transport protein SEC13





• Molecule 3: Protein transport protein SEC13



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of subtomograms used	192	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH TILTED IMAGE WITHIN TOMOGRAM	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	19500	Depositor
Image detector	GATAN MULTISCAN	Depositor
Maximum map value	6.592	Depositor
Minimum map value	-2.492	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2	Depositor
Map size (Å)	309.6, 309.6, 309.6	wwPDB
Map dimensions	72, 72, 72	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	4.3, 4.3, 4.3	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.50	0/5516	1.07	40/7479 (0.5%)
1	C	0.53	1/5533 (0.0%)	1.08	38/7502 (0.5%)
2	B	0.47	0/2256	0.99	6/3079 (0.2%)
3	F	0.48	0/2265	1.01	9/3085 (0.3%)
All	All	0.51	1/15570 (0.0%)	1.06	93/21145 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	384	ALA	CA-CB	-5.08	1.45	1.53

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	ARG	N-CA-C	-11.32	98.85	112.89
1	C	243	ARG	N-CA-C	-11.29	98.89	112.89
1	C	157	MET	N-CA-C	9.68	124.19	108.41
3	F	178	ALA	N-CA-C	-9.65	101.51	113.28
1	A	157	MET	N-CA-C	9.64	124.24	108.52
1	A	34	ALA	N-CA-C	-8.99	102.32	113.38
1	C	34	ALA	N-CA-C	-8.99	102.32	113.38
3	F	275	ASP	N-CA-C	-8.35	103.21	113.15
1	A	175	VAL	N-CA-C	8.04	121.53	108.99
1	C	175	VAL	N-CA-C	8.03	121.52	108.99
2	B	226	SER	N-CA-C	7.95	121.25	109.24
1	C	377	TYR	N-CA-C	7.37	120.61	109.41
1	A	312	ALA	CA-C-N	7.29	128.96	119.84
1	A	312	ALA	C-N-CA	7.29	128.96	119.84
1	C	312	ALA	CA-C-N	7.24	128.90	119.84
1	C	312	ALA	C-N-CA	7.24	128.90	119.84
1	C	26	GLY	N-CA-C	-7.21	102.88	112.82
1	A	26	GLY	N-CA-C	-7.19	102.90	112.82
1	C	713	THR	N-CA-C	-7.16	104.53	113.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	128	VAL	N-CA-C	7.08	118.32	108.12
1	A	206	SER	N-CA-C	-6.82	103.03	112.30
1	C	206	SER	N-CA-C	-6.80	103.05	112.30
1	C	533	ASN	N-CA-C	-6.76	99.21	109.95
1	A	286	ASN	CA-C-N	6.66	128.16	119.84
1	A	286	ASN	C-N-CA	6.66	128.16	119.84
1	C	286	ASN	CA-C-N	6.65	128.15	119.84
1	C	286	ASN	C-N-CA	6.65	128.15	119.84
3	F	122	ASP	N-CA-C	-6.61	105.52	112.93
1	C	308	PHE	N-CA-C	-6.60	99.77	110.20
2	B	120	SER	N-CA-C	6.58	119.90	109.50
1	A	308	PHE	N-CA-C	-6.57	99.82	110.20
1	A	156	SER	N-CA-C	6.53	124.72	110.80
1	C	156	SER	N-CA-C	6.53	124.72	110.80
3	F	121	SER	N-CA-C	-6.53	105.38	113.15
1	C	386	TRP	N-CA-C	-6.45	101.23	110.59
1	A	608	ILE	N-CA-C	6.45	117.20	110.62
1	A	309	ALA	N-CA-C	-6.45	98.30	109.58
1	C	309	ALA	N-CA-C	-6.39	98.40	109.58
1	A	314	ASP	N-CA-C	-6.37	105.26	113.16
1	C	314	ASP	N-CA-C	-6.36	105.28	113.16
1	A	377	TYR	N-CA-C	6.28	118.50	109.14
1	A	90	SER	N-CA-C	6.17	120.38	112.12
1	C	90	SER	N-CA-C	6.15	120.36	112.12
2	B	143	ALA	N-CA-C	6.10	121.65	113.72
1	C	406	ASN	CA-C-N	6.08	127.44	119.84
1	C	406	ASN	C-N-CA	6.08	127.44	119.84
3	F	266	GLY	N-CA-C	-6.08	107.31	115.21
1	C	173	ALA	CA-C-N	6.05	128.38	120.28
1	C	173	ALA	C-N-CA	6.05	128.38	120.28
1	A	173	ALA	CA-C-N	6.02	128.35	120.28
1	A	173	ALA	C-N-CA	6.02	128.35	120.28
1	A	378	GLY	N-CA-C	6.02	123.36	115.36
1	A	188	TRP	N-CA-C	5.98	118.65	108.90
1	C	188	TRP	N-CA-C	5.96	118.61	108.90
1	C	131	GLY	N-CA-C	-5.91	105.98	115.08
1	A	131	GLY	N-CA-C	-5.91	105.98	115.08
1	C	253	ASN	N-CA-C	5.86	119.02	110.17
1	A	253	ASN	N-CA-C	5.86	119.01	110.17
2	B	179	ASP	N-CA-C	-5.84	105.74	112.92
3	F	226	SER	N-CA-C	5.77	117.03	108.60
3	F	3	VAL	N-CA-C	5.76	117.93	109.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	ASN	N-CA-C	-5.71	106.94	114.31
1	C	336	THR	N-CA-C	-5.70	98.66	110.80
1	A	66	ASN	N-CA-C	-5.69	106.97	114.31
1	A	192	ALA	N-CA-C	-5.68	106.02	113.17
1	C	441	ASP	N-CA-C	5.68	117.47	111.28
1	A	336	THR	N-CA-C	-5.67	98.72	110.80
1	C	192	ALA	N-CA-C	-5.61	106.10	113.17
1	A	39	ASP	N-CA-C	5.58	117.80	109.59
1	C	39	ASP	N-CA-C	5.57	117.77	109.59
1	C	536	LEU	N-CA-C	5.55	117.02	110.97
1	C	732	GLU	N-CA-C	-5.52	104.09	112.04
3	F	181	LEU	N-CA-C	5.50	117.93	109.07
1	A	376	TRP	N-CA-C	5.47	116.92	111.07
1	A	533	ASN	N-CA-C	-5.44	100.66	108.60
3	F	36	PHE	N-CA-C	5.42	117.21	109.14
1	A	600	ILE	N-CA-C	-5.40	107.16	111.81
1	A	154	GLY	N-CA-C	5.36	125.89	113.18
2	B	287	GLY	N-CA-C	-5.34	107.65	115.72
1	C	154	GLY	N-CA-C	5.34	125.84	113.18
1	A	384	ALA	N-CA-C	5.34	117.18	110.24
1	C	177	ALA	N-CA-C	5.33	118.12	109.06
1	A	177	ALA	N-CA-C	5.32	118.10	109.06
1	A	547	ASN	N-CA-C	-5.30	107.36	113.88
1	A	219	PRO	N-CA-C	5.18	120.42	114.20
1	C	219	PRO	N-CA-C	5.10	120.32	114.20
1	C	648	TRP	N-CA-C	5.06	116.88	111.36
1	A	406	ASN	CA-C-N	5.05	125.05	119.89
1	A	406	ASN	C-N-CA	5.05	125.05	119.89
1	A	453	LEU	N-CA-C	-5.05	105.90	111.71
1	C	45	TRP	N-CA-C	5.01	116.99	109.23
1	A	191	LYS	N-CA-C	-5.00	107.02	113.23
1	A	45	TRP	N-CA-C	5.00	116.98	109.23

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	5410	0	5272	636	0
1	C	5427	0	5289	638	0
2	B	2196	0	2138	190	0
3	F	2205	0	2131	308	0
4	A	45	0	0	24	0
4	B	61	0	0	25	0
4	C	68	0	0	26	0
4	F	11	0	0	4	0
All	All	15423	0	14830	1643	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 55.

All (1643) 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:C:739:ARG:HA	3:F:20:TYR:CE1	1.28	1.64
1:C:664:LYS:C	3:F:285:LEU:HD21	1.30	1.56
1:C:739:ARG:CA	3:F:20:TYR:HE1	1.28	1.46
1:A:314:ASP:OD2	1:A:376:TRP:CD2	1.64	1.46
1:A:314:ASP:OD2	1:A:376:TRP:CE2	1.76	1.36
1:C:665:THR:N	3:F:285:LEU:HD21	1.38	1.35
1:C:665:THR:HA	3:F:285:LEU:CD2	1.58	1.32
1:A:313:PRO:HG3	4:A:3118:HOH:O	1.14	1.30
1:C:663:ASN:C	3:F:285:LEU:HD11	1.53	1.29
1:C:268:GLN:HB3	1:C:374:PRO:O	1.29	1.25
1:C:313:PRO:HG3	4:C:2145:HOH:O	1.32	1.25
1:A:268:GLN:HB3	1:A:374:PRO:O	1.15	1.25
1:A:268:GLN:HG3	4:A:3118:HOH:O	1.32	1.24
1:C:663:ASN:C	3:F:285:LEU:CD1	2.13	1.21
1:A:268:GLN:CB	1:A:374:PRO:O	1.87	1.20
1:C:665:THR:CA	3:F:285:LEU:CD2	2.19	1.19
1:C:331:GLN:NE2	4:C:2144:HOH:O	1.73	1.19
1:C:314:ASP:OD2	1:C:376:TRP:CD2	1.95	1.17
1:A:314:ASP:CG	1:A:376:TRP:CE2	2.22	1.16
1:C:314:ASP:OD2	1:C:376:TRP:CE2	2.01	1.13
1:A:22:LEU:HD11	1:A:94:ALA:HB1	1.30	1.13
1:C:313:PRO:CG	4:C:2145:HOH:O	1.86	1.13
1:C:314:ASP:OD1	4:C:2011:HOH:O	1.63	1.13
1:C:664:LYS:N	3:F:285:LEU:HD11	1.65	1.12
1:C:22:LEU:HD11	1:C:94:ALA:HB1	1.30	1.10
1:C:664:LYS:C	3:F:285:LEU:CD2	2.24	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ASP:OD2	1:A:376:TRP:CE3	2.06	1.08
1:C:665:THR:N	3:F:285:LEU:CD2	2.14	1.08
1:C:268:GLN:NE2	4:C:2146:HOH:O	1.87	1.08
1:C:739:ARG:CA	3:F:20:TYR:CE1	2.15	1.07
1:C:268:GLN:HA	1:C:373:ALA:HB1	1.34	1.07
3:F:256:VAL:HG12	3:F:257:LEU:H	1.11	1.06
1:C:665:THR:CA	3:F:285:LEU:HD21	1.83	1.06
1:C:93:GLU:HB2	1:C:96:ASN:HD22	1.16	1.05
1:C:268:GLN:HE21	1:C:313:PRO:HD3	1.19	1.05
3:F:24:MET:HG2	3:F:25:ALA:H	1.18	1.05
1:C:665:THR:HA	3:F:285:LEU:HD23	1.09	1.05
1:C:665:THR:CA	3:F:285:LEU:HD23	1.81	1.05
1:A:93:GLU:HB2	1:A:96:ASN:HD22	1.16	1.04
3:F:184:ILE:HD11	3:F:222:MET:HE1	1.34	1.04
1:A:268:GLN:HE21	1:A:313:PRO:HD3	1.19	1.04
1:C:425:LYS:HE2	1:C:686:ASN:HD21	1.21	1.02
1:C:304:PHE:HD1	1:C:304:PHE:H	1.04	1.02
3:F:46:ILE:HG22	3:F:47:ASP:H	1.20	1.02
1:C:664:LYS:O	3:F:285:LEU:HD21	1.58	1.01
1:C:688:ILE:HG13	1:C:689:ASN:H	1.20	1.01
1:C:408:LYS:HD3	1:C:408:LYS:H	1.22	1.00
2:B:11:LEU:O	2:B:28:SER:HB2	1.61	1.00
1:C:314:ASP:CG	4:C:2011:HOH:O	2.01	1.00
1:C:663:ASN:O	3:F:285:LEU:CD1	2.08	1.00
1:C:154:GLY:O	1:C:155:GLN:HG2	1.61	1.00
3:F:69:ILE:HD11	3:F:83:LYS:HE2	1.43	1.00
3:F:80:MET:HG2	3:F:94:VAL:HG23	1.43	0.99
1:A:304:PHE:HD1	1:A:304:PHE:H	1.04	0.99
1:C:377:TYR:CE2	3:F:75:TYR:HE1	1.80	0.99
1:C:623:LYS:HE3	1:C:647:ILE:HD12	1.44	0.98
1:A:268:GLN:HA	1:A:373:ALA:HB1	1.45	0.98
1:A:154:GLY:O	1:A:155:GLN:HG2	1.61	0.98
3:F:69:ILE:HG12	3:F:83:LYS:HG2	1.45	0.98
2:B:128:VAL:HG22	2:B:138:PRO:HB3	1.43	0.97
1:C:202:THR:C	1:C:204:PRO:HD2	1.89	0.97
1:A:431:ILE:HD11	1:A:683:VAL:HG11	1.42	0.97
1:C:268:GLN:CB	1:C:374:PRO:O	2.13	0.97
1:A:438:VAL:HG23	1:A:443:ASN:HD22	1.28	0.97
1:A:268:GLN:CG	4:A:3118:HOH:O	1.91	0.96
1:C:268:GLN:HA	1:C:373:ALA:CB	1.95	0.96
1:A:202:THR:C	1:A:204:PRO:HD2	1.89	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:720:THR:HA	1:A:723:LEU:HD12	1.46	0.95
1:C:535:LEU:HB3	1:C:538:GLU:HG3	1.48	0.95
1:A:93:GLU:HB2	1:A:96:ASN:ND2	1.81	0.95
1:C:93:GLU:HB2	1:C:96:ASN:ND2	1.81	0.95
1:C:407:PRO:HD2	4:C:2214:HOH:O	1.67	0.95
1:A:370:HIS:CE1	2:B:75:TYR:CE2	2.56	0.94
1:A:370:HIS:CE1	2:B:75:TYR:HE2	1.86	0.93
1:C:16:SER:O	1:C:310:PRO:HG3	1.69	0.93
1:A:10:THR:HG23	1:A:28:VAL:HG12	1.50	0.93
3:F:233:ILE:H	3:F:233:ILE:HD12	1.33	0.93
1:A:72:HIS:CE1	1:A:118:ALA:HA	2.04	0.93
1:A:16:SER:O	1:A:310:PRO:HG3	1.69	0.92
1:C:22:LEU:CD1	1:C:94:ALA:HB1	1.99	0.92
1:A:31:THR:HG22	1:A:32:VAL:H	1.33	0.92
1:A:22:LEU:CD1	1:A:94:ALA:HB1	1.99	0.92
1:A:364:GLU:O	1:A:365:LYS:HB2	1.66	0.92
1:C:72:HIS:CE1	1:C:118:ALA:HA	2.04	0.92
1:A:268:GLN:HG3	4:A:3079:HOH:O	1.67	0.92
1:C:31:THR:HG22	1:C:32:VAL:H	1.33	0.92
1:A:368:VAL:O	1:A:370:HIS:N	2.02	0.92
1:C:125:ALA:HB2	1:C:168:TRP:CH2	2.04	0.92
1:C:377:TYR:CE2	3:F:75:TYR:CE1	2.58	0.91
1:A:299:ARG:HE	1:A:323:ASN:HB2	1.33	0.91
1:C:368:VAL:O	1:C:370:HIS:N	2.02	0.91
1:A:125:ALA:HB2	1:A:168:TRP:CH2	2.05	0.91
1:A:639:GLY:HA2	1:A:688:ILE:HD11	1.51	0.91
1:A:314:ASP:N	1:A:376:TRP:HE1	1.69	0.91
1:C:10:THR:HG23	1:C:28:VAL:HG12	1.50	0.91
1:C:364:GLU:O	1:C:365:LYS:HB2	1.66	0.91
1:C:664:LYS:CA	3:F:285:LEU:HD11	2.00	0.91
1:A:313:PRO:C	1:A:376:TRP:HE1	1.79	0.90
1:A:370:HIS:HE1	2:B:75:TYR:CE2	1.90	0.90
1:A:244:ASN:HD21	1:A:246:ASN:ND2	1.70	0.90
1:C:739:ARG:CB	3:F:20:TYR:HE1	1.83	0.90
1:A:428:LYS:HB2	1:A:429:PRO:HD3	1.54	0.89
1:C:420:GLU:O	1:C:423:LYS:HG2	1.70	0.89
1:C:649:LEU:HD22	1:C:698:GLN:HG2	1.55	0.89
1:C:299:ARG:HE	1:C:323:ASN:HB2	1.33	0.89
1:A:106:ASN:N	1:A:106:ASN:HD22	1.70	0.89
3:F:249:LYS:HE3	3:F:251:GLU:HB2	1.54	0.89
1:A:536:LEU:HD23	1:C:537:MET:HE1	1.55	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:ASP:CG	1:C:376:TRP:CE2	2.50	0.88
1:A:202:THR:O	1:A:204:PRO:HD2	1.74	0.88
1:C:244:ASN:HD21	1:C:246:ASN:ND2	1.70	0.88
2:B:81:ILE:HB	4:B:2320:HOH:O	1.73	0.87
1:C:739:ARG:HA	3:F:20:TYR:CD1	2.08	0.87
3:F:180:ASN:HD22	3:F:180:ASN:N	1.72	0.87
1:A:592:GLN:HE21	1:C:506:LEU:HD12	1.40	0.87
1:C:377:TYR:HB3	3:F:57:TRP:CH2	2.10	0.87
1:A:314:ASP:CG	1:A:376:TRP:CD2	2.48	0.86
1:C:268:GLN:HE21	1:C:313:PRO:CD	1.87	0.86
1:C:313:PRO:HG3	4:C:2080:HOH:O	1.73	0.86
1:A:75:LYS:HZ1	1:A:94:ALA:H	1.23	0.86
1:A:314:ASP:OD2	1:A:376:TRP:CZ2	2.28	0.86
1:A:268:GLN:HE21	1:A:313:PRO:CD	1.87	0.86
2:B:81:ILE:HD13	2:B:93:ALA:HB3	1.54	0.86
1:C:202:THR:O	1:C:204:PRO:HD2	1.74	0.86
1:A:496:THR:HG23	1:C:557:ASN:HB3	1.54	0.86
4:A:3245:HOH:O	1:C:602:ASN:HB3	1.75	0.86
1:C:106:ASN:N	1:C:106:ASN:HD22	1.70	0.86
1:C:377:TYR:HB3	3:F:57:TRP:CZ2	2.11	0.86
1:C:663:ASN:O	3:F:285:LEU:HD11	1.69	0.86
1:C:663:ASN:O	3:F:285:LEU:HD12	1.74	0.86
2:B:83:LYS:O	2:B:89:TRP:HA	1.76	0.85
1:A:412:LEU:HD21	1:A:713:THR:HG22	1.57	0.85
1:C:425:LYS:O	1:C:425:LYS:HD3	1.75	0.85
1:C:314:ASP:OD2	1:C:376:TRP:CE3	2.30	0.85
1:A:75:LYS:NZ	1:A:94:ALA:H	1.74	0.85
3:F:73:CYS:HB3	3:F:79:VAL:HG12	1.59	0.85
1:C:494:ILE:HG13	1:C:495:GLU:H	1.42	0.85
1:A:10:THR:CG2	1:A:28:VAL:HG12	2.06	0.85
2:B:12:ILE:HA	2:B:28:SER:HB3	1.59	0.84
1:C:703:PHE:O	1:C:707:ILE:HG12	1.78	0.84
2:B:257:LEU:HD13	2:B:271:LEU:HD21	1.59	0.84
1:C:10:THR:CG2	1:C:28:VAL:HG12	2.06	0.84
1:C:117:ASN:HD22	1:C:118:ALA:N	1.75	0.84
3:F:69:ILE:CD1	3:F:83:LYS:HE2	2.07	0.84
1:C:73:ASN:O	1:C:75:LYS:N	2.11	0.84
1:C:75:LYS:NZ	1:C:94:ALA:H	1.74	0.83
1:A:30:GLY:HA3	1:A:321:PHE:HE2	1.44	0.83
1:A:73:ASN:O	1:A:75:LYS:N	2.11	0.83
1:A:119:LYS:HB2	1:A:173:ALA:HB2	1.59	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:24:MET:CG	3:F:25:ALA:H	1.90	0.83
1:A:268:GLN:NE2	1:A:313:PRO:HD3	1.94	0.83
1:C:665:THR:HG22	3:F:285:LEU:HA	1.61	0.83
1:A:117:ASN:HD22	1:A:118:ALA:N	1.75	0.82
3:F:150:SER:OG	3:F:209:ASP:HA	1.79	0.82
1:C:119:LYS:HB2	1:C:173:ALA:HB2	1.59	0.82
1:C:383:ALA:HB1	4:F:2302:HOH:O	1.80	0.82
1:C:268:GLN:NE2	1:C:313:PRO:HD3	1.94	0.82
3:F:83:LYS:HG3	3:F:92:ILE:HD13	1.62	0.82
1:C:74:ASN:HD22	1:C:74:ASN:N	1.77	0.82
1:C:31:THR:HG22	1:C:32:VAL:N	1.95	0.82
1:A:336:THR:HB	2:B:96:ALA:O	1.80	0.82
1:C:524:LYS:HG3	1:C:525:SER:H	1.43	0.81
3:F:46:ILE:HG22	3:F:47:ASP:N	1.95	0.81
1:A:221:ASN:HD22	1:A:222:SER:N	1.79	0.81
1:A:314:ASP:N	1:A:376:TRP:NE1	2.29	0.81
1:C:30:GLY:HA3	1:C:321:PHE:HE2	1.44	0.81
1:C:380:PRO:HG3	3:F:11:MET:CE	2.10	0.81
3:F:79:VAL:HG23	3:F:95:HIS:HB3	1.60	0.81
1:A:370:HIS:CG	1:A:371:LEU:H	1.99	0.81
1:C:133:ILE:HD11	1:C:163:VAL:HG21	1.62	0.81
1:C:202:THR:C	1:C:204:PRO:CD	2.55	0.80
1:C:427:PHE:O	1:C:431:ILE:HG12	1.81	0.80
1:A:292:GLN:O	1:A:368:VAL:HG23	1.81	0.80
1:C:221:ASN:HD22	1:C:222:SER:N	1.79	0.80
1:C:292:GLN:O	1:C:368:VAL:HG23	1.81	0.80
1:C:370:HIS:CG	1:C:371:LEU:H	1.99	0.80
1:A:518:LEU:HB3	1:C:576:ILE:HD13	1.63	0.80
1:C:300:GLY:O	1:C:301:ASN:HB2	1.81	0.80
1:A:420:GLU:HA	1:A:423:LYS:HE2	1.63	0.80
3:F:24:MET:HG2	3:F:25:ALA:N	1.96	0.80
1:A:315:LEU:HD11	2:B:146:ILE:HD12	1.64	0.80
1:C:314:ASP:H	1:C:376:TRP:HZ2	1.30	0.79
1:C:439:ILE:HG21	1:C:659:LEU:HD21	1.63	0.79
1:A:19:LYS:O	1:A:21:PRO:HD3	1.82	0.79
1:A:202:THR:C	1:A:204:PRO:CD	2.55	0.79
1:C:74:ASN:HD22	1:C:74:ASN:H	1.30	0.79
1:A:505:SER:HB3	1:C:589:ASP:HB2	1.63	0.79
1:A:74:ASN:HD22	1:A:74:ASN:H	1.30	0.79
1:A:133:ILE:HD11	1:A:163:VAL:HG21	1.62	0.79
1:C:652:PHE:HB3	1:C:653:PRO:HD3	1.64	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:GLY:O	1:A:301:ASN:HB2	1.81	0.79
1:A:31:THR:HG22	1:A:32:VAL:N	1.95	0.79
1:C:72:HIS:O	1:C:74:ASN:ND2	2.16	0.79
1:A:72:HIS:O	1:A:74:ASN:ND2	2.16	0.78
1:A:74:ASN:HD22	1:A:74:ASN:N	1.77	0.78
1:A:80:ALA:HB1	1:A:111:VAL:HG12	1.65	0.78
1:A:590:VAL:HG13	1:A:622:LEU:HD23	1.65	0.78
1:C:250:GLN:NE2	1:C:251:THR:H	1.81	0.78
1:C:56:ILE:HD13	1:C:95:ASN:HA	1.65	0.78
1:C:688:ILE:HG13	1:C:689:ASN:N	1.98	0.78
1:A:56:ILE:HD13	1:A:95:ASN:HA	1.65	0.78
1:C:19:LYS:O	1:C:21:PRO:HD3	1.82	0.78
1:C:80:ALA:HB1	1:C:111:VAL:HG12	1.65	0.78
3:F:37:GLU:HG2	3:F:46:ILE:HD11	1.65	0.78
1:A:268:GLN:HG3	1:A:313:PRO:HG3	1.65	0.78
1:A:73:ASN:C	1:A:75:LYS:H	1.92	0.78
1:A:250:GLN:NE2	1:A:251:THR:H	1.81	0.77
1:C:75:LYS:HZ1	1:C:94:ALA:H	1.32	0.77
1:C:380:PRO:HG3	3:F:11:MET:HE1	1.67	0.77
1:C:268:GLN:HG3	1:C:313:PRO:HG3	1.65	0.77
1:A:93:GLU:CB	1:A:96:ASN:HD22	1.97	0.77
1:C:196:VAL:HG23	1:C:197:ILE:HG13	1.66	0.77
1:C:80:ALA:HB2	1:C:114:VAL:HG23	1.67	0.76
1:C:513:THR:HB	4:C:2202:HOH:O	1.84	0.76
1:A:151:LEU:HD12	1:A:152:THR:H	1.50	0.76
3:F:33:ILE:HB	3:F:49:LEU:HD12	1.67	0.76
1:C:151:LEU:HD12	1:C:152:THR:H	1.50	0.76
1:C:372:GLN:O	1:C:372:GLN:HG3	1.86	0.76
1:A:174:HIS:NE2	1:A:191:LYS:HB2	1.99	0.76
1:C:739:ARG:HG3	3:F:20:TYR:CE1	2.20	0.76
1:C:304:PHE:CD1	1:C:304:PHE:N	2.52	0.76
3:F:65:LYS:HD3	3:F:110:HIS:HB2	1.68	0.76
3:F:71:ALA:HB2	3:F:81:ILE:HG22	1.67	0.75
1:A:196:VAL:HG23	1:A:197:ILE:HG13	1.66	0.75
1:C:174:HIS:NE2	1:C:191:LYS:HB2	1.99	0.75
1:A:589:ASP:HB2	1:C:505:SER:HB3	1.67	0.75
1:C:73:ASN:C	1:C:75:LYS:H	1.92	0.75
3:F:154:ALA:HB2	3:F:212:TRP:CZ3	2.21	0.75
1:A:652:PHE:HB3	1:A:653:PRO:HD3	1.69	0.75
3:F:256:VAL:CG1	3:F:257:LEU:H	1.94	0.75
1:A:304:PHE:CD1	1:A:304:PHE:N	2.52	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:VAL:HG22	1:A:404:ILE:HG13	1.67	0.75
2:B:10:GLU:HB2	4:B:2336:HOH:O	1.86	0.75
1:A:719:ALA:O	1:A:723:LEU:HG	1.87	0.75
1:A:80:ALA:HB2	1:A:114:VAL:HG23	1.67	0.74
1:C:133:ILE:CD1	1:C:163:VAL:HG21	2.17	0.74
1:A:372:GLN:O	1:A:372:GLN:HG3	1.86	0.74
1:C:524:LYS:HG3	1:C:525:SER:N	2.01	0.74
1:C:428:LYS:HB2	1:C:429:PRO:HD3	1.69	0.74
3:F:83:LYS:HG3	3:F:92:ILE:HG21	1.68	0.74
1:C:739:ARG:CB	3:F:20:TYR:CE1	2.64	0.74
1:C:592:GLN:HG3	1:C:595:PHE:HB3	1.69	0.74
1:A:314:ASP:CG	1:A:376:TRP:NE1	2.46	0.74
1:A:723:LEU:HD11	1:A:740:VAL:HG21	1.69	0.74
2:B:117:LEU:HA	4:B:2340:HOH:O	1.86	0.74
1:C:85:SER:HB2	1:C:104:PHE:O	1.88	0.74
3:F:52:HIS:CE1	3:F:80:MET:HE3	2.22	0.74
3:F:225:VAL:HG22	3:F:257:LEU:HB3	1.70	0.73
1:C:313:PRO:CD	4:C:2146:HOH:O	2.35	0.73
3:F:117:LEU:HD23	3:F:151:ALA:O	1.86	0.73
1:A:93:GLU:CB	1:A:96:ASN:ND2	2.52	0.73
1:C:78:ALA:CB	1:C:114:VAL:HG11	2.19	0.73
1:A:276:SER:OG	1:A:303:CYS:HB2	1.88	0.73
2:B:255:ASP:OD2	2:B:274:GLY:HA3	1.89	0.73
1:C:10:THR:HG23	1:C:28:VAL:CG1	2.18	0.73
3:F:29:SER:C	3:F:31:LYS:H	1.95	0.73
3:F:282:LYS:HA	4:F:2298:HOH:O	1.87	0.73
3:F:224:SER:HB2	3:F:234:TRP:HE1	1.53	0.73
1:C:31:THR:CG2	1:C:32:VAL:H	2.02	0.73
1:A:10:THR:HG23	1:A:28:VAL:CG1	2.18	0.72
1:C:425:LYS:HE2	1:C:686:ASN:ND2	2.02	0.72
1:A:133:ILE:CD1	1:A:163:VAL:HG21	2.17	0.72
1:A:578:LYS:O	1:A:580:GLU:HG3	1.88	0.72
1:C:377:TYR:CZ	3:F:75:TYR:HE1	2.06	0.72
1:A:31:THR:CG2	1:A:32:VAL:H	2.02	0.72
3:F:16:VAL:HG12	3:F:61:TRP:HD1	1.54	0.72
3:F:225:VAL:HG22	3:F:257:LEU:HD13	1.71	0.72
1:A:78:ALA:CB	1:A:114:VAL:HG11	2.19	0.72
1:C:276:SER:OG	1:C:303:CYS:HB2	1.88	0.72
1:A:85:SER:HB2	1:A:104:PHE:O	1.88	0.72
3:F:46:ILE:HD12	3:F:46:ILE:N	2.04	0.72
1:C:314:ASP:OD2	1:C:376:TRP:CZ2	2.42	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:256:VAL:HG12	3:F:257:LEU:N	1.92	0.72
1:A:393:VAL:HG21	2:B:17:LEU:HG	1.69	0.71
1:C:93:GLU:CB	1:C:96:ASN:ND2	2.52	0.71
1:A:431:ILE:HD13	1:A:447:TRP:HZ3	1.55	0.71
1:C:548:ASN:O	1:C:552:LYS:HB2	1.89	0.71
1:A:496:THR:O	1:A:497:ASN:HB2	1.89	0.71
1:A:171:SER:O	1:A:172:LEU:HD23	1.90	0.71
1:C:69:ASP:OD2	1:C:116:PHE:HB2	1.90	0.71
1:C:408:LYS:HD3	1:C:408:LYS:N	1.97	0.71
1:C:510:ILE:HD12	1:C:510:ILE:H	1.55	0.71
1:A:202:THR:OG1	1:A:209:LYS:HD3	1.90	0.71
1:C:331:GLN:OE1	1:C:333:LEU:HD21	1.91	0.71
1:A:420:GLU:HG3	1:A:423:LYS:HE2	1.72	0.71
1:C:93:GLU:CB	1:C:96:ASN:HD22	1.97	0.71
3:F:82:TRP:O	3:F:89:TRP:HZ3	1.74	0.71
3:F:73:CYS:CB	3:F:79:VAL:HG12	2.20	0.71
1:A:69:ASP:OD2	1:A:116:PHE:HB2	1.91	0.70
1:C:202:THR:OG1	1:C:209:LYS:HD3	1.90	0.70
1:A:388:PHE:HB2	1:A:739:ARG:HH21	1.56	0.70
1:A:331:GLN:OE1	1:A:333:LEU:HD21	1.91	0.70
1:A:518:LEU:HD13	1:C:576:ILE:HD12	1.73	0.70
1:C:664:LYS:O	3:F:285:LEU:CD2	2.31	0.70
3:F:196:LEU:HD11	3:F:198:SER:O	1.90	0.70
1:A:428:LYS:NZ	1:A:455:MET:HG2	2.06	0.70
2:B:74:SER:HB3	2:B:76:ASP:OD1	1.91	0.70
1:A:333:LEU:HD23	4:B:2298:HOH:O	1.59	0.70
1:C:171:SER:O	1:C:172:LEU:HD23	1.90	0.70
3:F:154:ALA:HB2	3:F:212:TRP:CE3	2.26	0.70
1:A:94:ALA:O	1:A:95:ASN:HB2	1.92	0.70
1:A:665:THR:OG1	1:A:668:GLU:HG3	1.91	0.70
1:C:567:SER:HB3	1:C:570:SER:HB2	1.73	0.70
1:C:212:LEU:HD13	1:C:227:THR:HG21	1.74	0.70
1:C:109:SER:O	1:C:110:SER:HB2	1.91	0.69
1:A:336:THR:CB	2:B:96:ALA:O	2.40	0.69
1:A:595:PHE:CZ	1:C:515:SER:HB2	2.28	0.69
1:C:203:SER:O	1:C:205:ASN:N	2.26	0.69
1:A:212:LEU:HD13	1:A:227:THR:HG21	1.74	0.69
1:A:109:SER:O	1:A:110:SER:HB2	1.91	0.69
1:A:164:ILE:HG12	1:A:180:GLY:HA2	1.74	0.69
1:A:203:SER:O	1:A:205:ASN:N	2.26	0.69
2:B:53:GLU:HG3	4:B:2337:HOH:O	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:ASN:HD22	1:C:118:ALA:H	1.40	0.69
1:C:304:PHE:HD1	1:C:304:PHE:N	1.87	0.69
1:C:314:ASP:CB	4:C:2011:HOH:O	2.34	0.69
1:A:75:LYS:NZ	1:A:94:ALA:HB2	2.08	0.69
1:C:444:GLU:HG2	1:C:448:ASN:ND2	2.08	0.69
3:F:227:GLN:HA	3:F:256:VAL:HG13	1.75	0.69
1:A:727:PRO:C	1:A:729:ASP:H	2.01	0.68
2:B:144:HIS:CE1	2:B:183:LYS:HD2	2.28	0.68
1:C:19:LYS:HD2	3:F:206:TRP:HE1	1.58	0.68
1:A:185:ALA:HB3	1:A:199:LEU:HB2	1.75	0.68
2:B:105:VAL:HG23	2:B:118:VAL:HG22	1.73	0.68
1:C:28:VAL:HG22	1:C:29:SER:H	1.58	0.68
1:C:185:ALA:HB3	1:C:199:LEU:HB2	1.75	0.68
3:F:105:VAL:HG22	3:F:116:LEU:HD11	1.75	0.68
1:A:402:VAL:HG11	2:B:24:LEU:HD21	1.76	0.68
1:A:107:HIS:ND1	1:A:111:VAL:HG22	2.09	0.68
1:C:221:ASN:HD22	1:C:221:ASN:C	2.01	0.68
1:C:509:ASN:N	1:C:509:ASN:HD22	1.92	0.68
1:C:280:ASN:C	1:C:298:ALA:HB3	2.19	0.68
1:A:86:LEU:CD2	1:A:104:PHE:HB2	2.24	0.68
1:A:280:ASN:C	1:A:298:ALA:HB3	2.19	0.68
1:A:736:GLU:O	1:A:740:VAL:HG23	1.93	0.68
1:C:107:HIS:ND1	1:C:111:VAL:HG22	2.09	0.68
1:C:164:ILE:HG12	1:C:180:GLY:HA2	1.74	0.68
1:A:117:ASN:HD22	1:A:118:ALA:H	1.39	0.68
1:A:249:LEU:O	1:A:249:LEU:HD23	1.94	0.68
1:A:314:ASP:OD2	1:A:376:TRP:CZ3	2.46	0.68
1:C:75:LYS:NZ	1:C:94:ALA:HB2	2.08	0.68
1:C:289:SER:OG	1:C:290:ALA:N	2.24	0.68
3:F:16:VAL:HG12	3:F:61:TRP:CD1	2.29	0.68
1:A:221:ASN:HD22	1:A:221:ASN:C	2.01	0.67
3:F:233:ILE:HD12	3:F:233:ILE:N	2.05	0.67
1:C:94:ALA:O	1:C:95:ASN:HB2	1.92	0.67
1:C:86:LEU:CD2	1:C:104:PHE:HB2	2.24	0.67
1:A:590:VAL:HG13	1:A:622:LEU:CD2	2.23	0.67
2:B:24:LEU:HB3	2:B:36:PHE:HB2	1.76	0.67
1:C:249:LEU:O	1:C:249:LEU:HD23	1.94	0.67
1:A:28:VAL:HG22	1:A:29:SER:H	1.58	0.67
1:A:241:ASP:C	1:A:243:ARG:H	2.02	0.67
1:A:528:LYS:HG3	1:C:493:GLN:HE22	1.58	0.67
3:F:153:TRP:O	3:F:212:TRP:HB3	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:ILE:HD11	2:B:248:LEU:HD13	1.76	0.67
1:A:124:LEU:HG	1:A:125:ALA:N	2.10	0.67
2:B:274:GLY:C	2:B:276:ASN:H	2.00	0.67
1:C:590:VAL:HG13	1:C:622:LEU:CD2	2.25	0.67
1:A:427:PHE:O	1:A:431:ILE:HG12	1.94	0.67
1:C:377:TYR:CB	3:F:57:TRP:CZ2	2.78	0.67
3:F:200:LEU:HB3	3:F:234:TRP:CZ3	2.30	0.67
1:A:639:GLY:CA	1:A:688:ILE:HD11	2.25	0.66
3:F:274:GLY:C	3:F:276:ASN:H	2.03	0.66
2:B:157:THR:OG1	2:B:170:SER:HB2	1.95	0.66
1:C:75:LYS:NZ	1:C:94:ALA:N	2.44	0.66
1:C:439:ILE:HG13	1:C:440:ASP:H	1.60	0.66
3:F:75:TYR:CD1	3:F:101:SER:HB2	2.31	0.66
3:F:144:HIS:HB2	3:F:147:GLY:O	1.95	0.66
1:A:557:ASN:HB3	1:C:496:THR:HG23	1.77	0.66
1:C:535:LEU:HB3	1:C:538:GLU:CG	2.23	0.66
1:A:414:SER:OG	1:A:715:ASN:HB2	1.96	0.66
2:B:3:VAL:C	2:B:4:ILE:HD12	2.21	0.66
1:C:124:LEU:HG	1:C:125:ALA:N	2.10	0.66
1:C:30:GLY:HA3	1:C:321:PHE:CE2	2.30	0.66
1:A:337:LEU:HD21	2:B:97:VAL:CG1	2.26	0.66
1:C:519:VAL:C	1:C:521:GLY:H	2.02	0.66
1:A:75:LYS:NZ	1:A:94:ALA:N	2.44	0.65
1:A:96:ASN:HB2	4:A:2420:HOH:O	1.96	0.65
1:C:250:GLN:HE21	1:C:251:THR:H	1.45	0.65
2:B:238:ASN:HD22	2:B:240:GLN:H	1.45	0.65
1:A:536:LEU:O	1:A:540:MET:HG3	1.96	0.65
1:A:557:ASN:HB3	1:C:496:THR:CG2	2.27	0.65
1:C:241:ASP:C	1:C:243:ARG:H	2.02	0.65
1:C:416:THR:HG22	1:C:420:GLU:OE2	1.96	0.65
3:F:225:VAL:CG2	3:F:257:LEU:HB3	2.26	0.65
1:A:438:VAL:HG23	1:A:443:ASN:ND2	2.07	0.65
3:F:2:VAL:HG13	3:F:41:GLU:HA	1.79	0.65
3:F:233:ILE:H	3:F:233:ILE:CD1	2.10	0.65
1:C:314:ASP:HB3	4:C:2011:HOH:O	1.93	0.65
1:A:314:ASP:H	1:A:376:TRP:HZ2	1.38	0.65
1:C:325:ILE:N	1:C:325:ILE:HD12	2.12	0.65
2:B:102:VAL:CG2	4:B:2353:HOH:O	2.45	0.65
1:C:96:ASN:HB2	4:C:3420:HOH:O	1.96	0.65
1:C:647:ILE:O	1:C:651:GLU:HG3	1.96	0.65
1:A:325:ILE:N	1:A:325:ILE:HD12	2.12	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:ILE:HB	1:A:611:ARG:HH12	1.62	0.64
1:C:125:ALA:HB2	1:C:168:TRP:HH2	1.62	0.64
1:C:400:LYS:O	3:F:7:ALA:N	2.29	0.64
1:A:124:LEU:HG	1:A:125:ALA:H	1.62	0.64
1:A:427:PHE:CD2	1:A:683:VAL:HG22	2.31	0.64
2:B:40:GLY:N	4:B:2335:HOH:O	2.30	0.64
1:A:30:GLY:HA3	1:A:321:PHE:CE2	2.30	0.64
1:A:498:PHE:HB2	1:C:561:ALA:HA	1.77	0.64
1:A:20:ILE:O	1:A:20:ILE:HG13	1.97	0.64
1:A:592:GLN:HG3	1:A:595:PHE:HB3	1.80	0.64
3:F:49:LEU:HD22	3:F:82:TRP:CD2	2.32	0.64
1:C:727:PRO:C	1:C:729:ASP:H	2.06	0.64
1:A:519:VAL:C	1:A:521:GLY:H	2.05	0.64
1:A:519:VAL:HG13	1:C:599:ALA:HA	1.79	0.64
1:C:212:LEU:HD22	1:C:227:THR:CG2	2.28	0.64
1:A:608:ILE:HD13	1:A:611:ARG:HH11	1.62	0.64
1:C:20:ILE:O	1:C:20:ILE:HG13	1.97	0.63
1:C:116:PHE:HE1	1:C:138:MET:HE3	1.63	0.63
1:A:537:MET:HE1	1:C:536:LEU:HD23	1.78	0.63
1:C:124:LEU:HG	1:C:125:ALA:H	1.62	0.63
1:C:395:ILE:HD13	3:F:12:ILE:O	1.98	0.63
1:C:739:ARG:CG	3:F:20:TYR:CE1	2.82	0.63
3:F:207:VAL:HA	3:F:226:SER:HB2	1.78	0.63
1:A:78:ALA:HB3	1:A:114:VAL:HG11	1.80	0.63
1:A:106:ASN:HD22	1:A:106:ASN:H	1.45	0.63
1:A:116:PHE:HE1	1:A:138:MET:HE3	1.63	0.63
1:C:661:LYS:C	1:C:663:ASN:H	2.06	0.63
1:A:206:SER:O	1:A:208:ILE:HG13	1.98	0.63
1:A:250:GLN:HE21	1:A:251:THR:H	1.45	0.63
1:C:78:ALA:HB3	1:C:114:VAL:HG11	1.80	0.63
3:F:105:VAL:CG2	3:F:116:LEU:HD11	2.28	0.63
3:F:224:SER:CB	3:F:234:TRP:HE1	2.11	0.63
1:A:458:THR:HG23	1:A:459:GLU:N	2.14	0.63
1:C:280:ASN:HB3	1:C:300:GLY:C	2.24	0.63
1:C:639:GLY:HA2	1:C:688:ILE:HD11	1.81	0.63
1:C:193:LYS:O	1:C:194:LYS:HB3	1.99	0.63
1:A:212:LEU:HD22	1:A:227:THR:CG2	2.28	0.62
1:C:377:TYR:CB	3:F:57:TRP:CH2	2.82	0.62
3:F:69:ILE:HD11	3:F:83:LYS:CE	2.25	0.62
1:A:280:ASN:HB3	1:A:300:GLY:C	2.24	0.62
2:B:33:ILE:HD11	2:B:56:VAL:HG11	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:225:VAL:CG2	3:F:257:LEU:HD13	2.28	0.62
2:B:23:ARG:NH1	2:B:68:THR:HG21	2.14	0.62
1:C:192:ALA:O	1:C:194:LYS:HG2	2.00	0.62
1:C:408:LYS:H	1:C:408:LYS:CD	2.05	0.62
1:C:206:SER:O	1:C:208:ILE:HG13	1.98	0.62
3:F:184:ILE:CD1	3:F:222:MET:HE1	2.21	0.62
1:A:592:GLN:HG3	1:A:592:GLN:O	1.99	0.62
1:A:147:ASN:O	1:A:148:TYR:C	2.42	0.62
2:B:18:ASP:HB2	4:B:2317:HOH:O	1.98	0.62
1:A:268:GLN:OE1	1:A:374:PRO:HD2	1.99	0.62
1:C:147:ASN:O	1:C:148:TYR:C	2.42	0.62
1:A:192:ALA:O	1:A:194:LYS:HG2	2.00	0.62
1:A:314:ASP:OD1	1:A:376:TRP:CD1	2.52	0.62
1:A:596:ILE:O	1:A:600:ILE:HG12	2.00	0.62
3:F:233:ILE:HD11	3:F:248:LEU:HD13	1.82	0.62
1:A:703:PHE:HA	4:A:3200:HOH:O	2.00	0.62
1:C:106:ASN:HD22	1:C:106:ASN:H	1.45	0.62
3:F:27:CYS:HB2	3:F:56:VAL:HG11	1.82	0.62
1:A:51:ASP:O	1:A:53:GLU:HG3	1.99	0.61
2:B:68:THR:C	2:B:69:ILE:HD12	2.23	0.61
2:B:66:PHE:HE1	2:B:114:PRO:HD3	1.65	0.61
1:A:193:LYS:O	1:A:194:LYS:HB3	1.99	0.61
2:B:155:PRO:HG3	2:B:214:PRO:HA	1.83	0.61
1:A:62:ASP:CG	1:A:103:ARG:HH12	2.08	0.61
2:B:157:THR:HG22	2:B:157:THR:O	2.00	0.61
1:C:153:PRO:HB2	1:C:188:TRP:CZ3	2.35	0.61
1:C:510:ILE:HA	4:C:2202:HOH:O	1.99	0.61
1:C:641:LEU:HD13	1:C:688:ILE:HG21	1.81	0.61
3:F:249:LYS:CE	3:F:251:GLU:HB2	2.28	0.61
1:A:559:TYR:CD2	1:C:541:VAL:HG21	2.35	0.61
2:B:257:LEU:CD1	2:B:271:LEU:HD21	2.30	0.61
1:A:370:HIS:HE1	2:B:75:TYR:CD2	2.18	0.61
1:C:51:ASP:O	1:C:53:GLU:HG3	1.99	0.61
1:C:241:ASP:OD1	1:C:243:ARG:HB2	2.00	0.61
3:F:81:ILE:HD13	3:F:81:ILE:H	1.66	0.61
3:F:118:VAL:O	3:F:125:VAL:HG13	2.00	0.61
3:F:147:GLY:N	3:F:178:ALA:HB3	2.15	0.61
1:A:514:ILE:HA	1:A:517:ASN:HD22	1.65	0.61
1:C:239:ILE:HB	1:C:250:GLN:HB3	1.81	0.61
3:F:115:MET:HG2	3:F:129:GLU:HB2	1.82	0.61
3:F:196:LEU:HD12	3:F:197:GLU:H	1.66	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:458:THR:HG23	1:C:459:GLU:H	1.65	0.61
1:A:241:ASP:OD1	1:A:243:ARG:HB2	2.00	0.61
1:A:608:ILE:CD1	1:A:611:ARG:HH11	2.14	0.61
1:C:244:ASN:ND2	1:C:246:ASN:ND2	2.47	0.61
1:C:665:THR:HG22	3:F:285:LEU:CA	2.30	0.61
1:A:187:ILE:HG22	1:A:196:VAL:HG22	1.83	0.60
1:A:239:ILE:HB	1:A:250:GLN:HB3	1.81	0.60
1:A:392:LEU:HD13	4:A:3219:HOH:O	2.00	0.60
3:F:23:ARG:HA	3:F:36:PHE:O	2.01	0.60
1:A:517:ASN:ND2	1:A:529:ASN:HD22	1.98	0.60
1:A:709:LEU:O	1:A:713:THR:HG23	2.02	0.60
1:A:742:ILE:HB	2:B:20:TYR:CD2	2.36	0.60
2:B:30:ASP:OD1	2:B:32:THR:N	2.34	0.60
1:C:78:ALA:HB1	1:C:114:VAL:HG11	1.84	0.60
3:F:106:GLN:O	3:F:116:LEU:HD12	2.02	0.60
1:A:153:PRO:HB2	1:A:188:TRP:CZ3	2.35	0.60
1:A:217:TRP:CD2	1:A:225:VAL:HG22	2.37	0.60
2:B:52:HIS:HA	4:B:2337:HOH:O	2.01	0.60
2:B:200:LEU:HB3	2:B:234:TRP:CZ3	2.36	0.60
1:C:75:LYS:HZ1	1:C:94:ALA:HB2	1.66	0.60
1:C:268:GLN:CA	1:C:373:ALA:HB1	2.21	0.60
1:A:675:THR:O	1:A:679:GLU:HG3	2.00	0.60
2:B:189:SER:C	2:B:191:ALA:H	2.09	0.60
1:C:62:ASP:CG	1:C:103:ARG:HH12	2.08	0.60
1:C:330:LEU:O	1:C:371:LEU:HD21	2.02	0.60
1:C:553:GLU:HG2	1:C:557:ASN:HD21	1.67	0.60
1:C:604:TYR:CE1	1:C:610:GLN:HG2	2.36	0.60
1:A:202:THR:O	1:A:202:THR:HG22	2.01	0.60
1:A:330:LEU:O	1:A:371:LEU:HD21	2.02	0.60
2:B:4:ILE:HG13	2:B:43:HIS:ND1	2.16	0.60
1:A:289:SER:OG	1:A:290:ALA:N	2.24	0.60
1:C:227:THR:HG22	1:C:227:THR:O	2.02	0.60
1:C:272:LEU:HD22	1:C:284:LEU:HD11	1.83	0.60
1:A:227:THR:HG22	1:A:227:THR:O	2.02	0.60
1:C:187:ILE:HG22	1:C:196:VAL:HG22	1.83	0.60
1:C:202:THR:O	1:C:202:THR:HG22	2.01	0.60
1:C:313:PRO:HG2	1:C:376:TRP:CE2	2.36	0.60
3:F:28:SER:OG	3:F:29:SER:N	2.35	0.60
3:F:172:LYS:HA	3:F:185:TRP:O	2.01	0.60
3:F:219:ARG:HG3	3:F:221:TYR:CE1	2.37	0.60
1:C:739:ARG:HG3	3:F:20:TYR:CD1	2.36	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:147:GLY:H	3:F:178:ALA:HB3	1.66	0.60
1:A:537:MET:O	1:A:541:VAL:HG23	2.02	0.60
2:B:12:ILE:HA	2:B:28:SER:CB	2.30	0.60
2:B:180:ASN:N	2:B:180:ASN:HD22	2.00	0.60
1:C:71:SER:O	1:C:73:ASN:N	2.34	0.60
1:C:105:SER:C	1:C:107:HIS:H	2.09	0.60
3:F:225:VAL:HG22	3:F:257:LEU:CD1	2.32	0.60
1:A:244:ASN:ND2	1:A:246:ASN:ND2	2.47	0.59
1:A:272:LEU:HD22	1:A:284:LEU:HD11	1.83	0.59
1:A:386:TRP:HA	4:A:3219:HOH:O	2.01	0.59
1:C:129:ASN:HA	1:C:162:GLU:HB3	1.84	0.59
1:C:217:TRP:CD2	1:C:225:VAL:HG22	2.36	0.59
3:F:247:LEU:HD13	3:F:249:LYS:O	2.02	0.59
1:A:40:SER:OG	1:A:61:VAL:HG23	2.02	0.59
1:A:458:THR:HG23	1:A:459:GLU:H	1.66	0.59
1:C:314:ASP:N	1:C:376:TRP:CZ2	2.68	0.59
3:F:249:LYS:HG2	3:F:251:GLU:OE1	2.03	0.59
1:A:71:SER:O	1:A:73:ASN:N	2.34	0.59
1:A:73:ASN:C	1:A:75:LYS:N	2.59	0.59
1:A:105:SER:C	1:A:107:HIS:H	2.09	0.59
1:A:370:HIS:CE1	2:B:75:TYR:CD2	2.90	0.59
1:C:667:TYR:CE2	3:F:266:GLY:HA2	2.37	0.59
2:B:216:VAL:HG12	2:B:216:VAL:O	2.03	0.59
1:C:40:SER:OG	1:C:61:VAL:HG23	2.03	0.59
3:F:14:ASP:OD2	3:F:59:VAL:HG22	2.01	0.59
3:F:52:HIS:N	4:F:2307:HOH:O	2.29	0.59
1:A:92:ASN:O	1:A:93:GLU:HB2	2.02	0.59
1:A:306:THR:HA	1:A:317:ALA:O	2.03	0.59
2:B:37:GLU:HG2	2:B:46:ILE:HG13	1.82	0.59
1:C:399:GLY:O	3:F:12:ILE:HG13	2.01	0.59
1:C:438:VAL:HG23	1:C:443:ASN:HD22	1.68	0.59
1:A:78:ALA:HB1	1:A:114:VAL:HG11	1.83	0.59
1:C:386:TRP:CZ2	3:F:280:LEU:HD22	2.37	0.59
1:A:15:TRP:HB3	1:A:310:PRO:HD3	1.85	0.59
1:A:396:THR:HG23	4:A:3251:HOH:O	2.01	0.59
1:C:377:TYR:HB3	4:C:2113:HOH:O	2.02	0.59
1:A:84:GLY:HA3	1:A:110:SER:H	1.68	0.59
1:A:175:VAL:HG12	1:A:176:PHE:N	2.18	0.59
1:A:289:SER:O	1:A:290:ALA:HB2	2.03	0.59
1:A:388:PHE:CD1	1:A:739:ARG:CZ	2.86	0.59
3:F:169:GLU:HG2	3:F:187:TYR:HD2	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:GLN:CD	4:A:3118:HOH:O	2.36	0.59
1:A:511:GLU:HG3	4:A:3107:HOH:O	2.03	0.59
1:C:670:HIS:HE1	1:C:705:GLU:OE1	1.86	0.59
1:A:74:ASN:ND2	1:A:74:ASN:N	2.50	0.58
1:A:75:LYS:HZ1	1:A:94:ALA:HB2	1.68	0.58
1:A:674:LEU:O	1:A:678:ILE:HG12	2.03	0.58
1:C:15:TRP:HB3	1:C:310:PRO:HD3	1.85	0.58
1:C:306:THR:HA	1:C:317:ALA:O	2.03	0.58
1:C:665:THR:CG2	3:F:285:LEU:HD23	2.33	0.58
3:F:17:MET:C	3:F:61:TRP:CD1	2.81	0.58
1:A:112:LYS:HG3	1:A:164:ILE:HG22	1.85	0.58
1:A:518:LEU:HB3	1:C:576:ILE:CD1	2.31	0.58
1:C:228:ALA:HB2	1:C:263:LEU:HD11	1.85	0.58
1:C:268:GLN:HG3	1:C:313:PRO:CG	2.33	0.58
1:A:509:ASN:N	1:A:509:ASN:HD22	2.01	0.58
3:F:4:ILE:N	3:F:4:ILE:HD12	2.18	0.58
3:F:37:GLU:HB2	3:F:44:LYS:HB3	1.85	0.58
1:A:88:LEU:HD13	1:A:138:MET:SD	2.43	0.58
1:A:228:ALA:HB1	1:A:260:ILE:HG21	1.85	0.58
1:A:314:ASP:OD2	1:A:376:TRP:CH2	2.55	0.58
1:A:496:THR:O	1:A:497:ASN:CB	2.51	0.58
1:A:612:ASN:O	1:A:616:ILE:HG12	2.03	0.58
2:B:19:TYR:CD2	2:B:64:PRO:HG2	2.38	0.58
3:F:81:ILE:HD13	3:F:81:ILE:N	2.18	0.58
1:A:11:ALA:HB1	1:A:26:GLY:O	2.04	0.58
2:B:102:VAL:HG23	4:B:2353:HOH:O	2.00	0.58
1:C:175:VAL:HG12	1:C:176:PHE:N	2.18	0.58
1:A:129:ASN:HA	1:A:162:GLU:HB3	1.84	0.58
1:A:314:ASP:CG	1:A:376:TRP:CD1	2.81	0.58
1:A:584:LEU:HD12	1:A:584:LEU:N	2.18	0.58
2:B:83:LYS:HB2	2:B:92:ILE:HD13	1.85	0.58
2:B:120:SER:HB3	2:B:122:ASP:OD1	2.03	0.58
2:B:222:LEU:HB2	2:B:234:TRP:HB2	1.85	0.58
1:C:370:HIS:CG	1:C:371:LEU:N	2.68	0.58
1:A:283:LEU:HD22	1:A:292:GLN:HE21	1.69	0.58
1:A:314:ASP:N	1:A:376:TRP:CE2	2.72	0.58
2:B:29:SER:HA	2:B:55:PRO:HB3	1.84	0.58
1:C:84:GLY:HA3	1:C:110:SER:H	1.68	0.58
3:F:29:SER:O	3:F:31:LYS:N	2.37	0.58
1:C:21:PRO:HB2	1:C:47:LEU:HD11	1.86	0.58
1:C:112:LYS:HG3	1:C:164:ILE:HG22	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:LEU:HD22	1:C:292:GLN:HE21	1.69	0.58
1:C:306:THR:O	1:C:307:LYS:HD3	2.04	0.58
1:C:313:PRO:HD2	4:C:2146:HOH:O	2.00	0.58
1:A:228:ALA:HB2	1:A:263:LEU:HD11	1.85	0.58
1:A:304:PHE:HD1	1:A:304:PHE:N	1.87	0.58
1:A:315:LEU:HD11	2:B:146:ILE:CD1	2.33	0.58
2:B:108:ALA:HB1	2:B:109:PRO:CD	2.34	0.58
3:F:130:PHE:HA	3:F:136:THR:HG22	1.86	0.58
2:B:225:VAL:HG13	2:B:257:LEU:HB2	1.84	0.58
1:C:289:SER:O	1:C:290:ALA:HB2	2.03	0.58
1:A:129:ASN:C	1:A:131:GLY:H	2.11	0.57
1:C:92:ASN:O	1:C:93:GLU:HB2	2.02	0.57
1:C:116:PHE:CE1	1:C:138:MET:HE3	2.39	0.57
1:C:386:TRP:HZ2	3:F:280:LEU:HD22	1.68	0.57
1:C:592:GLN:HG3	1:C:595:PHE:CB	2.33	0.57
1:A:306:THR:O	1:A:307:LYS:HD3	2.04	0.57
1:C:88:LEU:HD13	1:C:138:MET:SD	2.43	0.57
1:A:146:SER:O	1:A:147:ASN:HB2	2.02	0.57
1:A:551:LEU:C	1:A:553:GLU:H	2.11	0.57
1:C:365:LYS:HD2	1:C:365:LYS:O	2.05	0.57
3:F:187:TYR:CG	3:F:188:ASN:N	2.71	0.57
1:C:314:ASP:CG	1:C:376:TRP:CD2	2.80	0.57
1:A:221:ASN:ND2	1:A:223:THR:H	2.03	0.57
1:A:262:SER:HB2	1:A:304:PHE:O	2.05	0.57
1:C:146:SER:O	1:C:147:ASN:HB2	2.02	0.57
3:F:25:ALA:HB1	3:F:70:LEU:HD21	1.86	0.57
1:A:116:PHE:CE1	1:A:138:MET:HE3	2.39	0.57
1:A:145:PRO:O	1:A:146:SER:C	2.48	0.57
1:A:423:LYS:HG3	1:A:424:THR:HG23	1.86	0.57
1:A:730:ASN:O	1:A:733:VAL:HB	2.03	0.57
2:B:4:ILE:HG13	2:B:43:HIS:CG	2.40	0.57
1:C:11:ALA:HB1	1:C:26:GLY:O	2.04	0.57
1:C:221:ASN:ND2	1:C:223:THR:H	2.03	0.57
1:C:329:THR:HB	1:C:331:GLN:O	2.04	0.57
3:F:4:ILE:HG22	3:F:4:ILE:O	2.04	0.57
1:A:172:LEU:C	1:A:174:HIS:H	2.13	0.57
1:A:329:THR:HB	1:A:331:GLN:O	2.04	0.57
1:A:496:THR:HG23	1:C:557:ASN:CB	2.32	0.57
1:A:731:GLU:O	1:A:734:LYS:HB3	2.04	0.57
1:C:113:THR:HG22	1:C:114:VAL:N	2.20	0.57
1:C:244:ASN:HD21	1:C:246:ASN:HD22	1.49	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:PRO:HG3	3:F:11:MET:SD	2.43	0.57
1:C:656:GLU:OE2	1:C:670:HIS:HA	2.04	0.57
4:C:2135:HOH:O	3:F:282:LYS:NZ	2.37	0.57
1:A:74:ASN:H	1:A:74:ASN:ND2	2.02	0.57
1:A:647:ILE:O	1:A:651:GLU:HG3	2.04	0.57
1:C:228:ALA:HB1	1:C:260:ILE:HG21	1.85	0.57
1:C:313:PRO:C	1:C:376:TRP:HE1	2.12	0.57
1:A:241:ASP:O	1:A:243:ARG:N	2.38	0.57
1:A:365:LYS:HD2	1:A:365:LYS:O	2.04	0.57
1:A:468:PHE:CE1	1:A:598:LYS:HE3	2.40	0.57
1:C:72:HIS:ND1	1:C:118:ALA:HA	2.19	0.57
1:C:172:LEU:C	1:C:174:HIS:H	2.13	0.57
1:C:430:LEU:HD11	1:C:679:GLU:HG2	1.86	0.57
1:A:71:SER:HA	1:A:116:PHE:CG	2.40	0.57
1:A:268:GLN:HG3	1:A:313:PRO:CG	2.34	0.57
1:C:509:ASN:N	1:C:509:ASN:ND2	2.51	0.57
2:B:255:ASP:CG	2:B:256:VAL:H	2.14	0.56
1:C:44:LEU:HD23	1:C:56:ILE:HB	1.87	0.56
1:C:145:PRO:O	1:C:146:SER:C	2.48	0.56
1:C:241:ASP:O	1:C:243:ARG:N	2.38	0.56
1:A:155:GLN:CB	1:A:195:GLU:HB3	2.35	0.56
1:A:531:LEU:C	1:A:533:ASN:H	2.13	0.56
2:B:24:LEU:HG	2:B:25:ALA:N	2.20	0.56
2:B:56:VAL:HA	2:B:74:SER:HB2	1.87	0.56
1:C:71:SER:HA	1:C:116:PHE:CG	2.40	0.56
1:C:129:ASN:C	1:C:131:GLY:H	2.11	0.56
3:F:196:LEU:HG	3:F:197:GLU:N	2.20	0.56
1:A:292:GLN:O	1:A:368:VAL:CG2	2.53	0.56
1:A:593:TRP:C	1:A:595:PHE:H	2.12	0.56
3:F:81:ILE:HG12	3:F:92:ILE:HG13	1.88	0.56
3:F:180:ASN:CG	3:F:205:ASP:O	2.49	0.56
1:A:42:LEU:HD21	1:A:89:TYR:CD2	2.41	0.56
1:A:72:HIS:ND1	1:A:118:ALA:HA	2.19	0.56
1:C:17:HIS:HB2	1:C:73:ASN:HB2	1.87	0.56
3:F:10:GLU:HG3	3:F:30:ASP:HB3	1.87	0.56
1:A:314:ASP:N	1:A:376:TRP:CZ2	2.72	0.56
1:A:418:LEU:HG	1:A:718:LEU:HD11	1.87	0.56
1:C:145:PRO:O	1:C:147:ASN:N	2.39	0.56
1:A:113:THR:HG22	1:A:114:VAL:N	2.20	0.56
1:A:365:LYS:NZ	1:A:371:LEU:HD22	2.21	0.56
2:B:66:PHE:CE1	2:B:114:PRO:HD3	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:80:MET:CG	3:F:94:VAL:HG23	2.27	0.56
1:A:21:PRO:HB2	1:A:47:LEU:HD11	1.86	0.56
1:A:44:LEU:HD23	1:A:56:ILE:HB	1.87	0.56
1:A:153:PRO:HB2	1:A:188:TRP:CE3	2.41	0.56
2:B:8:HIS:ND1	2:B:30:ASP:OD2	2.39	0.56
3:F:239:GLU:N	4:F:2304:HOH:O	2.38	0.56
1:A:87:GLU:HG2	1:A:89:TYR:CE1	2.41	0.56
2:B:4:ILE:HD12	2:B:4:ILE:N	2.20	0.56
1:C:87:GLU:HG2	1:C:89:TYR:CE1	2.41	0.56
1:C:155:GLN:CB	1:C:195:GLU:HB3	2.35	0.56
1:C:262:SER:HB2	1:C:304:PHE:O	2.05	0.56
1:A:145:PRO:O	1:A:147:ASN:N	2.39	0.56
1:A:280:ASN:HB3	1:A:300:GLY:O	2.06	0.56
1:A:431:ILE:HD13	1:A:447:TRP:CZ3	2.40	0.56
1:C:129:ASN:ND2	1:C:162:GLU:OE1	2.38	0.56
1:C:153:PRO:HB2	1:C:188:TRP:CE3	2.41	0.56
1:C:280:ASN:HB3	1:C:300:GLY:O	2.06	0.56
1:A:438:VAL:HG22	1:A:439:ILE:N	2.20	0.55
1:C:178:SER:HB2	1:C:186:SER:HB2	1.88	0.55
1:A:74:ASN:O	1:A:76:ILE:HG12	2.06	0.55
1:A:268:GLN:HB2	1:A:374:PRO:O	1.98	0.55
1:C:292:GLN:O	1:C:368:VAL:CG2	2.53	0.55
3:F:184:ILE:HG12	3:F:198:SER:HB2	1.88	0.55
3:F:257:LEU:HD23	3:F:273:GLY:HA2	1.86	0.55
1:A:120:GLN:HG3	1:A:122:ASN:OD1	2.06	0.55
1:A:203:SER:N	1:A:204:PRO:CD	2.69	0.55
1:A:337:LEU:CD2	2:B:97:VAL:HG12	2.36	0.55
1:C:260:ILE:CG2	1:C:261:LEU:N	2.69	0.55
3:F:150:SER:HB2	3:F:210:VAL:HG22	1.88	0.55
1:A:17:HIS:HB2	1:A:73:ASN:HB2	1.87	0.55
1:A:260:ILE:CG2	1:A:261:LEU:N	2.69	0.55
1:A:314:ASP:CG	1:A:376:TRP:CG	2.84	0.55
1:A:537:MET:HE1	1:C:536:LEU:CD2	2.36	0.55
2:B:69:ILE:HD12	2:B:69:ILE:N	2.22	0.55
1:C:199:LEU:HD13	1:C:240:TRP:CG	2.42	0.55
1:C:462:LEU:HD22	1:C:637:ALA:HB2	1.87	0.55
1:C:519:VAL:HG23	1:C:520:SER:N	2.21	0.55
1:A:418:LEU:HD23	1:A:718:LEU:HD21	1.89	0.55
1:A:730:ASN:HB3	1:A:733:VAL:CG2	2.36	0.55
1:C:364:GLU:O	1:C:365:LYS:CB	2.47	0.55
1:C:365:LYS:NZ	1:C:371:LEU:HD22	2.21	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:145:ALA:HB3	3:F:179:ASP:HB3	1.89	0.55
1:A:12:THR:HG23	1:A:12:THR:O	2.06	0.55
1:A:80:ALA:CB	1:A:111:VAL:HG12	2.37	0.55
1:A:510:ILE:HB	4:A:3107:HOH:O	2.06	0.55
1:C:42:LEU:HD21	1:C:89:TYR:CD2	2.41	0.55
1:C:667:TYR:CD2	3:F:266:GLY:HA2	2.41	0.55
1:A:80:ALA:HB2	1:A:114:VAL:CG2	2.36	0.55
1:A:162:GLU:O	1:A:164:ILE:HG23	2.06	0.55
1:A:178:SER:HB2	1:A:186:SER:HB2	1.89	0.55
1:A:312:ALA:CB	1:A:315:LEU:HD12	2.36	0.55
1:C:268:GLN:HG3	4:C:2145:HOH:O	2.06	0.55
3:F:155:PRO:HG2	3:F:214:PRO:HA	1.88	0.55
1:A:104:PHE:CD1	1:A:104:PHE:N	2.75	0.55
1:A:125:ALA:HB2	1:A:168:TRP:HH2	1.62	0.55
1:A:129:ASN:ND2	1:A:162:GLU:OE1	2.38	0.55
1:A:199:LEU:HD13	1:A:240:TRP:CG	2.42	0.55
1:A:616:ILE:HD11	1:A:640:SER:HB2	1.88	0.55
1:C:120:GLN:HG3	1:C:122:ASN:OD1	2.06	0.55
1:C:312:ALA:CB	1:C:315:LEU:HD12	2.36	0.55
1:A:196:VAL:C	1:A:197:ILE:HG13	2.32	0.55
1:A:517:ASN:HD21	1:A:529:ASN:ND2	2.04	0.55
1:A:584:LEU:HD12	1:A:584:LEU:H	1.71	0.55
1:C:196:VAL:C	1:C:197:ILE:HG13	2.32	0.55
1:C:203:SER:N	1:C:204:PRO:CD	2.69	0.55
3:F:183:LYS:HB2	3:F:185:TRP:HE1	1.72	0.55
1:A:241:ASP:C	1:A:243:ARG:N	2.64	0.54
1:A:420:GLU:HG3	1:A:423:LYS:CE	2.37	0.54
1:A:434:ARG:HG3	1:A:447:TRP:CZ2	2.41	0.54
2:B:73:CYS:HB2	2:B:102:VAL:CG1	2.37	0.54
1:C:12:THR:HG23	1:C:12:THR:O	2.06	0.54
1:C:38:THR:O	1:C:64:LYS:HE2	2.07	0.54
1:C:80:ALA:HB2	1:C:114:VAL:CG2	2.36	0.54
1:C:104:PHE:N	1:C:104:PHE:CD1	2.75	0.54
1:A:247:THR:CG2	1:A:248:PRO:HD2	2.37	0.54
2:B:180:ASN:N	2:B:180:ASN:ND2	2.53	0.54
1:C:74:ASN:O	1:C:76:ILE:HG12	2.06	0.54
1:C:431:ILE:HD11	1:C:683:VAL:HG11	1.88	0.54
1:C:494:ILE:HG13	1:C:495:GLU:N	2.18	0.54
1:C:535:LEU:HD22	1:C:538:GLU:HG3	1.88	0.54
1:C:551:LEU:HD23	1:C:551:LEU:C	2.33	0.54
3:F:92:ILE:HG13	3:F:93:ALA:H	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:283:GLU:HA	3:F:288:LYS:O	2.07	0.54
1:A:26:GLY:HA2	1:A:42:LEU:HA	1.89	0.54
1:A:38:THR:O	1:A:64:LYS:HE2	2.07	0.54
1:C:402:VAL:HG11	3:F:24:MET:SD	2.47	0.54
1:C:444:GLU:HG2	1:C:448:ASN:HD21	1.71	0.54
3:F:2:VAL:HG12	3:F:2:VAL:O	2.07	0.54
3:F:74:SER:HB3	3:F:76:ASP:OD1	2.06	0.54
3:F:79:VAL:CG2	3:F:95:HIS:HB3	2.35	0.54
1:C:59:LEU:HD22	1:C:98:ILE:HG12	1.89	0.54
1:C:247:THR:CG2	1:C:248:PRO:HD2	2.37	0.54
1:C:733:VAL:O	1:C:737:LYS:HG3	2.07	0.54
2:B:80:LEU:CD2	2:B:94:VAL:HG23	2.38	0.54
2:B:80:LEU:HD23	2:B:94:VAL:HG23	1.90	0.54
3:F:46:ILE:N	3:F:46:ILE:CD1	2.71	0.54
1:C:26:GLY:HA2	1:C:42:LEU:HA	1.90	0.54
3:F:155:PRO:CG	3:F:214:PRO:HA	2.37	0.54
1:A:19:LYS:C	1:A:21:PRO:HD3	2.33	0.54
1:C:696:ASN:O	1:C:700:ILE:HG13	2.08	0.54
3:F:59:VAL:HG12	3:F:72:SER:HA	1.89	0.54
1:A:509:ASN:N	1:A:509:ASN:ND2	2.54	0.54
2:B:45:LEU:O	2:B:46:ILE:HD13	2.08	0.54
1:C:162:GLU:O	1:C:164:ILE:HG23	2.06	0.54
3:F:225:VAL:HG22	3:F:257:LEU:CB	2.37	0.54
1:A:7:PHE:O	1:A:324:LYS:HD3	2.08	0.54
1:C:48:LEU:O	1:C:49:ALA:O	2.25	0.54
1:A:175:VAL:HG13	1:A:188:TRP:O	2.09	0.53
1:A:259:GLY:HA3	1:A:278:ARG:HH11	1.74	0.53
1:C:604:TYR:CZ	1:C:610:GLN:HG2	2.43	0.53
3:F:25:ALA:HA	3:F:34:LYS:O	2.08	0.53
1:C:46:SER:HB2	1:C:56:ILE:HD11	1.90	0.53
1:C:110:SER:OG	1:C:129:ASN:ND2	2.41	0.53
1:C:175:VAL:HG13	1:C:188:TRP:O	2.09	0.53
3:F:184:ILE:CG1	3:F:198:SER:HB2	2.38	0.53
3:F:208:ARG:H	3:F:226:SER:HA	1.72	0.53
3:F:215:THR:HG23	3:F:215:THR:O	2.08	0.53
1:A:41:SER:O	1:A:42:LEU:HB3	2.07	0.53
1:A:59:LEU:HD22	1:A:98:ILE:HG12	1.89	0.53
1:A:528:LYS:HG3	1:C:493:GLN:NE2	2.22	0.53
1:A:593:TRP:C	1:A:595:PHE:N	2.66	0.53
1:A:623:LYS:HE3	1:A:647:ILE:HD12	1.89	0.53
2:B:29:SER:C	2:B:31:LYS:H	2.16	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:VAL:CG2	2:B:138:PRO:HB3	2.27	0.53
1:A:46:SER:HB2	1:A:56:ILE:HD11	1.90	0.53
1:A:62:ASP:OD1	1:A:62:ASP:N	2.36	0.53
1:C:510:ILE:HG21	1:C:533:ASN:ND2	2.23	0.53
1:A:110:SER:OG	1:A:129:ASN:ND2	2.41	0.53
2:B:25:ALA:HB2	2:B:61:TRP:CZ2	2.44	0.53
1:A:48:LEU:O	1:A:49:ALA:O	2.25	0.53
1:A:439:ILE:HG21	1:A:659:LEU:HD21	1.90	0.53
2:B:117:LEU:HD12	4:B:2340:HOH:O	2.08	0.53
1:C:7:PHE:O	1:C:324:LYS:HD3	2.09	0.53
1:C:13:PHE:HA	1:C:24:VAL:O	2.09	0.53
1:C:41:SER:O	1:C:42:LEU:HB3	2.07	0.53
1:C:665:THR:HG22	3:F:285:LEU:HD23	1.91	0.53
1:A:90:SER:O	1:A:91:THR:HB	2.08	0.53
1:A:285:TRP:CZ3	1:A:292:GLN:HG3	2.44	0.53
1:C:285:TRP:CZ3	1:C:292:GLN:HG3	2.44	0.53
1:C:519:VAL:C	1:C:521:GLY:N	2.62	0.53
1:C:590:VAL:HG13	1:C:622:LEU:HD23	1.90	0.53
1:A:75:LYS:HZ1	1:A:94:ALA:N	1.99	0.53
1:C:74:ASN:H	1:C:74:ASN:ND2	2.02	0.53
1:C:199:LEU:HD13	1:C:240:TRP:CD2	2.44	0.53
1:C:203:SER:C	1:C:205:ASN:H	2.16	0.53
1:C:707:ILE:O	1:C:710:THR:HB	2.09	0.53
3:F:29:SER:C	3:F:31:LYS:N	2.59	0.53
1:A:742:ILE:H	1:A:742:ILE:HD12	1.73	0.53
1:C:268:GLN:HA	1:C:373:ALA:HB3	1.88	0.53
1:C:386:TRP:NE1	3:F:270:ALA:HB2	2.24	0.53
1:C:614:MET:HA	1:C:614:MET:HE2	1.90	0.53
3:F:39:GLU:O	3:F:41:GLU:N	2.33	0.53
3:F:71:ALA:CB	3:F:81:ILE:HG22	2.37	0.53
3:F:75:TYR:C	3:F:77:GLY:H	2.17	0.53
3:F:119:ALA:HB2	3:F:151:ALA:HB2	1.91	0.53
3:F:229:ARG:HG2	3:F:256:VAL:HA	1.91	0.53
3:F:236:GLN:HG2	3:F:237:ASP:N	2.22	0.53
1:A:22:LEU:CD1	1:A:94:ALA:CB	2.82	0.52
1:A:199:LEU:HD13	1:A:240:TRP:CD2	2.44	0.52
1:A:203:SER:C	1:A:205:ASN:H	2.17	0.52
1:A:723:LEU:HA	4:A:3255:HOH:O	2.08	0.52
2:B:49:LEU:HB3	2:B:82:TRP:CZ3	2.44	0.52
1:C:57:ALA:O	1:C:98:ILE:HG22	2.09	0.52
1:C:423:LYS:CG	1:C:424:THR:N	2.71	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ASN:H	1:A:106:ASN:ND2	2.04	0.52
1:A:337:LEU:HD11	2:B:97:VAL:HB	1.91	0.52
1:A:420:GLU:CA	1:A:423:LYS:HE2	2.38	0.52
3:F:78:LYS:HG2	3:F:96:ALA:CB	2.39	0.52
3:F:206:TRP:N	3:F:206:TRP:CD1	2.78	0.52
3:F:260:ALA:HA	3:F:271:LEU:HD12	1.89	0.52
1:A:57:ALA:O	1:A:98:ILE:HG22	2.09	0.52
2:B:39:GLU:HB2	4:B:2335:HOH:O	2.08	0.52
1:C:90:SER:O	1:C:91:THR:HB	2.09	0.52
3:F:188:ASN:HB3	3:F:191:ALA:HB3	1.91	0.52
1:C:252:LEU:HD13	1:C:285:TRP:CG	2.45	0.52
1:C:312:ALA:HB1	1:C:315:LEU:HD12	1.92	0.52
1:A:27:THR:HB	1:A:40:SER:CB	2.40	0.52
1:A:244:ASN:HD21	1:A:246:ASN:HD22	1.49	0.52
1:A:13:PHE:HA	1:A:24:VAL:O	2.09	0.52
1:A:388:PHE:CD1	1:A:739:ARG:NH2	2.77	0.52
1:A:451:GLU:O	1:A:454:SER:HB3	2.09	0.52
1:A:584:LEU:H	1:A:584:LEU:CD1	2.23	0.52
1:A:688:ILE:HD13	1:A:689:ASN:N	2.25	0.52
2:B:33:ILE:CD1	2:B:56:VAL:HG11	2.39	0.52
1:C:259:GLY:HA3	1:C:278:ARG:HH11	1.74	0.52
1:C:727:PRO:C	1:C:729:ASP:N	2.67	0.52
1:A:268:GLN:CA	1:A:373:ALA:HB1	2.27	0.52
1:A:412:LEU:C	1:A:412:LEU:HD23	2.35	0.52
1:C:27:THR:HB	1:C:40:SER:CB	2.40	0.52
1:C:268:GLN:CA	1:C:373:ALA:CB	2.80	0.52
3:F:108:ALA:HB2	3:F:153:TRP:CZ2	2.44	0.52
1:A:155:GLN:HG3	1:A:194:LYS:HB2	1.92	0.52
1:A:649:LEU:HB3	1:A:698:GLN:OE1	2.09	0.52
1:C:75:LYS:HZ2	1:C:94:ALA:N	2.07	0.52
1:C:137:ASP:OD1	1:C:139:ASN:HB2	2.10	0.52
1:C:408:LYS:HE2	3:F:292:ALA:O	2.09	0.52
1:C:674:LEU:HD21	1:C:705:GLU:HB3	1.91	0.52
3:F:231:CYS:HB3	3:F:248:LEU:HD22	1.92	0.52
1:A:505:SER:CB	1:C:589:ASP:HB2	2.37	0.51
1:A:519:VAL:CG1	1:C:599:ALA:HA	2.40	0.51
1:C:19:LYS:C	1:C:21:PRO:HD3	2.33	0.51
1:C:286:ASN:HB2	1:C:293:LEU:HD11	1.92	0.51
3:F:99:SER:O	3:F:100:ALA:CB	2.58	0.51
3:F:123:GLY:HA2	3:F:147:GLY:HA2	1.92	0.51
1:A:137:ASP:OD1	1:A:139:ASN:HB2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:MET:HE1	1:C:541:VAL:HG23	1.91	0.51
3:F:71:ALA:HB2	3:F:81:ILE:CG2	2.40	0.51
1:A:608:ILE:HD13	1:A:611:ARG:NH1	2.24	0.51
1:C:377:TYR:HA	4:C:2113:HOH:O	2.11	0.51
1:C:80:ALA:CB	1:C:111:VAL:HG12	2.37	0.51
1:C:677:PHE:CD2	1:C:678:ILE:HD12	2.46	0.51
3:F:27:CYS:HB2	3:F:56:VAL:CG1	2.41	0.51
1:C:261:LEU:HB2	1:C:277:GLY:HA2	1.92	0.51
3:F:23:ARG:NH1	3:F:68:THR:CG2	2.74	0.51
3:F:180:ASN:N	3:F:180:ASN:ND2	2.46	0.51
2:B:238:ASN:HD22	2:B:240:GLN:N	2.07	0.51
1:C:51:ASP:O	1:C:52:SER:C	2.54	0.51
1:C:283:LEU:HD13	1:C:292:GLN:NE2	2.26	0.51
1:C:314:ASP:OD2	1:C:376:TRP:CZ3	2.62	0.51
1:C:636:LEU:HD12	1:C:688:ILE:HD12	1.93	0.51
1:A:203:SER:C	1:A:205:ASN:N	2.69	0.51
1:A:212:LEU:HD13	1:A:227:THR:CG2	2.41	0.51
1:A:286:ASN:HB2	1:A:293:LEU:HD11	1.92	0.51
2:B:105:VAL:CG2	2:B:116:LEU:HD21	2.41	0.51
3:F:85:GLU:O	3:F:86:ASN:HB2	2.11	0.51
3:F:233:ILE:HG21	3:F:289:TRP:CZ2	2.45	0.51
3:F:274:GLY:C	3:F:276:ASN:N	2.66	0.51
1:A:274:LEU:HG	1:A:308:PHE:CZ	2.46	0.51
1:A:432:ASN:O	1:A:436:VAL:HG23	2.11	0.51
1:A:664:LYS:HA	1:A:668:GLU:OE1	2.11	0.51
2:B:33:ILE:HB	2:B:49:LEU:HB2	1.92	0.51
1:C:155:GLN:HG3	1:C:194:LYS:HB2	1.92	0.51
3:F:29:SER:HA	3:F:55:PRO:HB3	1.93	0.51
1:A:70:TRP:HD1	1:A:71:SER:O	1.94	0.51
1:A:117:ASN:HD22	1:A:117:ASN:C	2.17	0.51
1:A:252:LEU:HD13	1:A:285:TRP:CG	2.45	0.51
2:B:69:ILE:HG22	2:B:70:LEU:N	2.25	0.51
1:C:335:ASN:OD1	3:F:99:SER:HB3	2.11	0.51
1:C:430:LEU:HD23	1:C:430:LEU:O	2.11	0.51
3:F:63:HIS:ND1	3:F:64:PRO:HD2	2.26	0.51
3:F:171:ARG:O	3:F:186:LYS:HA	2.11	0.51
3:F:259:ARG:HG3	3:F:259:ARG:HH11	1.76	0.51
3:F:284:ASN:HB3	3:F:290:GLU:CD	2.36	0.51
1:A:51:ASP:O	1:A:52:SER:C	2.54	0.50
1:C:333:LEU:HG	3:F:100:ALA:HA	1.93	0.50
3:F:92:ILE:HG13	3:F:93:ALA:N	2.27	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LEU:C	1:A:174:HIS:N	2.69	0.50
1:A:283:LEU:HD13	1:A:292:GLN:NE2	2.26	0.50
2:B:95:HIS:CE1	2:B:128:VAL:HG21	2.46	0.50
1:C:70:TRP:HD1	1:C:71:SER:O	1.94	0.50
1:C:204:PRO:C	1:C:206:SER:H	2.19	0.50
1:C:268:GLN:HE21	1:C:313:PRO:CG	2.25	0.50
1:C:271:HIS:O	1:C:272:LEU:HD23	2.12	0.50
1:A:66:ASN:N	1:A:80:ALA:O	2.39	0.50
1:A:370:HIS:CG	1:A:371:LEU:N	2.68	0.50
1:A:663:ASN:HA	2:B:285:LEU:HD11	1.94	0.50
2:B:30:ASP:OD1	2:B:30:ASP:C	2.55	0.50
2:B:200:LEU:HD13	2:B:234:TRP:CE3	2.47	0.50
3:F:65:LYS:CD	3:F:110:HIS:HB2	2.40	0.50
3:F:78:LYS:HG2	3:F:96:ALA:HB1	1.94	0.50
1:A:364:GLU:O	1:A:365:LYS:CB	2.47	0.50
1:A:371:LEU:O	1:A:372:GLN:C	2.55	0.50
1:A:731:GLU:HA	1:A:734:LYS:HB3	1.93	0.50
1:C:106:ASN:H	1:C:106:ASN:ND2	2.04	0.50
1:C:400:LYS:O	3:F:6:ASN:HA	2.11	0.50
1:A:268:GLN:HE21	1:A:313:PRO:CG	2.25	0.50
1:A:537:MET:HE2	1:C:540:MET:SD	2.52	0.50
1:C:237:ILE:HB	1:C:252:LEU:HB2	1.93	0.50
3:F:286:GLU:HG3	3:F:288:LYS:HD2	1.94	0.50
1:A:261:LEU:HB2	1:A:277:GLY:HA2	1.92	0.50
1:C:203:SER:C	1:C:205:ASN:N	2.69	0.50
1:C:212:LEU:HD13	1:C:227:THR:CG2	2.41	0.50
1:C:601:GLN:HE22	1:C:611:ARG:HD3	1.77	0.50
1:A:312:ALA:HB1	1:A:315:LEU:HD12	1.92	0.50
1:A:524:LYS:HG3	1:A:525:SER:N	2.26	0.50
1:A:540:MET:HE1	1:C:541:VAL:CG2	2.42	0.50
2:B:112:TYR:CZ	2:B:171:ARG:HG2	2.46	0.50
1:C:22:LEU:CD1	1:C:94:ALA:CB	2.82	0.50
2:B:4:ILE:O	2:B:4:ILE:HG22	2.11	0.50
1:C:274:LEU:HG	1:C:308:PHE:CZ	2.46	0.50
3:F:94:VAL:O	3:F:94:VAL:HG13	2.11	0.50
1:A:75:LYS:HZ1	1:A:94:ALA:CB	2.25	0.50
2:B:29:SER:C	2:B:31:LYS:N	2.70	0.50
1:C:172:LEU:C	1:C:174:HIS:N	2.69	0.50
1:A:11:ALA:HB3	1:A:325:ILE:HD11	1.93	0.49
1:C:124:LEU:CG	1:C:125:ALA:H	2.24	0.49
1:C:249:LEU:HD23	1:C:249:LEU:C	2.37	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ALA:O	1:A:98:ILE:CG2	2.60	0.49
1:A:314:ASP:OD1	1:A:376:TRP:CG	2.65	0.49
1:C:15:TRP:HB3	1:C:310:PRO:CD	2.41	0.49
1:C:439:ILE:HG13	1:C:440:ASP:N	2.27	0.49
1:C:494:ILE:HG23	1:C:495:GLU:N	2.26	0.49
3:F:131:LYS:HB3	3:F:132:GLU:OE2	2.12	0.49
1:A:15:TRP:HB3	1:A:310:PRO:CD	2.41	0.49
1:C:264:ASP:HB2	1:C:307:LYS:HD3	1.94	0.49
1:A:204:PRO:C	1:A:206:SER:H	2.19	0.49
1:A:543:ALA:C	1:A:545:ASP:H	2.19	0.49
2:B:26:THR:O	2:B:33:ILE:HG23	2.12	0.49
2:B:95:HIS:HE1	2:B:138:PRO:HG3	1.77	0.49
1:C:154:GLY:O	1:C:155:GLN:CG	2.48	0.49
3:F:121:SER:C	3:F:123:GLY:H	2.20	0.49
1:C:439:ILE:CG2	1:C:659:LEU:HD21	2.39	0.49
1:A:124:LEU:CG	1:A:125:ALA:H	2.24	0.49
1:A:187:ILE:HB	1:A:197:ILE:HB	1.95	0.49
1:A:237:ILE:HB	1:A:252:LEU:HB2	1.93	0.49
1:A:271:HIS:O	1:A:272:LEU:HD23	2.12	0.49
1:A:314:ASP:CB	1:A:376:TRP:CE2	2.95	0.49
1:C:284:LEU:HD23	1:C:371:LEU:HD11	1.95	0.49
1:C:665:THR:HG22	3:F:285:LEU:N	2.27	0.49
1:C:733:VAL:HG12	1:C:737:LYS:HE3	1.95	0.49
1:A:268:GLN:CB	4:A:3118:HOH:O	2.46	0.49
1:A:466:LEU:O	1:A:598:LYS:HE2	2.13	0.49
1:A:555:VAL:O	1:A:558:ALA:HB3	2.12	0.49
1:A:585:VAL:HA	1:A:596:ILE:HG21	1.95	0.49
2:B:184:ILE:N	2:B:184:ILE:HD12	2.28	0.49
1:C:75:LYS:HZ1	1:C:94:ALA:CB	2.25	0.49
1:A:15:TRP:HZ3	1:A:307:LYS:O	1.96	0.49
1:A:29:SER:HB2	1:A:82:ASP:OD1	2.13	0.49
1:C:221:ASN:C	1:C:221:ASN:ND2	2.69	0.49
1:C:371:LEU:O	1:C:372:GLN:C	2.55	0.49
1:C:530:SER:O	1:C:533:ASN:O	2.31	0.49
3:F:52:HIS:ND1	3:F:74:SER:HB2	2.28	0.49
1:A:496:THR:HG22	1:A:497:ASN:N	2.27	0.49
2:B:8:HIS:CE1	2:B:34:LYS:HE2	2.48	0.49
2:B:233:ILE:CD1	2:B:248:LEU:HD13	2.43	0.49
1:C:130:ASN:HB3	1:C:132:GLU:HG3	1.95	0.49
1:A:130:ASN:HB3	1:A:132:GLU:HG3	1.95	0.49
1:A:568:SER:HB2	1:C:511:GLU:OE1	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:535:LEU:CB	1:C:538:GLU:HG3	2.31	0.49
3:F:179:ASP:C	3:F:180:ASN:HD22	2.20	0.49
3:F:240:GLN:O	3:F:241:GLY:C	2.55	0.49
1:A:325:ILE:N	1:A:325:ILE:CD1	2.76	0.48
1:A:608:ILE:HB	1:A:611:ARG:NH1	2.27	0.48
2:B:259:ARG:HG3	2:B:259:ARG:HH11	1.77	0.48
1:C:57:ALA:O	1:C:98:ILE:CG2	2.60	0.48
1:C:187:ILE:HB	1:C:197:ILE:HB	1.95	0.48
1:C:219:PRO:HG3	1:C:266:CYS:O	2.13	0.48
3:F:59:VAL:HA	3:F:71:ALA:O	2.12	0.48
1:A:31:THR:O	1:A:32:VAL:HG23	2.13	0.48
1:A:105:SER:C	1:A:107:HIS:N	2.71	0.48
1:A:284:LEU:HD23	1:A:371:LEU:HD11	1.95	0.48
1:A:365:LYS:HZ3	1:A:371:LEU:HD22	1.77	0.48
2:B:74:SER:C	2:B:76:ASP:N	2.71	0.48
2:B:148:VAL:O	4:B:2338:HOH:O	2.20	0.48
1:C:29:SER:HB2	1:C:82:ASP:OD1	2.13	0.48
1:C:664:LYS:C	3:F:285:LEU:HD11	2.38	0.48
3:F:24:MET:HB3	3:F:36:PHE:HB2	1.96	0.48
1:A:28:VAL:HG22	1:A:29:SER:N	2.26	0.48
2:B:57:TRP:O	2:B:58:ARG:HG2	2.14	0.48
2:B:172:LYS:HA	2:B:185:TRP:O	2.13	0.48
1:C:15:TRP:HZ3	1:C:307:LYS:O	1.96	0.48
1:C:331:GLN:HG2	1:C:371:LEU:HD23	1.96	0.48
3:F:82:TRP:N	3:F:82:TRP:CD1	2.82	0.48
3:F:108:ALA:HB3	3:F:115:MET:HB2	1.96	0.48
1:A:264:ASP:HB2	1:A:307:LYS:HD3	1.94	0.48
1:A:331:GLN:HG2	1:A:371:LEU:HD23	1.96	0.48
1:A:567:SER:HB3	1:A:570:SER:HB2	1.93	0.48
1:A:644:VAL:HG11	1:A:684:PHE:CE2	2.48	0.48
1:C:115:LYS:O	1:C:124:LEU:HD12	2.13	0.48
1:C:553:GLU:HG2	1:C:557:ASN:ND2	2.28	0.48
3:F:10:GLU:CG	3:F:30:ASP:HB3	2.42	0.48
1:A:75:LYS:HD2	1:A:91:THR:HG22	1.95	0.48
1:A:219:PRO:HG3	1:A:266:CYS:O	2.13	0.48
1:A:249:LEU:HD23	1:A:249:LEU:C	2.37	0.48
1:A:514:ILE:HA	1:A:517:ASN:ND2	2.28	0.48
1:A:519:VAL:C	1:A:521:GLY:N	2.71	0.48
1:C:11:ALA:HB3	1:C:325:ILE:HD11	1.93	0.48
3:F:129:GLU:HG2	3:F:130:PHE:N	2.27	0.48
1:A:337:LEU:CD2	2:B:97:VAL:CG1	2.90	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:ASP:OD1	1:A:429:PRO:HD3	2.14	0.48
2:B:63:HIS:CD2	4:B:2334:HOH:O	2.65	0.48
1:C:33:ASP:OD1	1:C:37:SER:HB3	2.13	0.48
1:C:424:THR:O	1:C:425:LYS:CB	2.62	0.48
1:C:456:ASP:O	1:C:460:GLU:HB2	2.14	0.48
3:F:47:ASP:OD2	3:F:89:TRP:HB2	2.12	0.48
3:F:259:ARG:HB2	3:F:272:SER:HB2	1.95	0.48
1:A:186:SER:HB3	1:A:188:TRP:NE1	2.29	0.48
1:C:124:LEU:CG	1:C:125:ALA:N	2.76	0.48
1:C:186:SER:HB3	1:C:188:TRP:NE1	2.29	0.48
3:F:95:HIS:CE1	3:F:128:VAL:HG21	2.48	0.48
1:A:115:LYS:O	1:A:124:LEU:HD12	2.13	0.48
2:B:18:ASP:OD2	2:B:23:ARG:HB3	2.14	0.48
1:C:31:THR:O	1:C:32:VAL:HG23	2.13	0.48
1:C:70:TRP:C	1:C:71:SER:O	2.55	0.48
1:C:73:ASN:C	1:C:75:LYS:N	2.58	0.48
3:F:109:PRO:HD2	3:F:112:TYR:CD2	2.49	0.48
3:F:131:LYS:HD2	3:F:135:THR:O	2.14	0.48
3:F:157:THR:HB	3:F:170:SER:OG	2.14	0.48
1:A:114:VAL:HA	1:A:125:ALA:O	2.14	0.48
1:A:392:LEU:CD1	4:A:3219:HOH:O	2.61	0.48
1:C:75:LYS:HD2	1:C:91:THR:HG22	1.95	0.48
3:F:196:LEU:CG	3:F:197:GLU:N	2.77	0.48
1:A:33:ASP:OD1	1:A:37:SER:HB3	2.13	0.48
1:A:430:LEU:O	1:A:430:LEU:HD23	2.13	0.48
1:A:517:ASN:HD21	1:A:529:ASN:HD22	1.61	0.48
1:A:551:LEU:C	1:A:553:GLU:N	2.71	0.48
2:B:59:VAL:HA	2:B:71:ALA:O	2.14	0.48
1:C:10:THR:O	1:C:11:ALA:HB2	2.14	0.48
1:C:19:LYS:HD2	3:F:206:TRP:NE1	2.27	0.48
1:C:92:ASN:O	1:C:93:GLU:CB	2.62	0.48
3:F:102:VAL:HA	3:F:120:SER:HA	1.95	0.48
1:A:412:LEU:CD2	1:A:713:THR:HG22	2.38	0.47
1:A:542:ILE:HD11	1:C:573:LEU:CD2	2.44	0.47
2:B:31:LYS:O	4:B:2321:HOH:O	2.20	0.47
2:B:37:GLU:HG2	2:B:46:ILE:CG1	2.44	0.47
2:B:72:SER:O	2:B:79:VAL:HG13	2.14	0.47
2:B:87:GLY:C	2:B:88:ARG:HG3	2.39	0.47
1:C:388:PHE:CE1	1:C:739:ARG:HD3	2.49	0.47
1:A:10:THR:O	1:A:11:ALA:HB2	2.14	0.47
1:A:72:HIS:HE1	1:A:118:ALA:HA	1.72	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LEU:CD1	1:A:152:THR:H	2.25	0.47
1:A:154:GLY:O	1:A:155:GLN:CG	2.48	0.47
2:B:34:LYS:HB3	2:B:36:PHE:HE1	1.80	0.47
2:B:255:ASP:CG	2:B:256:VAL:N	2.72	0.47
1:C:16:SER:HB2	1:C:18:ASP:OD1	2.14	0.47
1:C:28:VAL:HG22	1:C:29:SER:N	2.26	0.47
1:A:42:LEU:CD2	1:A:98:ILE:HD11	2.44	0.47
2:B:108:ALA:HA	2:B:153:TRP:CD1	2.49	0.47
1:C:271:HIS:CE1	1:C:288:GLU:OE2	2.67	0.47
1:C:514:ILE:HA	1:C:517:ASN:HD22	1.79	0.47
1:C:536:LEU:O	1:C:537:MET:C	2.57	0.47
2:B:29:SER:O	2:B:31:LYS:HG3	2.14	0.47
1:C:114:VAL:HA	1:C:125:ALA:O	2.14	0.47
1:C:661:LYS:C	1:C:663:ASN:N	2.72	0.47
1:A:42:LEU:HD23	1:A:98:ILE:HD11	1.96	0.47
1:A:115:LYS:O	1:A:168:TRP:HZ3	1.97	0.47
2:B:18:ASP:CG	2:B:23:ARG:HB3	2.39	0.47
2:B:119:ALA:HB1	2:B:148:VAL:HG12	1.96	0.47
1:C:728:SER:HB3	1:C:737:LYS:NZ	2.29	0.47
3:F:40:GLY:O	3:F:41:GLU:CG	2.62	0.47
3:F:141:ILE:HD13	3:F:141:ILE:O	2.14	0.47
1:A:16:SER:HB2	1:A:18:ASP:OD1	2.14	0.47
1:A:91:THR:HG22	1:A:91:THR:O	2.14	0.47
1:A:78:ALA:HB3	1:A:114:VAL:CG1	2.45	0.47
1:A:92:ASN:O	1:A:93:GLU:CB	2.62	0.47
1:A:117:ASN:ND2	1:A:118:ALA:N	2.54	0.47
1:A:271:HIS:CE1	1:A:288:GLU:OE2	2.67	0.47
1:A:336:THR:OG1	2:B:96:ALA:O	2.33	0.47
1:A:517:ASN:ND2	1:A:529:ASN:ND2	2.63	0.47
1:A:593:TRP:O	1:A:595:PHE:N	2.48	0.47
1:A:664:LYS:HB3	1:A:668:GLU:HB2	1.96	0.47
1:A:739:ARG:HD2	2:B:19:TYR:CZ	2.50	0.47
2:B:27:CYS:HB2	2:B:56:VAL:CG1	2.44	0.47
2:B:69:ILE:CG2	2:B:70:LEU:N	2.77	0.47
2:B:119:ALA:HB1	2:B:148:VAL:CG1	2.45	0.47
2:B:124:LYS:HE2	2:B:142:ASP:OD1	2.15	0.47
2:B:212:TRP:CD2	2:B:222:LEU:HD21	2.49	0.47
2:B:225:VAL:HG13	2:B:257:LEU:CB	2.43	0.47
1:C:42:LEU:HD23	1:C:98:ILE:HD11	1.96	0.47
1:C:115:LYS:O	1:C:168:TRP:HZ3	1.97	0.47
1:C:731:GLU:HA	1:C:734:LYS:HB3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:31:LYS:HB3	3:F:52:HIS:O	2.15	0.47
3:F:205:ASP:H	3:F:228:ASP:HB3	1.78	0.47
3:F:250:GLU:C	3:F:251:GLU:OE1	2.58	0.47
1:A:402:VAL:HG11	2:B:24:LEU:CD2	2.42	0.47
1:A:652:PHE:HB3	1:A:653:PRO:CD	2.44	0.47
2:B:15:ALA:HA	2:B:25:ALA:O	2.14	0.47
1:C:313:PRO:HG2	4:C:2145:HOH:O	1.82	0.47
1:C:314:ASP:OD2	1:C:376:TRP:CH2	2.67	0.47
3:F:24:MET:O	3:F:61:TRP:HZ2	1.96	0.47
3:F:209:ASP:HB2	3:F:258:TRP:O	2.14	0.47
1:A:639:GLY:HA2	1:A:688:ILE:CD1	2.35	0.47
1:A:727:PRO:C	1:A:729:ASP:N	2.69	0.47
2:B:109:PRO:HD2	2:B:112:TYR:CD2	2.50	0.47
1:C:589:ASP:C	1:C:591:SER:H	2.23	0.47
3:F:23:ARG:NH1	3:F:68:THR:HG21	2.29	0.47
3:F:69:ILE:CG1	3:F:83:LYS:HG2	2.32	0.47
1:A:15:TRP:CZ3	1:A:317:ALA:N	2.83	0.47
1:A:86:LEU:HD23	1:A:104:PHE:HB2	1.96	0.47
2:B:259:ARG:HG3	2:B:259:ARG:NH1	2.30	0.47
3:F:216:VAL:HG12	3:F:216:VAL:O	2.15	0.47
1:A:462:LEU:HD13	1:A:637:ALA:HB2	1.97	0.46
1:C:15:TRP:CZ3	1:C:317:ALA:N	2.83	0.46
1:C:382:PRO:CB	3:F:278:VAL:HG23	2.46	0.46
1:C:412:LEU:CD2	1:C:713:THR:HG22	2.45	0.46
3:F:99:SER:O	3:F:100:ALA:HB2	2.15	0.46
1:A:68:LEU:HA	1:A:78:ALA:O	2.15	0.46
2:B:74:SER:CB	2:B:76:ASP:OD1	2.61	0.46
1:C:252:LEU:HD13	1:C:285:TRP:CB	2.45	0.46
1:C:325:ILE:N	1:C:325:ILE:CD1	2.76	0.46
1:C:329:THR:C	1:C:331:GLN:N	2.73	0.46
1:C:386:TRP:HZ3	4:C:2214:HOH:O	1.98	0.46
1:C:674:LEU:O	1:C:678:ILE:HD13	2.15	0.46
3:F:52:HIS:NE2	3:F:80:MET:HE3	2.30	0.46
1:A:45:TRP:CD1	1:A:45:TRP:N	2.84	0.46
1:A:252:LEU:HD13	1:A:285:TRP:CB	2.45	0.46
1:A:542:ILE:HD11	1:C:573:LEU:HD21	1.96	0.46
1:C:68:LEU:HA	1:C:78:ALA:O	2.16	0.46
1:C:78:ALA:HB3	1:C:114:VAL:CG1	2.45	0.46
1:C:93:GLU:O	1:C:94:ALA:C	2.57	0.46
3:F:37:GLU:O	3:F:43:HIS:HA	2.15	0.46
3:F:146:ILE:HB	3:F:178:ALA:HB3	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:200:LEU:HD13	3:F:234:TRP:CE3	2.51	0.46
3:F:210:VAL:HG23	3:F:210:VAL:O	2.14	0.46
1:A:329:THR:C	1:A:331:GLN:N	2.73	0.46
1:A:337:LEU:HD21	2:B:97:VAL:HG11	1.97	0.46
1:A:608:ILE:CD1	1:A:611:ARG:NH1	2.78	0.46
1:C:42:LEU:CD2	1:C:98:ILE:HD11	2.44	0.46
1:C:91:THR:HG22	1:C:91:THR:O	2.14	0.46
1:C:279:ASP:OD2	1:C:281:THR:HG22	2.16	0.46
1:A:563:TYR:C	1:A:565:SER:H	2.24	0.46
1:C:438:VAL:HG21	1:C:444:GLU:HA	1.96	0.46
3:F:118:VAL:HB	3:F:126:SER:OG	2.15	0.46
3:F:124:LYS:HG2	3:F:142:ASP:OD1	2.15	0.46
3:F:152:SER:CB	3:F:211:ALA:HA	2.45	0.46
1:C:66:ASN:N	1:C:80:ALA:O	2.39	0.46
1:C:183:ASN:HA	1:C:211:GLN:HA	1.97	0.46
3:F:194:TYR:H	3:F:194:TYR:HD1	1.63	0.46
1:A:93:GLU:O	1:A:94:ALA:C	2.57	0.46
1:A:428:LYS:HB2	1:A:429:PRO:CD	2.38	0.46
1:C:259:GLY:HA3	1:C:278:ARG:NH1	2.31	0.46
1:C:432:ASN:O	1:C:436:VAL:HG23	2.16	0.46
1:C:641:LEU:HD12	1:C:684:PHE:HE2	1.80	0.46
1:A:68:LEU:HD22	1:A:77:ILE:HG22	1.98	0.46
1:A:663:ASN:CA	2:B:285:LEU:HD11	2.46	0.46
2:B:93:ALA:HB1	4:B:2344:HOH:O	2.14	0.46
1:A:70:TRP:C	1:A:71:SER:O	2.55	0.46
1:A:124:LEU:CG	1:A:125:ALA:N	2.76	0.46
1:A:219:PRO:HD3	1:A:265:TRP:CD1	2.51	0.46
1:A:564:GLY:HA2	1:A:570:SER:OG	2.16	0.46
2:B:117:LEU:HB2	2:B:153:TRP:NE1	2.31	0.46
1:C:212:LEU:HD22	1:C:227:THR:HG22	1.98	0.46
1:C:268:GLN:HG3	1:C:313:PRO:CB	2.46	0.46
1:C:312:ALA:O	1:C:314:ASP:N	2.48	0.46
1:A:392:LEU:HA	4:A:3219:HOH:O	2.16	0.46
2:B:121:SER:HA	4:B:2338:HOH:O	2.15	0.46
1:C:45:TRP:CD1	1:C:45:TRP:N	2.84	0.46
1:C:120:GLN:C	1:C:122:ASN:H	2.22	0.46
1:C:212:LEU:HB3	1:C:227:THR:HG23	1.98	0.46
1:C:438:VAL:HG23	1:C:443:ASN:ND2	2.30	0.46
1:C:641:LEU:HD12	1:C:684:PHE:CE2	2.51	0.46
3:F:75:TYR:O	3:F:77:GLY:N	2.49	0.46
3:F:85:GLU:HG2	3:F:86:ASN:ND2	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:271:LEU:HD12	3:F:271:LEU:HA	1.57	0.46
1:A:202:THR:CG2	1:A:209:LYS:HD3	2.46	0.45
1:A:260:ILE:HG23	1:A:261:LEU:N	2.31	0.45
1:A:337:LEU:HD21	2:B:140:ILE:HD11	1.97	0.45
2:B:200:LEU:HB3	2:B:234:TRP:CH2	2.50	0.45
1:C:68:LEU:HD22	1:C:77:ILE:HG22	1.98	0.45
1:C:202:THR:CG2	1:C:209:LYS:HD3	2.46	0.45
1:C:219:PRO:HD3	1:C:265:TRP:CD1	2.51	0.45
1:A:120:GLN:C	1:A:122:ASN:H	2.22	0.45
1:A:129:ASN:C	1:A:131:GLY:N	2.74	0.45
1:A:169:ASN:OD1	1:A:172:LEU:HB2	2.16	0.45
1:A:572:ILE:CD1	1:C:504:PHE:HE2	2.28	0.45
1:A:718:LEU:O	1:A:722:PHE:HD1	1.98	0.45
1:C:105:SER:C	1:C:107:HIS:N	2.71	0.45
1:C:129:ASN:C	1:C:131:GLY:N	2.74	0.45
1:A:279:ASP:OD2	1:A:281:THR:HG22	2.16	0.45
1:A:312:ALA:O	1:A:314:ASP:N	2.49	0.45
1:A:581:VAL:HG11	1:A:600:ILE:HD13	1.98	0.45
2:B:284:ASN:HB2	4:B:2352:HOH:O	2.16	0.45
1:C:377:TYR:CA	4:C:2113:HOH:O	2.64	0.45
3:F:59:VAL:HG12	3:F:72:SER:CB	2.46	0.45
3:F:191:ALA:C	3:F:192:GLN:HG2	2.41	0.45
1:A:221:ASN:C	1:A:221:ASN:ND2	2.69	0.45
1:A:504:PHE:CZ	1:C:588:LEU:HD13	2.52	0.45
1:A:595:PHE:C	1:A:597:SER:N	2.72	0.45
1:C:117:ASN:ND2	1:C:118:ALA:N	2.54	0.45
1:C:169:ASN:OD1	1:C:172:LEU:HB2	2.16	0.45
1:C:431:ILE:HD13	1:C:447:TRP:HZ3	1.82	0.45
3:F:14:ASP:HB3	3:F:27:CYS:SG	2.55	0.45
1:A:83:ASN:O	1:A:84:GLY:C	2.59	0.45
1:A:162:GLU:HG3	1:A:164:ILE:HG23	1.99	0.45
1:A:436:VAL:O	1:A:436:VAL:HG12	2.16	0.45
1:A:441:ASP:HA	4:A:3212:HOH:O	2.15	0.45
1:A:551:LEU:C	1:A:551:LEU:HD23	2.41	0.45
1:A:559:TYR:CE2	1:C:541:VAL:HG21	2.52	0.45
1:C:15:TRP:CH2	1:C:317:ALA:HB2	2.52	0.45
1:C:497:ASN:O	1:C:497:ASN:CG	2.59	0.45
3:F:226:SER:OG	3:F:227:GLN:N	2.49	0.45
3:F:247:LEU:C	3:F:249:LYS:N	2.74	0.45
1:A:127:GLY:HA2	1:A:132:GLU:O	2.16	0.45
2:B:66:PHE:CD1	2:B:114:PRO:HB3	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:ASN:O	1:C:84:GLY:C	2.59	0.45
1:C:260:ILE:HG23	1:C:261:LEU:N	2.31	0.45
1:C:665:THR:CB	3:F:285:LEU:HD23	2.46	0.45
3:F:120:SER:O	3:F:148:VAL:HG23	2.16	0.45
3:F:255:ASP:HB2	3:F:275:ASP:HB3	1.98	0.45
1:A:155:GLN:HB2	1:A:195:GLU:HB3	1.99	0.45
1:A:193:LYS:O	1:A:194:LYS:CB	2.65	0.45
1:A:573:LEU:HD23	1:C:518:LEU:CD1	2.47	0.45
1:A:688:ILE:HG12	1:A:689:ASN:H	1.82	0.45
1:C:86:LEU:HD23	1:C:104:PHE:HB2	1.96	0.45
1:C:457:GLY:O	1:C:458:THR:C	2.59	0.45
1:C:590:VAL:O	1:C:590:VAL:CG1	2.64	0.45
1:C:596:ILE:O	1:C:600:ILE:HG13	2.16	0.45
1:C:622:LEU:O	1:C:627:HIS:HB2	2.16	0.45
1:A:232:ASP:O	1:A:258:LYS:HA	2.17	0.45
1:A:259:GLY:HA3	1:A:278:ARG:NH1	2.31	0.45
1:C:169:ASN:HB3	1:C:172:LEU:O	2.16	0.45
1:C:193:LYS:O	1:C:194:LYS:CB	2.65	0.45
3:F:196:LEU:CD1	3:F:197:GLU:H	2.30	0.45
1:A:183:ASN:HA	1:A:211:GLN:HA	1.97	0.45
1:A:232:ASP:HA	1:A:259:GLY:H	1.82	0.45
1:A:289:SER:O	1:A:290:ALA:CB	2.65	0.45
1:A:601:GLN:HE22	1:A:611:ARG:HD3	1.82	0.45
1:C:127:GLY:HA2	1:C:132:GLU:O	2.16	0.45
1:C:155:GLN:HB3	1:C:195:GLU:HB3	1.99	0.45
1:C:241:ASP:C	1:C:243:ARG:N	2.65	0.45
1:C:244:ASN:C	1:C:244:ASN:HD22	2.24	0.45
1:A:169:ASN:HB3	1:A:172:LEU:O	2.16	0.45
1:A:399:GLY:O	2:B:11:LEU:HD12	2.17	0.45
1:A:536:LEU:CD2	1:C:537:MET:HE1	2.38	0.45
1:C:193:LYS:NZ	4:C:3427:HOH:O	2.46	0.45
3:F:46:ILE:CG2	3:F:47:ASP:N	2.66	0.45
3:F:224:SER:HB2	3:F:234:TRP:NE1	2.28	0.45
1:A:5:ALA:N	4:A:2426:HOH:O	2.49	0.44
1:A:212:LEU:HB3	1:A:227:THR:HG23	1.98	0.44
1:A:449:LEU:O	1:A:453:LEU:HB2	2.17	0.44
2:B:102:VAL:HG22	4:B:2353:HOH:O	2.14	0.44
2:B:127:VAL:HA	4:B:2340:HOH:O	2.15	0.44
2:B:239:GLU:HG3	4:B:2327:HOH:O	2.16	0.44
1:C:5:ALA:N	4:C:3426:HOH:O	2.49	0.44
1:C:62:ASP:OD1	1:C:62:ASP:N	2.36	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:LEU:HD21	1:C:104:PHE:HB2	1.99	0.44
1:C:162:GLU:HG3	1:C:164:ILE:HG23	1.99	0.44
1:C:412:LEU:C	1:C:412:LEU:HD23	2.42	0.44
1:A:212:LEU:HD22	1:A:227:THR:HG22	1.98	0.44
1:A:244:ASN:C	1:A:244:ASN:HD22	2.24	0.44
2:B:35:ILE:HG13	2:B:89:TRP:CE2	2.52	0.44
1:C:27:THR:O	1:C:65:PHE:HB2	2.17	0.44
1:C:129:ASN:HA	1:C:162:GLU:CB	2.47	0.44
1:C:232:ASP:O	1:C:258:LYS:HA	2.17	0.44
1:C:727:PRO:O	1:C:729:ASP:N	2.50	0.44
1:A:20:ILE:O	1:A:20:ILE:CG1	2.65	0.44
1:A:496:THR:CG2	1:A:497:ASN:N	2.81	0.44
1:A:584:LEU:N	1:A:584:LEU:CD1	2.81	0.44
1:C:63:SER:HB3	1:C:82:ASP:HB2	1.98	0.44
1:C:365:LYS:HZ3	1:C:371:LEU:HD22	1.80	0.44
3:F:24:MET:CG	3:F:25:ALA:N	2.60	0.44
1:A:75:LYS:NZ	1:A:94:ALA:CB	2.80	0.44
1:A:197:ILE:HG22	1:A:198:HIS:N	2.32	0.44
1:A:538:GLU:O	1:A:539:ALA:C	2.60	0.44
2:B:105:VAL:HG22	2:B:116:LEU:HD11	1.99	0.44
2:B:181:LEU:CD2	2:B:201:GLU:HG2	2.47	0.44
1:C:66:ASN:HD22	1:C:66:ASN:HA	1.64	0.44
1:C:116:PHE:CE1	1:C:124:LEU:HD13	2.53	0.44
1:A:63:SER:HB3	1:A:82:ASP:HB2	1.98	0.44
1:A:242:LEU:N	1:A:242:LEU:HD23	2.33	0.44
1:A:299:ARG:HA	1:A:299:ARG:HD2	1.86	0.44
1:A:379:GLU:HG2	2:B:258:TRP:CZ2	2.53	0.44
2:B:213:SER:HB2	2:B:262:TRP:CE2	2.53	0.44
1:C:314:ASP:CG	1:C:376:TRP:NE1	2.76	0.44
1:A:15:TRP:CH2	1:A:317:ALA:HB2	2.52	0.44
1:A:155:GLN:HB3	1:A:195:GLU:HB3	1.99	0.44
1:A:232:ASP:HA	1:A:259:GLY:N	2.33	0.44
1:A:504:PHE:CE2	1:C:588:LEU:HD13	2.53	0.44
1:A:511:GLU:HG2	1:C:569:LEU:HB2	1.99	0.44
2:B:4:ILE:HG21	2:B:36:PHE:CE2	2.52	0.44
1:C:151:LEU:CD1	1:C:152:THR:H	2.25	0.44
1:C:242:LEU:N	1:C:242:LEU:HD23	2.33	0.44
1:C:665:THR:CG2	3:F:285:LEU:N	2.80	0.44
1:A:119:LYS:CB	1:A:173:ALA:HB2	2.41	0.44
1:A:133:ILE:HD11	1:A:163:VAL:CG2	2.41	0.44
1:C:162:GLU:HG3	1:C:164:ILE:CG2	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:ILE:HG22	1:C:198:HIS:N	2.32	0.44
3:F:3:VAL:C	3:F:4:ILE:HD12	2.42	0.44
1:A:88:LEU:CD1	1:A:138:MET:SD	3.06	0.44
1:A:129:ASN:HA	1:A:162:GLU:CB	2.47	0.44
1:A:162:GLU:HG3	1:A:164:ILE:CG2	2.48	0.44
1:A:252:LEU:HD13	1:A:285:TRP:CD2	2.53	0.44
2:B:14:ASP:HB3	2:B:27:CYS:SG	2.58	0.44
2:B:30:ASP:OD1	2:B:32:THR:HG23	2.17	0.44
2:B:85:GLU:O	2:B:86:ASN:HB2	2.18	0.44
1:C:42:LEU:O	1:C:42:LEU:HG	2.18	0.44
1:C:543:ALA:C	1:C:545:ASP:H	2.25	0.44
1:C:155:GLN:HB2	1:C:195:GLU:HB3	1.99	0.44
1:C:312:ALA:N	1:C:313:PRO:CD	2.80	0.44
1:C:677:PHE:HD2	1:C:678:ILE:HD12	1.83	0.44
3:F:38:VAL:HA	3:F:42:THR:O	2.18	0.44
1:A:604:TYR:N	1:A:605:PRO:CD	2.81	0.43
1:A:688:ILE:CG1	1:A:689:ASN:H	2.31	0.43
2:B:63:HIS:CE1	2:B:65:LYS:HB3	2.53	0.43
2:B:191:ALA:HB1	2:B:193:THR:HG22	1.99	0.43
2:B:238:ASN:HD22	2:B:238:ASN:C	2.26	0.43
1:C:74:ASN:N	1:C:74:ASN:ND2	2.50	0.43
1:C:152:THR:HA	1:C:153:PRO:HD3	1.81	0.43
1:C:232:ASP:HA	1:C:259:GLY:H	1.83	0.43
1:C:232:ASP:HA	1:C:259:GLY:N	2.33	0.43
1:C:551:LEU:C	1:C:553:GLU:N	2.76	0.43
3:F:72:SER:O	3:F:79:VAL:HA	2.17	0.43
1:A:204:PRO:HG2	1:A:208:ILE:O	2.18	0.43
1:A:706:PHE:CB	4:A:3200:HOH:O	2.66	0.43
1:C:236:SER:C	1:C:237:ILE:HD12	2.44	0.43
1:C:519:VAL:O	1:C:521:GLY:N	2.51	0.43
1:A:24:VAL:CG2	1:A:70:TRP:CZ3	3.01	0.43
1:A:438:VAL:CG2	1:A:439:ILE:N	2.81	0.43
1:C:22:LEU:HD21	1:C:95:ASN:ND2	2.34	0.43
1:C:67:ASP:OD2	1:C:113:THR:HG23	2.18	0.43
1:C:72:HIS:HE1	1:C:118:ALA:HA	1.72	0.43
1:C:74:ASN:O	1:C:75:LYS:C	2.61	0.43
1:C:289:SER:O	1:C:290:ALA:CB	2.65	0.43
3:F:52:HIS:ND1	3:F:74:SER:CB	2.81	0.43
1:A:223:THR:O	1:A:241:ASP:HA	2.19	0.43
2:B:25:ALA:HB2	2:B:61:TRP:HZ2	1.81	0.43
2:B:152:SER:OG	2:B:210:VAL:O	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:281:TRP:CD1	2:B:281:TRP:N	2.87	0.43
1:C:201:TYR:CD2	1:C:238:LEU:HD11	2.54	0.43
1:A:42:LEU:O	1:A:42:LEU:HG	2.18	0.43
1:A:66:ASN:HD22	1:A:66:ASN:HA	1.64	0.43
1:A:201:TYR:CD2	1:A:238:LEU:HD11	2.54	0.43
1:A:312:ALA:N	1:A:313:PRO:CD	2.80	0.43
2:B:64:PRO:HD2	4:B:2334:HOH:O	2.17	0.43
2:B:74:SER:C	2:B:76:ASP:H	2.26	0.43
1:C:20:ILE:O	1:C:20:ILE:CG1	2.65	0.43
1:C:88:LEU:CD1	1:C:138:MET:SD	3.06	0.43
1:C:299:ARG:HA	1:C:299:ARG:HD2	1.86	0.43
1:C:571:ARG:O	1:C:574:TYR:HB3	2.19	0.43
1:C:636:LEU:HD12	1:C:688:ILE:CD1	2.48	0.43
2:B:46:ILE:O	2:B:46:ILE:HG22	2.19	0.43
1:C:24:VAL:CG2	1:C:70:TRP:CZ3	3.01	0.43
1:C:252:LEU:HD13	1:C:285:TRP:CD2	2.53	0.43
1:C:608:ILE:HD13	1:C:611:ARG:NH1	2.33	0.43
3:F:63:HIS:HB3	3:F:66:PHE:CE1	2.53	0.43
3:F:213:SER:OG	3:F:214:PRO:HD2	2.18	0.43
3:F:219:ARG:CG	3:F:221:TYR:CE1	3.02	0.43
1:A:27:THR:O	1:A:65:PHE:HB2	2.17	0.43
1:A:204:PRO:HG3	1:A:210:GLN:HG3	2.00	0.43
1:A:314:ASP:CB	1:A:376:TRP:CZ2	3.02	0.43
1:A:429:PRO:HD2	4:A:3159:HOH:O	2.19	0.43
2:B:107:TRP:CH2	2:B:130:PHE:HE2	2.37	0.43
1:C:551:LEU:C	1:C:553:GLU:H	2.27	0.43
3:F:109:PRO:O	3:F:110:HIS:C	2.61	0.43
1:A:116:PHE:CE1	1:A:124:LEU:HD13	2.53	0.43
1:A:196:VAL:O	1:A:197:ILE:HG13	2.19	0.43
1:C:695:ASN:ND2	4:C:2100:HOH:O	2.52	0.43
3:F:39:GLU:HB2	3:F:42:THR:OG1	2.18	0.43
3:F:184:ILE:O	3:F:196:LEU:HD12	2.18	0.43
3:F:201:GLU:O	3:F:234:TRP:HH2	2.02	0.43
3:F:257:LEU:HD23	3:F:257:LEU:HA	1.80	0.43
3:F:259:ARG:HG3	3:F:259:ARG:NH1	2.33	0.43
1:A:109:SER:O	1:A:110:SER:CB	2.61	0.43
1:A:423:LYS:HG3	1:A:424:THR:N	2.32	0.43
1:A:549:GLU:HA	1:A:552:LYS:HB3	2.01	0.43
2:B:112:TYR:N	2:B:112:TYR:CD1	2.86	0.43
1:C:424:THR:O	1:C:425:LYS:HB3	2.19	0.43
3:F:26:THR:O	3:F:33:ILE:HA	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:233:ILE:HG21	3:F:289:TRP:HZ2	1.82	0.43
1:A:67:ASP:OD2	1:A:113:THR:HG23	2.18	0.43
1:A:86:LEU:HD21	1:A:104:PHE:HB2	1.99	0.43
1:A:152:THR:HA	1:A:153:PRO:HD3	1.81	0.43
1:A:314:ASP:CG	1:A:376:TRP:CZ2	2.87	0.43
2:B:226:SER:HB3	2:B:228:ASP:OD1	2.19	0.43
1:C:211:GLN:O	1:C:229:THR:HA	2.19	0.43
1:A:74:ASN:O	1:A:75:LYS:C	2.61	0.42
1:A:236:SER:C	1:A:237:ILE:HD12	2.44	0.42
1:A:330:LEU:HD12	1:A:330:LEU:HA	1.87	0.42
1:A:537:MET:HE1	1:C:536:LEU:CG	2.48	0.42
1:A:639:GLY:C	1:A:688:ILE:HD11	2.44	0.42
2:B:63:HIS:CD2	2:B:110:HIS:HB3	2.54	0.42
1:C:41:SER:O	1:C:42:LEU:CB	2.67	0.42
1:C:204:PRO:HG2	1:C:208:ILE:O	2.18	0.42
1:C:531:LEU:C	1:C:533:ASN:N	2.77	0.42
1:A:22:LEU:HD21	1:A:95:ASN:ND2	2.33	0.42
1:A:187:ILE:HD13	1:A:187:ILE:HA	1.88	0.42
2:B:227:GLN:HA	2:B:256:VAL:HG13	2.01	0.42
1:C:144:SER:C	1:C:146:SER:N	2.78	0.42
1:C:313:PRO:HG2	1:C:376:TRP:NE1	2.34	0.42
1:C:420:GLU:HA	1:C:423:LYS:HD3	2.01	0.42
1:A:302:TRP:CD1	1:A:321:PHE:CD1	3.07	0.42
1:A:500:PRO:O	1:A:501:GLU:HG2	2.20	0.42
2:B:30:ASP:OD1	2:B:32:THR:OG1	2.36	0.42
1:C:72:HIS:C	1:C:74:ASN:H	2.27	0.42
1:C:223:THR:O	1:C:241:ASP:HA	2.19	0.42
3:F:23:ARG:HD3	3:F:61:TRP:CH2	2.54	0.42
2:B:16:VAL:HG12	2:B:61:TRP:HD1	1.85	0.42
1:C:412:LEU:HD21	1:C:713:THR:HG22	2.01	0.42
1:C:420:GLU:HA	1:C:423:LYS:CD	2.50	0.42
3:F:233:ILE:HD11	3:F:248:LEU:CD1	2.48	0.42
1:A:7:PHE:CD1	1:A:7:PHE:N	2.87	0.42
1:A:144:SER:C	1:A:146:SER:N	2.77	0.42
1:A:388:PHE:CE2	1:A:716:PHE:HE2	2.37	0.42
2:B:4:ILE:N	2:B:4:ILE:CD1	2.83	0.42
1:C:458:THR:HG23	1:C:459:GLU:N	2.30	0.42
1:C:639:GLY:HA2	1:C:688:ILE:CD1	2.47	0.42
3:F:62:ALA:HB2	3:F:107:TRP:CE2	2.55	0.42
3:F:231:CYS:HB2	3:F:271:LEU:HD21	2.00	0.42
1:A:15:TRP:HZ3	1:A:317:ALA:H	1.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:HIS:C	1:A:74:ASN:H	2.28	0.42
1:A:497:ASN:OD1	1:A:498:PHE:N	2.53	0.42
1:C:29:SER:OG	1:C:66:ASN:ND2	2.53	0.42
1:C:70:TRP:O	1:C:71:SER:C	2.63	0.42
1:C:196:VAL:O	1:C:197:ILE:HG13	2.19	0.42
1:C:302:TRP:CD1	1:C:321:PHE:CD1	3.07	0.42
1:C:379:GLU:HB3	3:F:258:TRP:CZ2	2.54	0.42
3:F:3:VAL:HG12	3:F:5:ALA:N	2.34	0.42
1:A:29:SER:OG	1:A:66:ASN:ND2	2.53	0.42
1:A:399:GLY:HA3	2:B:11:LEU:CD1	2.49	0.42
1:A:422:LEU:CD2	1:A:721:GLU:HG2	2.49	0.42
2:B:238:ASN:ND2	2:B:240:GLN:H	2.14	0.42
1:C:493:GLN:HG3	1:C:494:ILE:N	2.35	0.42
3:F:33:ILE:HD13	3:F:72:SER:HB3	2.02	0.42
1:A:59:LEU:O	1:A:60:GLN:C	2.62	0.42
1:A:215:VAL:HA	1:A:226:ALA:O	2.20	0.42
1:A:420:GLU:O	1:A:423:LYS:HG2	2.20	0.42
2:B:49:LEU:HA	4:B:2355:HOH:O	2.20	0.42
2:B:233:ILE:HD12	2:B:233:ILE:N	2.35	0.42
1:C:6:GLU:OE2	1:C:324:LYS:HB2	2.20	0.42
3:F:68:THR:HG22	3:F:89:TRP:CH2	2.54	0.42
3:F:105:VAL:HG21	3:F:116:LEU:HD21	2.02	0.42
1:A:9:ARG:O	1:A:10:THR:C	2.63	0.42
1:A:193:LYS:NZ	4:A:2427:HOH:O	2.46	0.42
1:A:434:ARG:HG3	1:A:447:TRP:CH2	2.55	0.42
1:A:556:LYS:C	1:A:558:ALA:N	2.78	0.42
1:A:563:TYR:C	1:A:565:SER:N	2.77	0.42
1:C:9:ARG:HB3	1:C:10:THR:H	1.65	0.42
1:C:59:LEU:O	1:C:60:GLN:C	2.62	0.42
3:F:60:ASP:O	3:F:107:TRP:NE1	2.52	0.42
3:F:247:LEU:C	3:F:249:LYS:H	2.27	0.42
1:A:6:GLU:OE2	1:A:324:LYS:HB2	2.20	0.42
1:A:70:TRP:O	1:A:71:SER:C	2.63	0.42
1:A:301:ASN:N	1:A:322:ASP:OD2	2.51	0.42
1:A:447:TRP:O	1:A:451:GLU:N	2.53	0.42
1:A:519:VAL:O	1:A:521:GLY:N	2.52	0.42
1:C:204:PRO:HG3	1:C:210:GLN:HG3	2.00	0.42
1:C:247:THR:HG23	1:C:248:PRO:HD2	2.02	0.42
1:C:261:LEU:N	1:C:277:GLY:HA2	2.35	0.42
1:C:438:VAL:HG21	1:C:444:GLU:CA	2.50	0.42
3:F:232:ILE:HG21	3:F:234:TRP:CZ2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:262:TRP:CE3	3:F:262:TRP:HA	2.55	0.42
1:A:202:THR:O	1:A:202:THR:CG2	2.67	0.41
1:A:204:PRO:C	1:A:205:ASN:CG	2.88	0.41
1:A:268:GLN:CA	1:A:374:PRO:O	2.63	0.41
1:A:431:ILE:HG21	1:A:451:GLU:HA	2.02	0.41
1:A:458:THR:CG2	1:A:459:GLU:N	2.81	0.41
1:A:644:VAL:HG21	1:A:684:PHE:CZ	2.55	0.41
1:A:706:PHE:HB2	4:A:3200:HOH:O	2.19	0.41
2:B:225:VAL:CG1	2:B:257:LEU:O	2.69	0.41
1:C:31:THR:OG1	1:C:321:PHE:HD2	2.03	0.41
1:C:590:VAL:HG13	1:C:622:LEU:HD22	1.99	0.41
1:C:646:SER:O	1:C:647:ILE:C	2.62	0.41
1:A:16:SER:HB2	1:A:17:HIS:H	1.70	0.41
1:A:27:THR:HB	1:A:40:SER:HB2	2.01	0.41
1:A:211:GLN:O	1:A:229:THR:HA	2.19	0.41
1:A:237:ILE:HD12	1:A:237:ILE:N	2.35	0.41
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.69	0.41
1:A:694:ILE:HG23	1:A:699:LEU:HD23	2.02	0.41
1:C:271:HIS:HB3	1:C:286:ASN:OD1	2.21	0.41
1:C:739:ARG:CD	3:F:19:TYR:CE2	2.71	0.41
3:F:49:LEU:HD22	3:F:82:TRP:CG	2.54	0.41
1:A:9:ARG:HA	1:A:324:LYS:HA	2.02	0.41
1:A:75:LYS:HZ2	1:A:94:ALA:N	2.15	0.41
1:A:247:THR:HG23	1:A:248:PRO:HD2	2.02	0.41
1:A:733:VAL:HG13	4:A:3255:HOH:O	2.19	0.41
2:B:52:HIS:CD2	2:B:56:VAL:HG22	2.55	0.41
1:C:468:PHE:O	1:C:469:ASP:C	2.62	0.41
1:C:510:ILE:O	1:C:511:GLU:C	2.63	0.41
1:C:596:ILE:O	1:C:597:SER:C	2.63	0.41
3:F:102:VAL:HG22	3:F:120:SER:HB2	2.02	0.41
1:A:31:THR:OG1	1:A:321:PHE:HD2	2.03	0.41
1:A:125:ALA:HB2	1:A:168:TRP:CZ3	2.53	0.41
1:A:412:LEU:HD23	1:A:413:GLU:N	2.36	0.41
1:A:598:LYS:O	1:A:602:ASN:HB2	2.20	0.41
1:A:653:PRO:O	1:A:656:GLU:N	2.54	0.41
1:C:215:VAL:HA	1:C:226:ALA:O	2.20	0.41
1:C:447:TRP:CE3	1:C:450:LEU:HD12	2.55	0.41
3:F:112:TYR:HA	3:F:171:ARG:NH2	2.36	0.41
1:A:430:LEU:C	1:A:430:LEU:CD2	2.94	0.41
1:A:439:ILE:HG13	1:A:440:ASP:H	1.85	0.41
1:A:610:GLN:HA	1:A:610:GLN:OE1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:ASP:C	1:C:281:THR:H	2.29	0.41
1:C:592:GLN:NE2	4:C:2229:HOH:O	2.53	0.41
3:F:194:TYR:CD1	3:F:194:TYR:N	2.88	0.41
1:A:252:LEU:HB3	1:A:285:TRP:CE3	2.55	0.41
1:A:300:GLY:O	1:A:301:ASN:CB	2.59	0.41
1:A:404:ILE:N	1:A:404:ILE:HD12	2.34	0.41
1:A:497:ASN:O	1:A:498:PHE:HB3	2.20	0.41
2:B:213:SER:HB2	2:B:262:TRP:CD2	2.55	0.41
1:C:9:ARG:HA	1:C:324:LYS:HA	2.01	0.41
1:C:272:LEU:HD23	1:C:272:LEU:HA	1.81	0.41
1:A:261:LEU:N	1:A:277:GLY:HA2	2.35	0.41
1:A:271:HIS:HB3	1:A:286:ASN:OD1	2.20	0.41
1:A:608:ILE:HA	1:A:611:ARG:NH1	2.34	0.41
2:B:205:ASP:O	2:B:206:TRP:C	2.62	0.41
2:B:238:ASN:HB2	4:B:2327:HOH:O	2.20	0.41
1:C:9:ARG:O	1:C:10:THR:C	2.63	0.41
1:C:117:ASN:HD22	1:C:117:ASN:C	2.17	0.41
1:C:202:THR:O	1:C:202:THR:CG2	2.67	0.41
1:C:252:LEU:HB3	1:C:285:TRP:CE3	2.55	0.41
1:C:400:LYS:C	3:F:12:ILE:HD11	2.45	0.41
1:A:444:GLU:HG2	1:A:448:ASN:ND2	2.36	0.41
2:B:121:SER:CA	4:B:2338:HOH:O	2.68	0.41
1:C:125:ALA:CB	1:C:168:TRP:CH2	2.92	0.41
1:C:365:LYS:O	1:C:366:PRO:C	2.64	0.41
3:F:10:GLU:HG3	3:F:30:ASP:CA	2.51	0.41
3:F:213:SER:OG	3:F:215:THR:HG22	2.20	0.41
1:A:96:ASN:O	1:A:97:ALA:HB2	2.21	0.41
1:A:127:GLY:HA3	1:A:163:VAL:HB	2.03	0.41
1:A:217:TRP:CE3	1:A:225:VAL:HG22	2.56	0.41
1:A:537:MET:CE	1:C:536:LEU:HD23	2.48	0.41
1:A:581:VAL:O	1:A:582:ASP:C	2.63	0.41
1:A:704:LEU:O	1:A:707:ILE:HB	2.21	0.41
2:B:46:ILE:O	2:B:47:ASP:HB2	2.21	0.41
2:B:120:SER:C	2:B:122:ASP:H	2.29	0.41
2:B:282:LYS:HB3	2:B:292:ALA:HB2	2.02	0.41
1:C:15:TRP:HZ3	1:C:317:ALA:H	1.67	0.41
1:C:27:THR:HB	1:C:40:SER:HB2	2.01	0.41
1:C:48:LEU:O	1:C:49:ALA:C	2.64	0.41
1:C:96:ASN:O	1:C:97:ALA:HB2	2.21	0.41
1:C:144:SER:C	1:C:146:SER:H	2.28	0.41
1:C:214:VAL:HB	1:C:228:ALA:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:TRP:CE3	1:C:225:VAL:HG22	2.56	0.41
1:C:237:ILE:HD12	1:C:237:ILE:N	2.35	0.41
1:C:331:GLN:NE2	3:F:75:TYR:CZ	2.88	0.41
1:C:572:ILE:HG22	1:C:573:LEU:N	2.35	0.41
1:C:643:LYS:O	1:C:647:ILE:HG12	2.21	0.41
3:F:152:SER:O	3:F:173:PHE:HB2	2.21	0.41
3:F:227:GLN:C	3:F:229:ARG:H	2.27	0.41
1:A:48:LEU:O	1:A:49:ALA:C	2.64	0.41
1:A:119:LYS:NZ	1:A:171:SER:O	2.54	0.41
1:A:421:ALA:O	1:A:425:LYS:HA	2.21	0.41
1:A:541:VAL:HG23	1:C:540:MET:HE1	2.03	0.41
2:B:145:ALA:O	2:B:147:GLY:N	2.50	0.41
1:C:119:LYS:CB	1:C:173:ALA:HB2	2.41	0.41
3:F:4:ILE:HG13	3:F:43:HIS:HB3	2.03	0.41
3:F:30:ASP:O	3:F:31:LYS:HB2	2.21	0.41
3:F:35:ILE:HG13	3:F:89:TRP:NE1	2.35	0.41
1:A:365:LYS:O	1:A:366:PRO:C	2.64	0.40
2:B:17:LEU:HD23	2:B:24:LEU:HA	2.03	0.40
1:C:7:PHE:CD1	1:C:7:PHE:N	2.87	0.40
1:C:7:PHE:HB2	1:C:8:SER:H	1.51	0.40
1:C:113:THR:CG2	1:C:114:VAL:N	2.84	0.40
1:C:589:ASP:C	1:C:591:SER:N	2.80	0.40
3:F:27:CYS:HB3	3:F:33:ILE:HG23	2.02	0.40
3:F:59:VAL:HG12	3:F:72:SER:CA	2.50	0.40
1:A:84:GLY:HA2	1:A:111:VAL:HG23	2.03	0.40
1:A:229:THR:HG22	1:A:230:GLY:N	2.35	0.40
1:A:614:MET:HA	1:A:614:MET:HE2	2.03	0.40
2:B:225:VAL:CG2	2:B:271:LEU:HD11	2.50	0.40
1:C:133:ILE:HD11	1:C:163:VAL:CG2	2.41	0.40
1:C:203:SER:O	1:C:204:PRO:C	2.64	0.40
1:C:314:ASP:N	1:C:376:TRP:HE1	2.20	0.40
1:A:578:LYS:HD3	1:A:580:GLU:OE2	2.21	0.40
1:A:592:GLN:O	1:A:595:PHE:HB3	2.21	0.40
2:B:17:LEU:HB3	2:B:21:GLY:HA2	2.03	0.40
1:C:15:TRP:HH2	1:C:316:PHE:C	2.29	0.40
1:C:652:PHE:CE2	1:C:702:LYS:HE2	2.56	0.40
1:C:702:LYS:HA	1:C:705:GLU:HB2	2.03	0.40
1:C:730:ASN:C	1:C:732:GLU:N	2.79	0.40
3:F:206:TRP:O	3:F:226:SER:OG	2.23	0.40
3:F:224:SER:O	3:F:231:CYS:HA	2.21	0.40
1:A:279:ASP:C	1:A:281:THR:H	2.29	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:ALA:O	1:A:388:PHE:C	2.65	0.40
2:B:155:PRO:CG	2:B:214:PRO:HA	2.49	0.40
1:C:400:LYS:HA	3:F:12:ILE:HG13	2.04	0.40
1:C:423:LYS:HG2	1:C:424:THR:H	1.86	0.40
3:F:83:LYS:CG	3:F:92:ILE:HG21	2.45	0.40
1:A:116:PHE:CD1	1:A:124:LEU:HD13	2.57	0.40
1:A:216:GLU:OE1	1:A:217:TRP:N	2.55	0.40
1:A:301:ASN:O	1:A:302:TRP:CB	2.70	0.40
1:A:396:THR:HB	1:A:398:ASP:OD2	2.21	0.40
1:A:727:PRO:O	1:A:729:ASP:N	2.54	0.40
2:B:2:VAL:HG13	2:B:41:GLU:HA	2.03	0.40
2:B:81:ILE:HD13	2:B:93:ALA:CB	2.40	0.40
2:B:143:ALA:O	2:B:144:HIS:CG	2.75	0.40
1:C:84:GLY:HA2	1:C:111:VAL:HG23	2.03	0.40
1:C:229:THR:HG22	1:C:230:GLY:N	2.35	0.40
1:C:289:SER:HG	1:C:291:GLU:HG3	1.86	0.40
1:C:535:LEU:CD2	1:C:538:GLU:HG3	2.52	0.40
3:F:105:VAL:HG13	3:F:105:VAL:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	681/1273 (54%)	519 (76%)	106 (16%)	56 (8%)	0	9
1	C	683/1273 (54%)	532 (78%)	97 (14%)	54 (8%)	1	10
2	B	275/297 (93%)	241 (88%)	30 (11%)	4 (2%)	8	40
3	F	276/297 (93%)	214 (78%)	37 (13%)	25 (9%)	0	8
All	All	1915/3140 (61%)	1506 (79%)	270 (14%)	139 (7%)	1	10

All (139) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	49	ALA
1	A	74	ASN
1	A	110	SER
1	A	143	GLU
1	A	146	SER
1	A	147	ASN
1	A	159	SER
1	A	203	SER
1	A	242	LEU
1	A	290	ALA
1	A	301	ASN
1	A	313	PRO
1	A	335	ASN
1	A	336	THR
1	A	365	LYS
1	A	369	PHE
1	A	497	ASN
2	B	131	LYS
1	C	33	ASP
1	C	49	ALA
1	C	74	ASN
1	C	110	SER
1	C	143	GLU
1	C	146	SER
1	C	147	ASN
1	C	159	SER
1	C	203	SER
1	C	242	LEU
1	C	290	ALA
1	C	301	ASN
1	C	313	PRO
1	C	335	ASN
1	C	336	THR
1	C	365	LYS
1	C	369	PHE
1	C	715	ASN
3	F	76	ASP
3	F	100	ALA
3	F	131	LYS
1	A	10	THR
1	A	84	GLY
1	A	105	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	160	VAL
1	A	194	LYS
1	A	238	LEU
1	A	266	CYS
1	A	322	ASP
1	A	332	ASN
1	A	337	LEU
1	A	388	PHE
1	A	425	LYS
1	A	518	LEU
2	B	135	THR
1	C	10	THR
1	C	84	GLY
1	C	105	SER
1	C	160	VAL
1	C	194	LYS
1	C	238	LEU
1	C	266	CYS
1	C	322	ASP
1	C	332	ASN
1	C	337	LEU
1	C	425	LYS
3	F	30	ASP
3	F	41	GLU
3	F	133	ASN
3	F	241	GLY
3	F	254	PRO
3	F	256	VAL
3	F	273	GLY
1	A	16	SER
1	A	52	SER
1	A	60	GLN
1	A	93	GLU
1	A	121	ASP
1	A	148	TYR
1	A	153	PRO
1	A	204	PRO
1	A	299	ARG
1	A	363	LYS
1	A	520	SER
1	A	728	SER
2	B	190	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	16	SER
1	C	52	SER
1	C	60	GLN
1	C	93	GLU
1	C	121	ASP
1	C	153	PRO
1	C	204	PRO
1	C	299	ARG
1	C	363	LYS
1	C	439	ILE
1	C	552	LYS
1	C	728	SER
3	F	40	GLY
3	F	47	ASP
3	F	101	SER
3	F	145	ALA
3	F	240	GLN
3	F	291	PRO
1	A	91	THR
1	A	302	TRP
1	A	368	VAL
1	A	439	ILE
1	A	498	PHE
1	A	561	ALA
2	B	202	GLY
1	C	91	THR
1	C	148	TYR
1	C	302	TRP
1	C	368	VAL
1	C	407	PRO
3	F	46	ILE
3	F	218	LEU
3	F	267	ASN
3	F	274	GLY
1	A	9	ARG
1	A	94	ALA
1	A	109	SER
1	A	207	GLY
1	A	548	ASN
1	A	653	PRO
1	C	9	ARG
1	C	94	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	109	SER
1	C	207	GLY
1	C	520	SER
1	C	662	ASP
3	F	51	GLY
3	F	170	SER
3	F	187	TYR
3	F	21	GLY
3	F	287	GLY
1	A	287	PRO
1	C	287	PRO
1	C	494	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	608/1113 (55%)	562 (92%)	46 (8%)	12	33
1	C	610/1113 (55%)	558 (92%)	52 (8%)	10	29
2	B	237/252 (94%)	230 (97%)	7 (3%)	36	57
3	F	238/252 (94%)	215 (90%)	23 (10%)	8	24
All	All	1693/2730 (62%)	1565 (92%)	128 (8%)	14	33

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	PHE
1	A	10	THR
1	A	15	TRP
1	A	18	ASP
1	A	20	ILE
1	A	51	ASP
1	A	61	VAL
1	A	62	ASP
1	A	66	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	73	ASN
1	A	74	ASN
1	A	91	THR
1	A	98	ILE
1	A	104	PHE
1	A	106	ASN
1	A	133	ILE
1	A	136	TRP
1	A	156	SER
1	A	168	TRP
1	A	170	GLN
1	A	183	ASN
1	A	198	HIS
1	A	204	PRO
1	A	216	GLU
1	A	223	THR
1	A	227	THR
1	A	232	ASP
1	A	243	ARG
1	A	260	ILE
1	A	261	LEU
1	A	266	CYS
1	A	268	GLN
1	A	281	THR
1	A	304	PHE
1	A	325	ILE
1	A	327	VAL
1	A	334	THR
1	A	336	THR
1	A	430	LEU
1	A	509	ASN
1	A	537	MET
1	A	545	ASP
1	A	572	ILE
1	A	688	ILE
1	A	703	PHE
1	A	720	THR
2	B	50	THR
2	B	92	ILE
2	B	180	ASN
2	B	204	SER
2	B	225	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	238	ASN
2	B	242	PRO
1	C	7	PHE
1	C	10	THR
1	C	15	TRP
1	C	18	ASP
1	C	20	ILE
1	C	51	ASP
1	C	61	VAL
1	C	62	ASP
1	C	66	ASN
1	C	73	ASN
1	C	74	ASN
1	C	91	THR
1	C	98	ILE
1	C	104	PHE
1	C	106	ASN
1	C	133	ILE
1	C	136	TRP
1	C	156	SER
1	C	168	TRP
1	C	170	GLN
1	C	183	ASN
1	C	198	HIS
1	C	204	PRO
1	C	216	GLU
1	C	223	THR
1	C	227	THR
1	C	232	ASP
1	C	243	ARG
1	C	260	ILE
1	C	261	LEU
1	C	266	CYS
1	C	268	GLN
1	C	281	THR
1	C	304	PHE
1	C	325	ILE
1	C	327	VAL
1	C	334	THR
1	C	336	THR
1	C	377	TYR
1	C	381	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	407	PRO
1	C	408	LYS
1	C	413	GLU
1	C	432	ASN
1	C	509	ASN
1	C	510	ILE
1	C	538	GLU
1	C	545	ASP
1	C	572	ILE
1	C	590	VAL
1	C	629	GLN
1	C	655	LEU
3	F	33	ILE
3	F	38	VAL
3	F	43	HIS
3	F	46	ILE
3	F	66	PHE
3	F	81	ILE
3	F	82	TRP
3	F	122	ASP
3	F	129	GLU
3	F	132	GLU
3	F	133	ASN
3	F	141	ILE
3	F	148	VAL
3	F	180	ASN
3	F	199	THR
3	F	200	LEU
3	F	206	TRP
3	F	225	VAL
3	F	233	ILE
3	F	237	ASP
3	F	247	LEU
3	F	255	ASP
3	F	286	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	66	ASN
1	A	72	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	73	ASN
1	A	74	ASN
1	A	96	ASN
1	A	99	ASN
1	A	106	ASN
1	A	117	ASN
1	A	129	ASN
1	A	130	ASN
1	A	139	ASN
1	A	147	ASN
1	A	210	GLN
1	A	221	ASN
1	A	244	ASN
1	A	246	ASN
1	A	250	GLN
1	A	268	GLN
1	A	271	HIS
1	A	292	GLN
1	A	301	ASN
1	A	370	HIS
1	A	372	GLN
1	A	433	GLN
1	A	443	ASN
1	A	448	ASN
1	A	509	ASN
1	A	512	GLN
1	A	517	ASN
1	A	529	ASN
1	A	592	GLN
1	A	601	GLN
1	A	612	ASN
2	B	91	GLN
2	B	95	HIS
2	B	149	ASN
2	B	180	ASN
2	B	238	ASN
2	B	240	GLN
1	C	35	ASN
1	C	66	ASN
1	C	72	HIS
1	C	73	ASN
1	C	74	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	96	ASN
1	C	99	ASN
1	C	106	ASN
1	C	117	ASN
1	C	129	ASN
1	C	130	ASN
1	C	139	ASN
1	C	147	ASN
1	C	210	GLN
1	C	221	ASN
1	C	244	ASN
1	C	246	ASN
1	C	250	GLN
1	C	268	GLN
1	C	292	GLN
1	C	301	ASN
1	C	372	GLN
1	C	443	ASN
1	C	448	ASN
1	C	493	GLN
1	C	509	ASN
1	C	512	GLN
1	C	517	ASN
1	C	557	ASN
1	C	601	GLN
1	C	602	ASN
1	C	606	ASN
1	C	670	HIS
1	C	686	ASN
3	F	86	ASN
3	F	149	ASN
3	F	180	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	372:GLN	C	373:ALA	N	16.58
1	C	372:GLN	C	373:ALA	N	16.33

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2431. These allow visual inspection of the internal detail of the map and identification of artifacts.

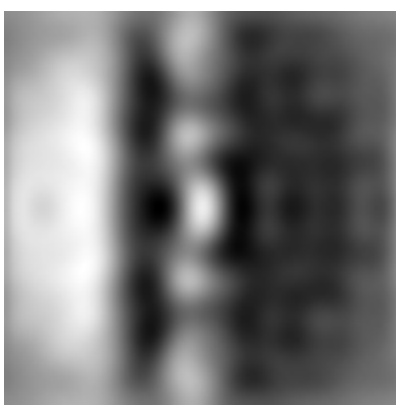
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y



Z

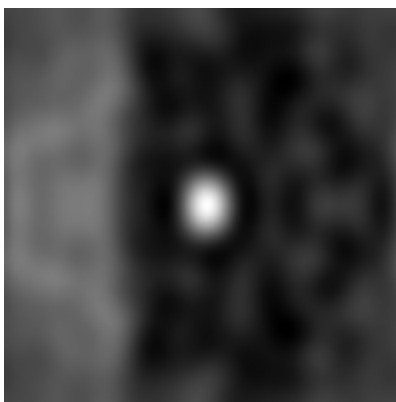
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

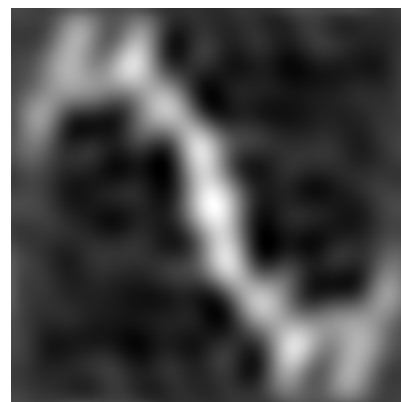
6.2.1 Primary map



X Index: 36



Y Index: 36



Z Index: 36

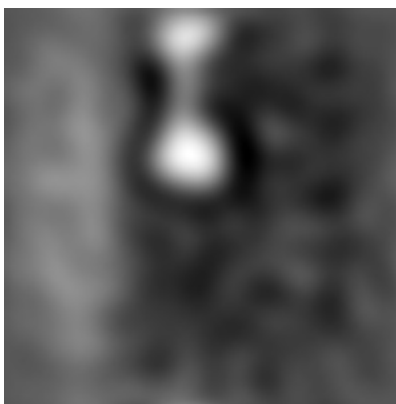
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

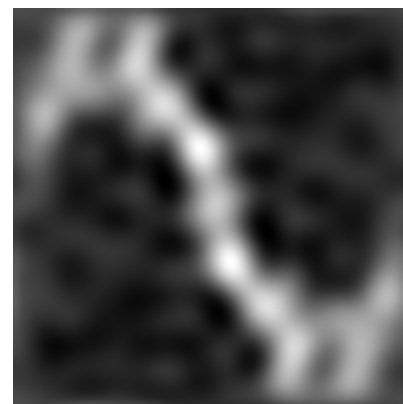
6.3.1 Primary map



X Index: 36



Y Index: 19

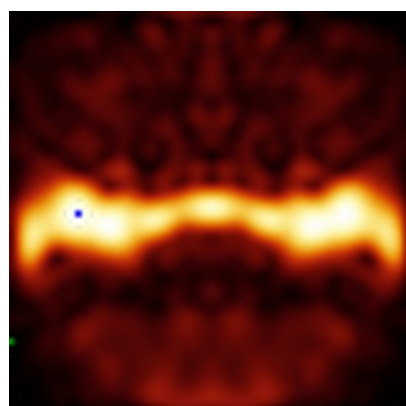


Z Index: 34

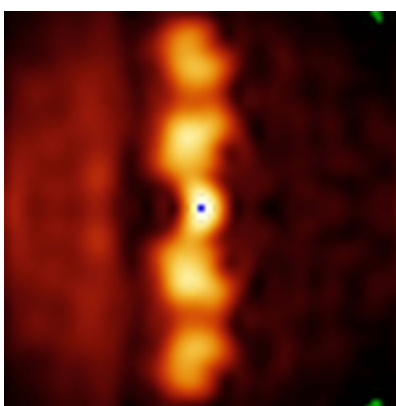
The images above show the largest variance slices of the map in three orthogonal directions.

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

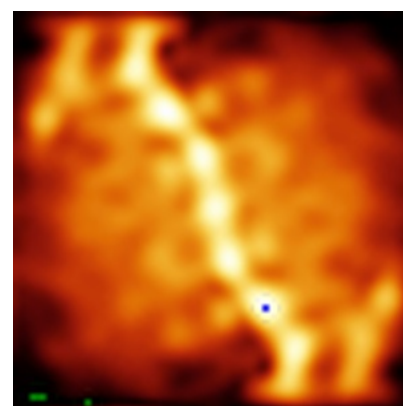
6.4.1 Primary map



X



Y

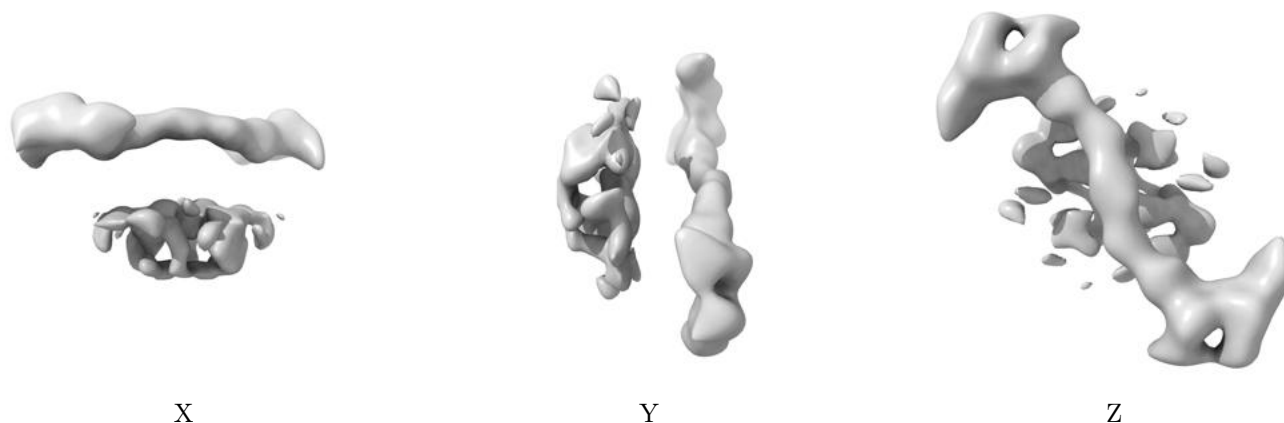


Z

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 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

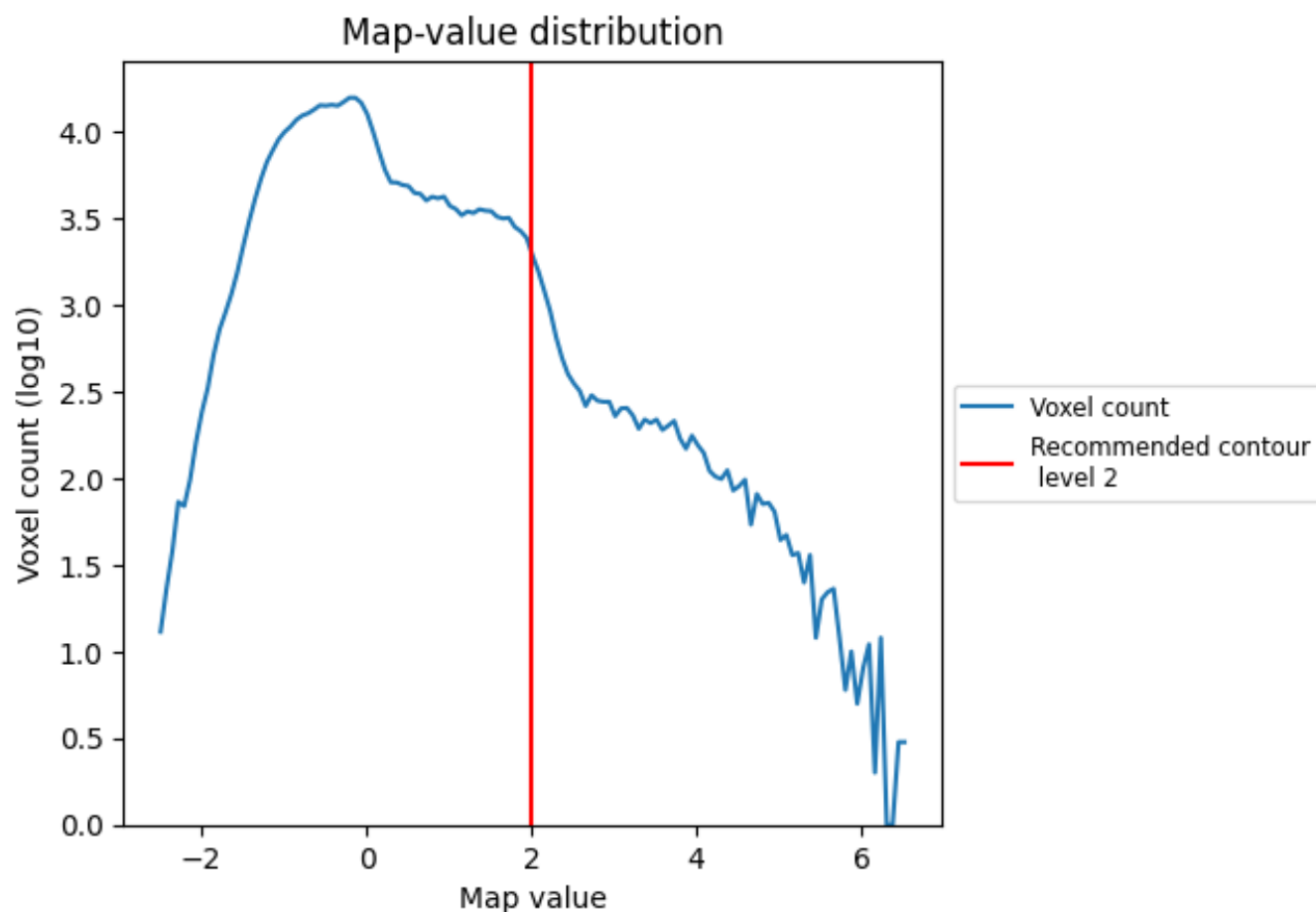
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

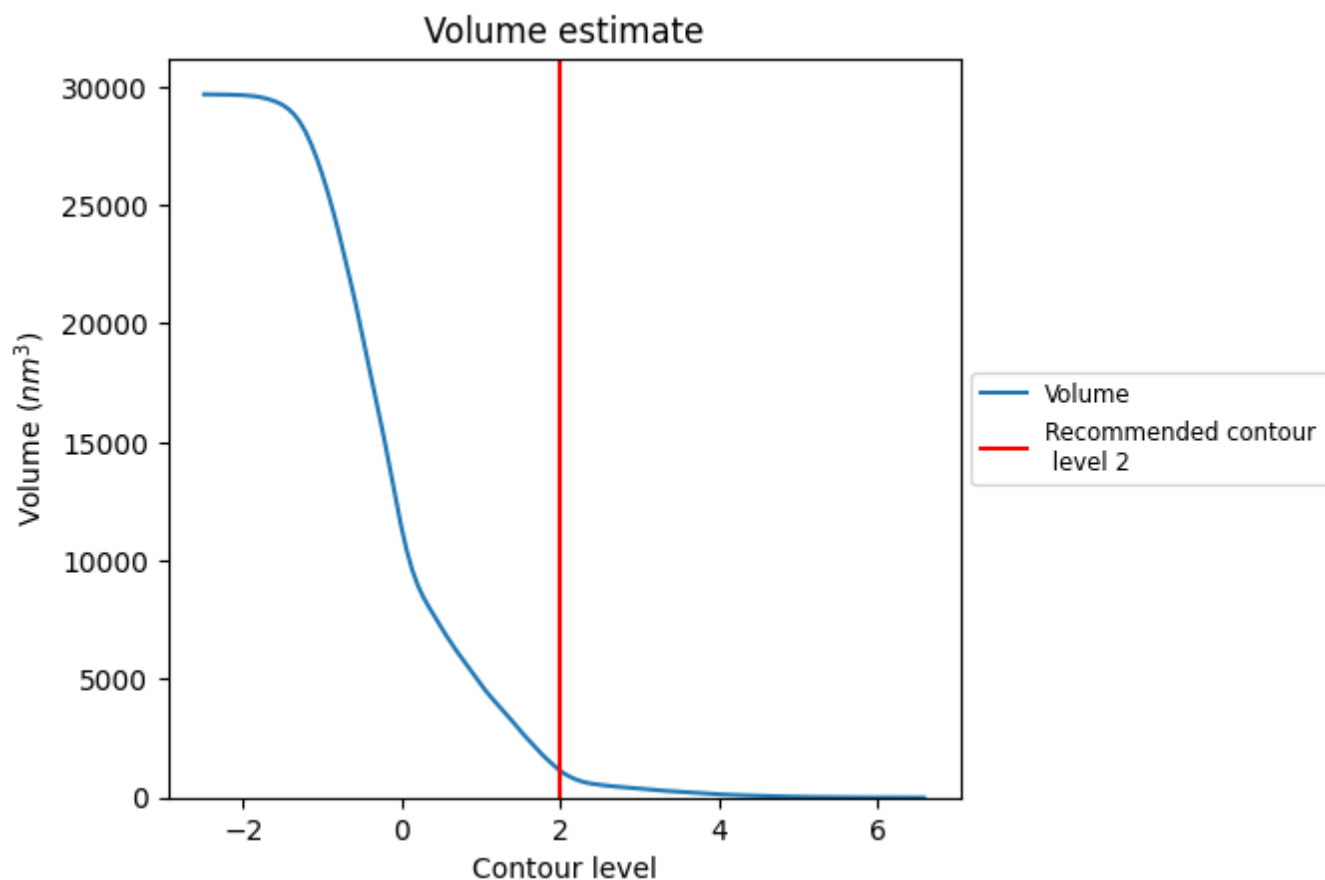
This section contains the results of statistical analysis of the map.

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.

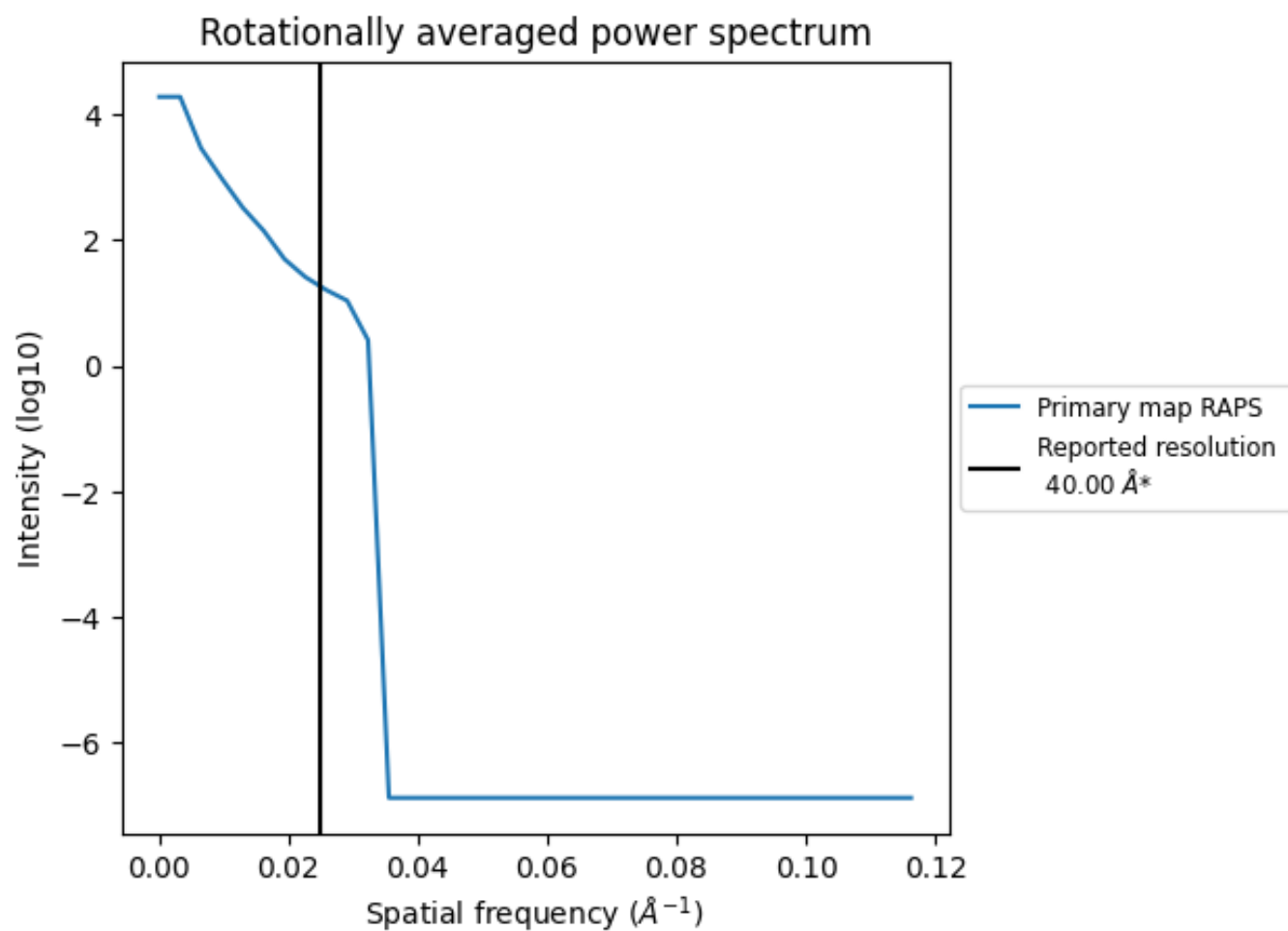
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1136 nm³; this corresponds to an approximate mass of 1026 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 0.025 Å⁻¹

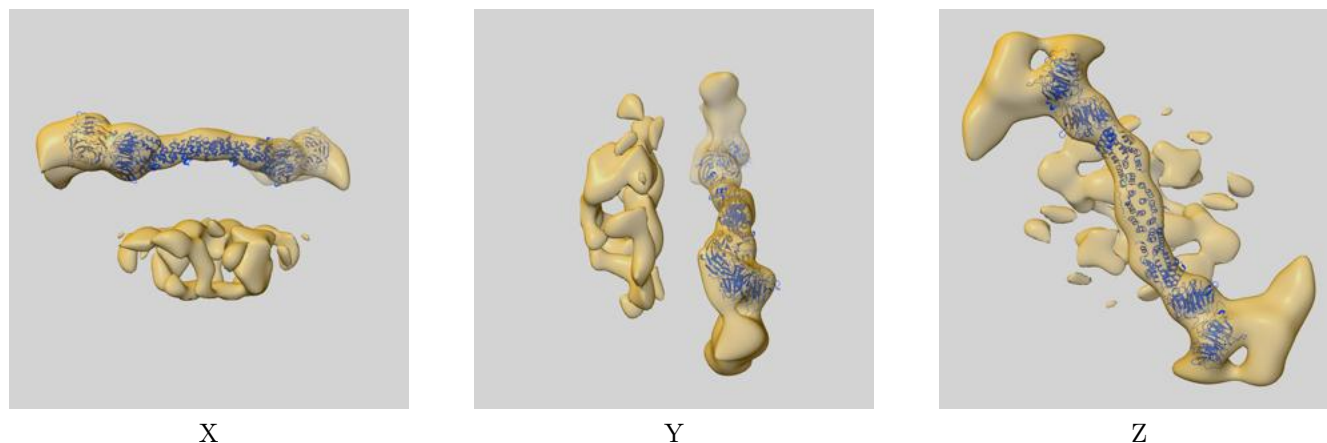
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

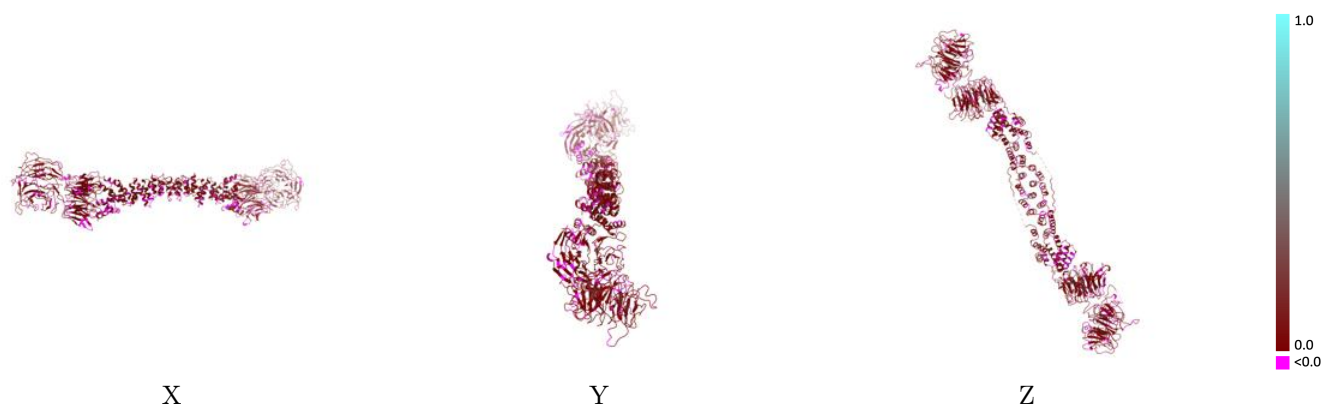
This section contains information regarding the fit between EMDB map EMD-2431 and PDB model 4BZK. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



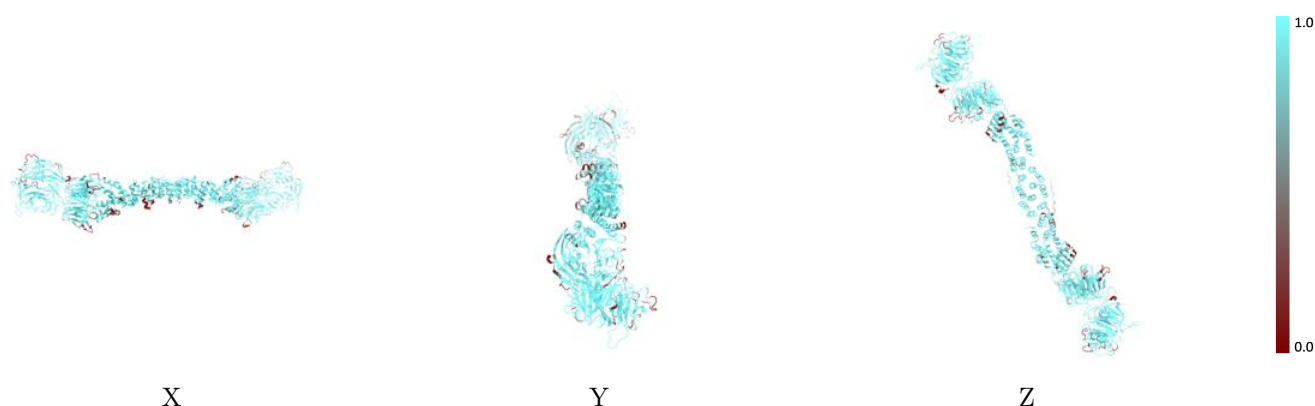
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



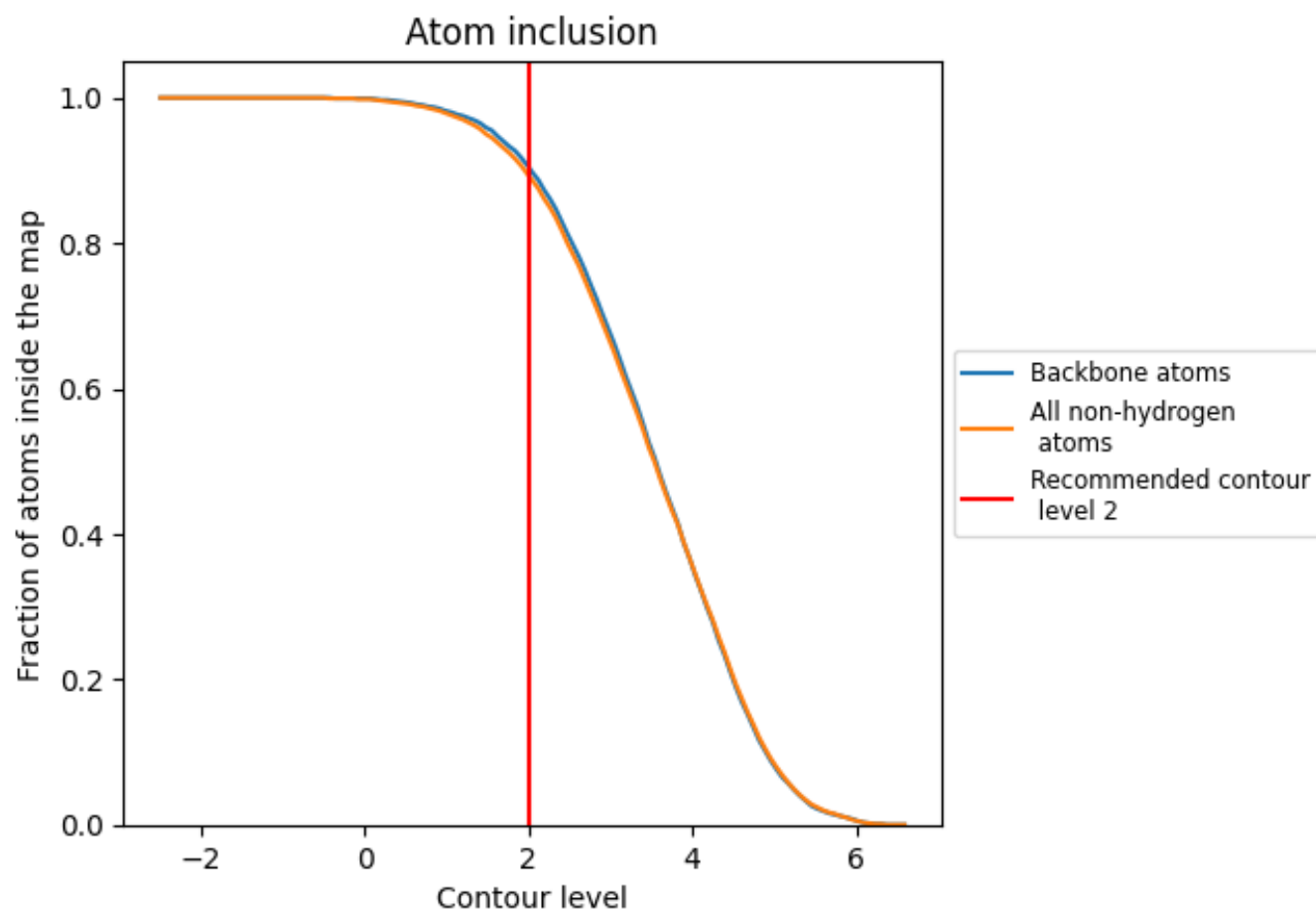
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 89% 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 (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8930	0.0520
A	0.8870	0.0530
B	0.8790	0.0450
C	0.9130	0.0560
F	0.8690	0.0510

