



Full wwPDB EM Validation Report ⓘ

Oct 19, 2024 – 06:21 PM EDT

PDB ID : 5VHZ
EMDB ID : EMD-8688
Title : GluA2-2xGSG1L bound to L-Quisqualate
Authors : Twomey, E.C.; Yelshanskaya, M.V.; Grassucci, R.A.; Frank, J.; Sobolevsky, A.I.
Deposited on : 2017-04-13
Resolution : 8.40 Å(reported)

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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

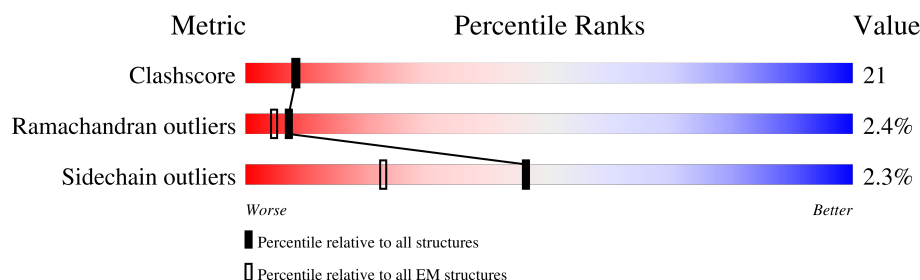
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.40 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1057	<div> <div>9%</div> <div>47%</div> <div>24%</div> <div>•</div> <div>26%</div> </div>
1	B	1057	<div> <div>13%</div> <div>47%</div> <div>24%</div> <div>•</div> <div>26%</div> </div>
1	C	1057	<div> <div>10%</div> <div>48%</div> <div>24%</div> <div>•</div> <div>26%</div> </div>
1	D	1057	<div> <div>13%</div> <div>48%</div> <div>23%</div> <div>•</div> <div>26%</div> </div>
1	E	1057	<div> <div>7%</div> <div>9%</div> <div>7%</div> <div>•</div> <div>83%</div> </div>
1	F	1057	<div> <div>7%</div> <div>9%</div> <div>8%</div> <div>•</div> <div>83%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 27460 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 Glutamate receptor 2, Germ cell-specific gene 1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	783	Total	C	N	O	S	0	0
			6159	3950	1023	1156	30		
1	B	780	Total	C	N	O	S	0	0
			6137	3938	1017	1152	30		
1	C	783	Total	C	N	O	S	0	0
			6159	3950	1023	1156	30		
1	D	780	Total	C	N	O	S	0	0
			6137	3938	1017	1152	30		
1	E	179	Total	C	N	O	S	0	0
			1408	920	231	245	12		
1	F	179	Total	C	N	O	S	0	0
			1408	920	231	245	12		

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	conflict	UNP P19491
A	382	LEU	VAL	conflict	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	conflict	UNP P19491
A	385	ASP	ASN	conflict	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
A	827	GLY	-	linker	UNP P19491
A	828	THR	-	linker	UNP P19491
A	829	GLY	-	linker	UNP P19491
B	241	GLU	ASN	conflict	UNP P19491
B	382	LEU	VAL	conflict	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491

Continued on next page...

Continued from previous page...

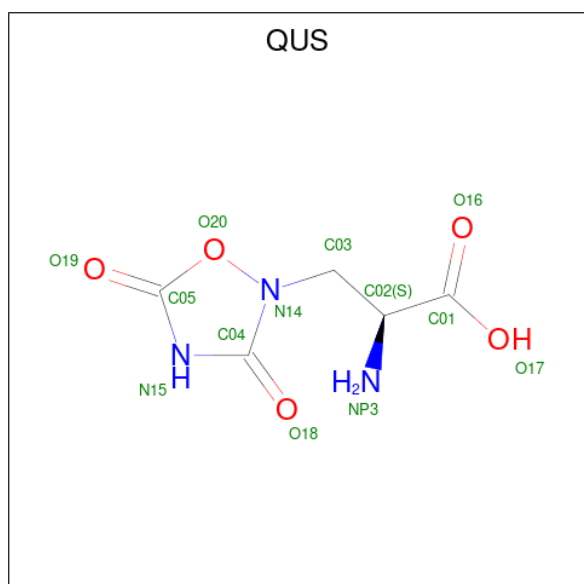
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	conflict	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	827	GLY	-	linker	UNP P19491
B	828	THR	-	linker	UNP P19491
B	829	GLY	-	linker	UNP P19491
C	241	GLU	ASN	conflict	UNP P19491
C	382	LEU	VAL	conflict	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	384	GLU	GLY	conflict	UNP P19491
C	385	ASP	ASN	conflict	UNP P19491
C	392	GLN	ASN	conflict	UNP P19491
C	827	GLY	-	linker	UNP P19491
C	828	THR	-	linker	UNP P19491
C	829	GLY	-	linker	UNP P19491
D	241	GLU	ASN	conflict	UNP P19491
D	382	LEU	VAL	conflict	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	conflict	UNP P19491
D	385	ASP	ASN	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	827	GLY	-	linker	UNP P19491
D	828	THR	-	linker	UNP P19491
D	829	GLY	-	linker	UNP P19491
E	-588	GLU	ASN	conflict	UNP P19491
E	-447	LEU	VAL	conflict	UNP P19491
E	?	-	LEU	deletion	UNP P19491
E	?	-	THR	deletion	UNP P19491

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	GLU	deletion	UNP P19491
E	?	-	LEU	deletion	UNP P19491
E	?	-	PRO	deletion	UNP P19491
E	?	-	SER	deletion	UNP P19491
E	-445	GLU	GLY	conflict	UNP P19491
E	-444	ASP	ASN	conflict	UNP P19491
E	-437	GLN	ASN	conflict	UNP P19491
E	-2	GLY	-	linker	UNP P19491
E	-1	THR	-	linker	UNP P19491
E	0	GLY	-	linker	UNP P19491
F	-588	GLU	ASN	conflict	UNP P19491
F	-447	LEU	VAL	conflict	UNP P19491
F	?	-	LEU	deletion	UNP P19491
F	?	-	THR	deletion	UNP P19491
F	?	-	GLU	deletion	UNP P19491
F	?	-	LEU	deletion	UNP P19491
F	?	-	PRO	deletion	UNP P19491
F	?	-	SER	deletion	UNP P19491
F	-445	GLU	GLY	conflict	UNP P19491
F	-444	ASP	ASN	conflict	UNP P19491
F	-437	GLN	ASN	conflict	UNP P19491
F	-2	GLY	-	linker	UNP P19491
F	-1	THR	-	linker	UNP P19491
F	0	GLY	-	linker	UNP P19491

- Molecule 2 is (S)-2-AMINO-3-(3,5-DIOXO-[1,2,4]OXADIAZOLIDIN-2-YL)-PROPIONIC ACID (three-letter code: QUS) (formula: C₅H₇N₃O₅).

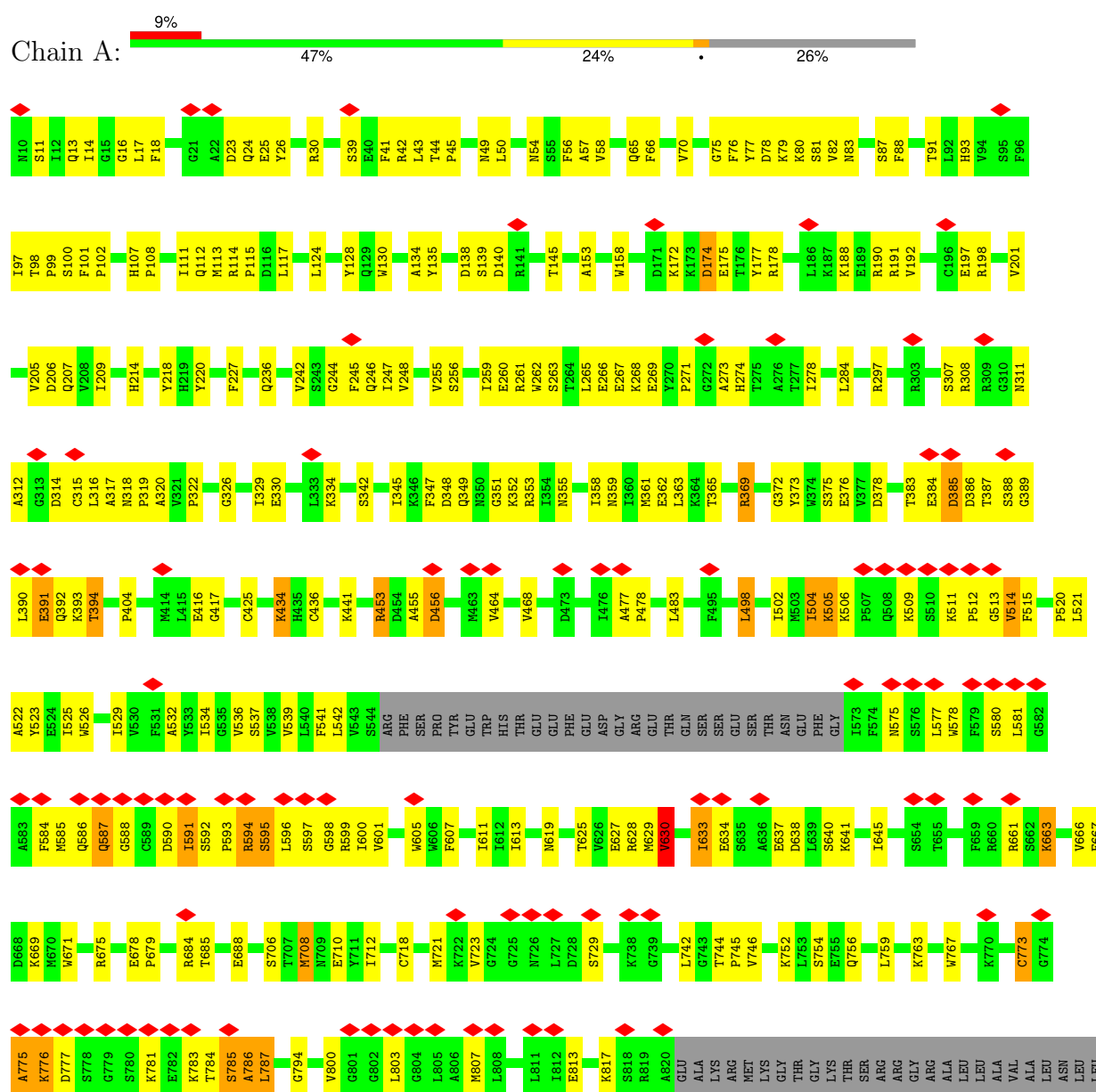


Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total 13	C 5	N 3	O 5	0
2	B	1	Total 13	C 5	N 3	O 5	0
2	C	1	Total 13	C 5	N 3	O 5	0
2	D	1	Total 13	C 5	N 3	O 5	0

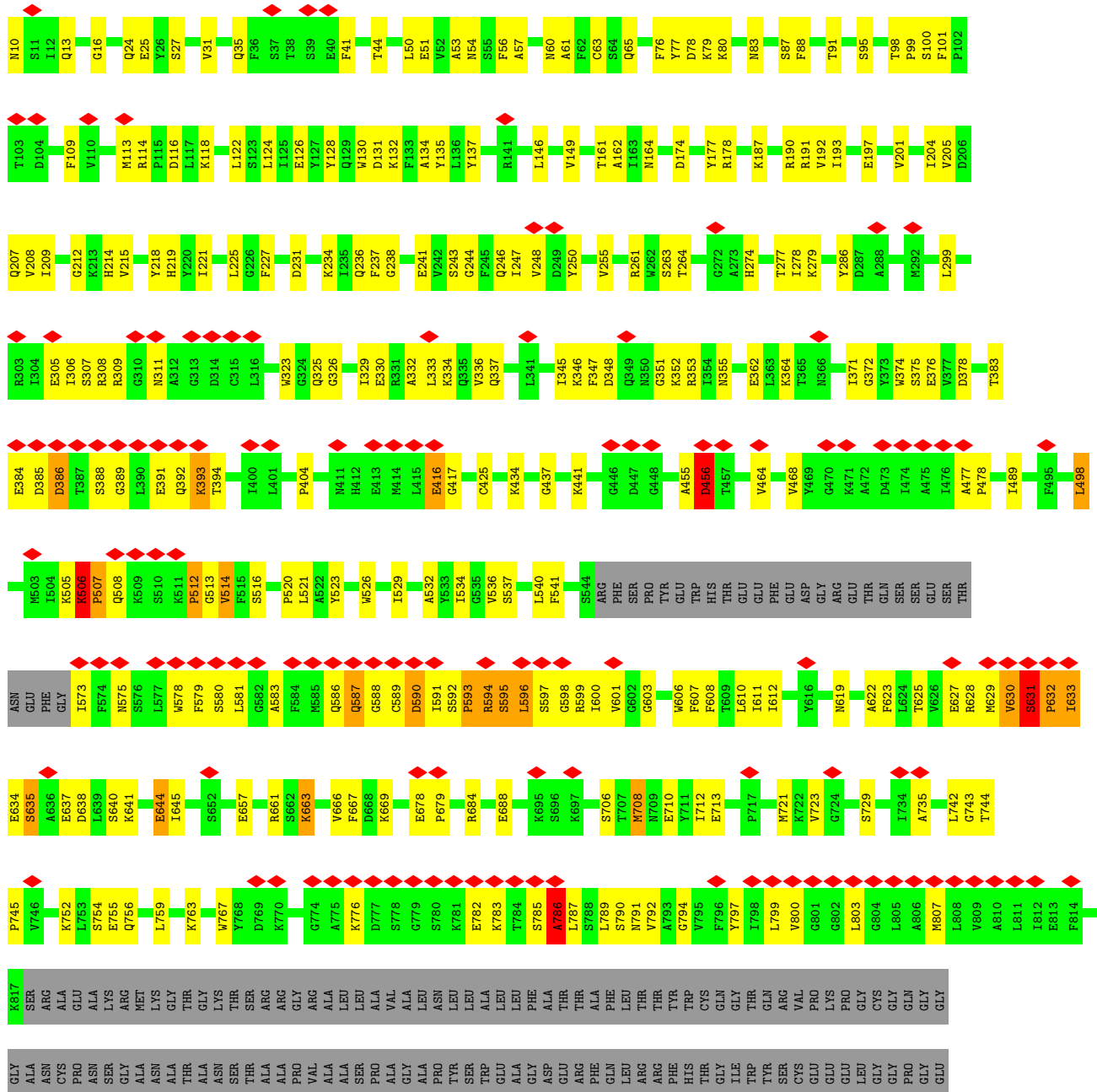
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glutamate receptor 2, Germ cell-specific gene 1-like protein

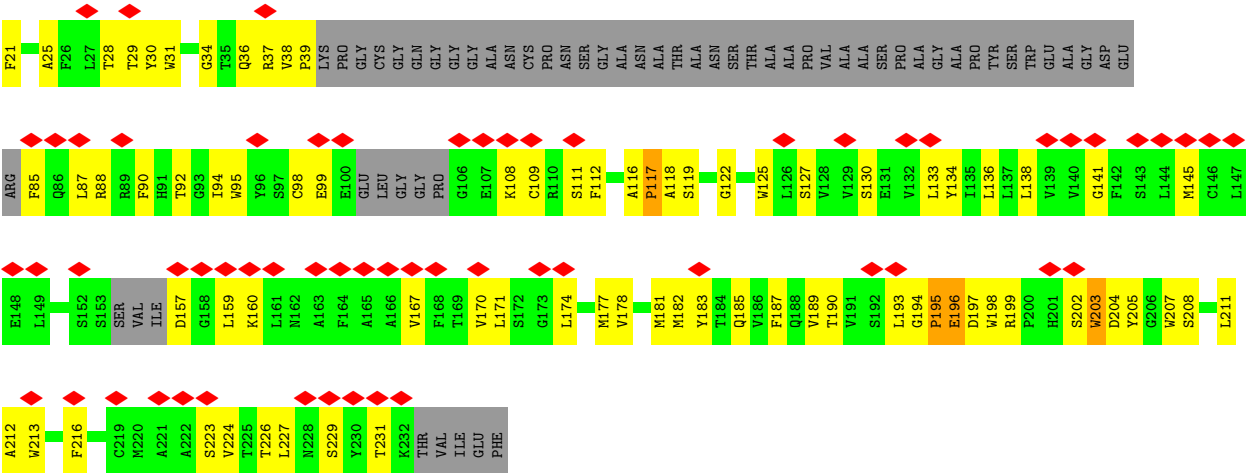


- Molecule 1: Glutamate receptor 2, Germ cell-specific gene 1-like protein









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	51130	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	67	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.053	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	352.80002, 352.80002, 352.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9800001, 0.9800001, 0.9800001	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.32	0/6287	0.50	0/8493
1	B	0.33	0/6265	0.56	4/8464 (0.0%)
1	C	0.32	0/6287	0.50	1/8493 (0.0%)
1	D	0.35	1/6265 (0.0%)	0.57	5/8464 (0.1%)
1	E	0.29	0/1443	0.49	0/1959
1	F	0.29	0/1443	0.48	0/1959
All	All	0.33	1/27990 (0.0%)	0.53	10/37832 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	786	ALA	C-N	-11.69	1.07	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	506	LYS	C-N-CD	-17.67	81.72	120.60
1	D	506	LYS	C-N-CD	-17.65	81.76	120.60
1	B	631	SER	C-N-CD	-16.78	83.69	120.60
1	D	631	SER	C-N-CD	-16.76	83.72	120.60
1	D	786	ALA	O-C-N	-8.83	108.58	122.70
1	D	386	ASP	CB-CG-OD2	5.23	123.00	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	386	ASP	CB-CG-OD2	5.21	122.99	118.30
1	C	456	ASP	CB-CG-OD2	5.21	122.98	118.30
1	D	456	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	456	ASP	CB-CG-OD2	5.19	122.97	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	786	ALA	Mainchain

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	6159	0	6157	283	0
1	B	6137	0	6132	321	0
1	C	6159	0	6157	309	0
1	D	6137	0	6131	291	0
1	E	1408	0	1406	61	0
1	F	1408	0	1406	54	0
2	A	13	0	6	0	0
2	B	13	0	6	0	0
2	C	13	0	6	0	0
2	D	13	0	6	0	0
All	All	27460	0	27413	1177	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 21.

All (1177) 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:506:LYS:CE	1:C:721:MET:HB2	1.20	1.65
1:A:506:LYS:CE	1:A:721:MET:HB2	1.16	1.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:LYS:HE3	1:A:721:MET:CB	1.33	1.57
1:C:506:LYS:HE3	1:C:721:MET:CB	1.35	1.56
1:A:506:LYS:CE	1:A:721:MET:CB	1.86	1.53
1:C:506:LYS:HE2	1:C:721:MET:CG	1.41	1.51
1:C:506:LYS:CE	1:C:721:MET:CB	1.87	1.48
1:A:506:LYS:HE2	1:A:721:MET:CG	1.43	1.45
1:B:512:PRO:HB3	1:B:516:SER:CB	1.46	1.43
1:A:483:LEU:CD2	1:D:755:GLU:OE2	1.71	1.37
1:B:512:PRO:CB	1:B:516:SER:CB	2.03	1.36
1:B:453:ARG:HD2	1:B:460:TRP:NE1	1.40	1.33
1:B:755:GLU:OE2	1:C:483:LEU:CD2	1.77	1.30
1:B:512:PRO:HB2	1:B:516:SER:OG	1.18	1.28
1:C:627:GLU:O	1:C:630:VAL:HG13	1.34	1.28
1:B:512:PRO:CB	1:B:516:SER:HB3	1.64	1.24
1:B:453:ARG:HD2	1:B:460:TRP:CE2	1.73	1.23
1:A:512:PRO:HB2	1:A:515:PHE:CD2	1.75	1.22
1:C:512:PRO:HB2	1:C:515:PHE:CD2	1.75	1.22
1:B:512:PRO:CB	1:B:516:SER:OG	1.89	1.21
1:D:512:PRO:HB2	1:D:516:SER:OG	1.43	1.18
1:C:634:GLU:CG	1:C:723:VAL:HB	1.73	1.18
1:A:483:LEU:HD21	1:D:755:GLU:OE2	1.30	1.17
1:C:663:LYS:HE2	1:C:663:LYS:HA	1.29	1.14
1:D:631:SER:HB3	1:D:632:PRO:CD	1.78	1.14
1:B:631:SER:HB3	1:B:632:PRO:CD	1.78	1.13
1:B:657:GLU:OE2	1:B:661:ARG:NH1	1.81	1.12
1:D:512:PRO:CB	1:D:516:SER:CB	2.27	1.12
1:B:755:GLU:OE2	1:C:483:LEU:HD21	1.40	1.10
1:A:504:ILE:HD11	1:A:723:VAL:HG13	1.25	1.10
1:A:506:LYS:HE2	1:A:721:MET:SD	1.93	1.09
1:A:627:GLU:O	1:A:630:VAL:HG13	1.51	1.09
1:D:633:ILE:HD11	1:D:645:ILE:CD1	1.83	1.08
1:C:506:LYS:CE	1:C:721:MET:CG	2.19	1.08
1:D:633:ILE:CD1	1:D:645:ILE:CD1	2.32	1.07
1:B:393:LYS:HG2	1:B:394:THR:N	1.69	1.07
1:B:633:ILE:CD1	1:B:645:ILE:CD1	2.33	1.06
1:B:633:ILE:HD11	1:B:645:ILE:CD1	1.84	1.06
1:B:453:ARG:CD	1:B:460:TRP:CE2	2.39	1.05
1:C:506:LYS:HE3	1:C:721:MET:CA	1.86	1.05
1:D:663:LYS:HE2	1:D:663:LYS:HA	1.32	1.05
1:B:713:GLU:OE2	1:B:776:LYS:HE3	1.57	1.04
1:C:506:LYS:HE2	1:C:721:MET:SD	1.97	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:506:LYS:HE2	1:C:721:MET:HG3	1.38	1.04
1:A:512:PRO:HB2	1:A:515:PHE:HD2	0.89	1.03
1:C:506:LYS:HE2	1:C:721:MET:CB	1.67	1.03
1:A:663:LYS:HE2	1:A:663:LYS:HA	1.39	1.02
1:D:393:LYS:HG2	1:D:394:THR:N	1.69	1.02
1:D:631:SER:HB3	1:D:632:PRO:HD2	1.02	1.02
1:A:506:LYS:CE	1:A:721:MET:CG	2.20	1.02
1:C:512:PRO:HB2	1:C:515:PHE:HD2	0.89	1.02
1:A:506:LYS:HE3	1:A:721:MET:CA	1.90	1.02
1:B:512:PRO:HB3	1:B:516:SER:HB3	1.18	1.01
1:A:634:GLU:HG3	1:A:723:VAL:HB	1.43	1.01
1:B:631:SER:HB3	1:B:632:PRO:HD2	1.02	1.01
1:C:742:LEU:O	1:C:745:PRO:HG2	1.61	1.01
1:B:742:LEU:O	1:B:745:PRO:HG2	1.61	1.01
1:C:634:GLU:HG2	1:C:723:VAL:HB	1.39	1.01
1:D:742:LEU:O	1:D:745:PRO:HG2	1.61	1.00
1:B:631:SER:CB	1:B:632:PRO:HD2	1.89	1.00
1:B:755:GLU:OE2	1:C:483:LEU:HD23	1.58	1.00
1:D:631:SER:CB	1:D:632:PRO:HD2	1.89	1.00
1:C:634:GLU:HG3	1:C:723:VAL:HB	1.44	1.00
1:A:506:LYS:HE2	1:A:721:MET:CB	1.68	0.99
1:C:512:PRO:CB	1:C:515:PHE:HD2	1.76	0.99
1:C:513:GLY:O	1:C:514:VAL:HG23	1.63	0.99
1:A:744:THR:OG1	1:A:745:PRO:HD3	1.63	0.98
1:D:713:GLU:OE2	1:D:776:LYS:HE3	1.61	0.98
1:A:512:PRO:CB	1:A:515:PHE:HD2	1.76	0.98
1:A:775:ALA:C	1:A:777:ASP:H	1.63	0.98
1:A:513:GLY:O	1:A:514:VAL:HG23	1.63	0.97
1:D:634:GLU:N	1:D:638:ASP:OD2	1.97	0.97
1:B:633:ILE:HD11	1:B:645:ILE:HD11	1.44	0.97
1:D:512:PRO:HB3	1:D:516:SER:CB	1.90	0.97
1:D:633:ILE:HD11	1:D:645:ILE:HD11	1.45	0.97
1:D:684:ARG:NH1	1:D:688:GLU:OE1	1.97	0.97
1:C:504:ILE:HD11	1:C:723:VAL:CG1	1.94	0.96
1:A:525:ILE:HG12	1:B:789:LEU:HB2	1.45	0.96
1:C:503:MET:HB2	1:C:709:ASN:OD1	1.64	0.96
1:D:512:PRO:CB	1:D:516:SER:HB3	1.92	0.96
1:C:504:ILE:HD13	1:C:504:ILE:H	1.30	0.95
1:A:506:LYS:HE2	1:A:721:MET:HG3	1.45	0.95
1:B:663:LYS:HA	1:B:663:LYS:HE2	1.46	0.95
1:A:483:LEU:HD23	1:D:755:GLU:OE2	1.61	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:PRO:HB2	1:B:516:SER:HG	1.30	0.95
1:A:504:ILE:HD11	1:A:723:VAL:CG1	1.96	0.95
1:F:31:TRP:HE1	1:F:208:SER:HG	1.15	0.94
1:B:455:ALA:O	1:B:456:ASP:HB2	1.66	0.94
1:C:506:LYS:CD	1:C:721:MET:HB2	1.97	0.94
1:C:775:ALA:C	1:C:777:ASP:H	1.63	0.93
1:D:455:ALA:O	1:D:456:ASP:HB2	1.66	0.93
1:C:455:ALA:O	1:C:456:ASP:HB2	1.66	0.93
1:A:436:CYS:SG	1:A:745:PRO:HB2	2.09	0.93
1:C:627:GLU:O	1:C:630:VAL:CG1	2.16	0.92
1:A:56:PHE:CE2	1:B:91:THR:HG21	2.03	0.92
1:A:742:LEU:O	1:A:746:VAL:HG23	1.69	0.92
1:C:512:PRO:CB	1:C:515:PHE:CD2	2.52	0.90
1:D:633:ILE:HG23	1:D:638:ASP:HB3	1.53	0.90
1:A:634:GLU:CG	1:A:723:VAL:HB	2.01	0.90
1:D:595:SER:HA	1:D:599:ARG:HB3	1.53	0.90
1:A:506:LYS:CD	1:A:721:MET:HB2	2.00	0.90
1:B:663:LYS:HA	1:B:663:LYS:CE	2.00	0.90
1:E:31:TRP:HE1	1:E:208:SER:HG	1.14	0.89
1:B:512:PRO:HB3	1:B:516:SER:HB2	1.52	0.89
1:D:512:PRO:HB2	1:D:516:SER:CB	1.95	0.88
1:B:178:ARG:NH2	1:D:237:PHE:CE2	2.43	0.86
1:A:512:PRO:CB	1:A:515:PHE:CD2	2.52	0.86
1:D:634:GLU:O	1:D:635:SER:HB3	1.75	0.86
1:B:633:ILE:HD13	1:B:645:ILE:CD1	2.07	0.85
1:B:453:ARG:CD	1:B:460:TRP:NE1	2.33	0.85
1:D:633:ILE:HD13	1:D:645:ILE:CD1	2.04	0.85
1:C:56:PHE:CE2	1:D:91:THR:HG21	2.12	0.85
1:B:453:ARG:HD2	1:B:460:TRP:HE1	1.38	0.84
1:A:513:GLY:O	1:A:514:VAL:CG2	2.26	0.84
1:C:87:SER:OG	1:D:54:ASN:OD1	1.95	0.83
1:C:506:LYS:CE	1:C:721:MET:HG3	2.01	0.83
1:C:513:GLY:O	1:C:514:VAL:CG2	2.26	0.83
1:B:634:GLU:N	1:B:638:ASP:OD2	2.10	0.83
1:A:744:THR:OG1	1:A:745:PRO:CD	2.27	0.82
1:C:455:ALA:O	1:C:456:ASP:CB	2.27	0.81
1:B:455:ALA:O	1:B:456:ASP:CB	2.27	0.81
1:C:504:ILE:HD11	1:C:723:VAL:HG13	1.62	0.81
1:B:453:ARG:CD	1:B:460:TRP:CZ2	2.63	0.81
1:B:512:PRO:CA	1:B:516:SER:HB3	2.10	0.81
1:A:188:LYS:HD2	1:A:190:ARG:HH22	1.46	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:633:ILE:CD1	1:D:645:ILE:HD12	2.10	0.80
1:B:393:LYS:CG	1:B:394:THR:N	2.45	0.80
1:B:631:SER:CB	1:B:632:PRO:CD	2.40	0.80
1:C:775:ALA:O	1:C:777:ASP:N	2.15	0.80
1:D:455:ALA:O	1:D:456:ASP:CB	2.27	0.80
1:A:16:GLY:H	1:A:65:GLN:HE22	1.30	0.80
1:B:729:SER:HB3	1:C:729:SER:CB	2.12	0.80
1:A:56:PHE:CD2	1:B:91:THR:HG21	2.17	0.79
1:A:627:GLU:O	1:A:630:VAL:CG1	2.30	0.79
1:C:337:GLN:HE21	1:C:346:LYS:HE2	1.47	0.79
1:C:684:ARG:HH21	1:C:684:ARG:HG3	1.45	0.79
1:C:786:ALA:O	1:C:787:LEU:HB2	1.81	0.79
1:B:453:ARG:HD3	1:B:460:TRP:CZ2	2.16	0.79
1:B:633:ILE:HD13	1:B:645:ILE:HD13	1.65	0.79
1:C:663:LYS:HA	1:C:663:LYS:CE	2.04	0.79
1:A:786:ALA:O	1:A:787:LEU:HB2	1.81	0.79
1:C:595:SER:H	1:C:599:ARG:HE	1.28	0.79
1:B:729:SER:HB3	1:C:729:SER:OG	1.83	0.78
1:C:742:LEU:O	1:C:745:PRO:CG	2.31	0.78
1:D:742:LEU:O	1:D:745:PRO:CG	2.31	0.78
1:A:775:ALA:O	1:A:777:ASP:N	2.15	0.78
1:B:742:LEU:O	1:B:745:PRO:CG	2.31	0.78
1:A:455:ALA:O	1:A:456:ASP:CB	2.32	0.78
1:A:506:LYS:CE	1:A:721:MET:HG3	2.05	0.78
1:D:134:ALA:HB3	1:D:192:VAL:HG22	1.66	0.78
1:D:393:LYS:CG	1:D:394:THR:N	2.45	0.78
1:B:134:ALA:HB3	1:B:192:VAL:HG22	1.66	0.78
1:D:372:GLY:HA2	1:D:383:THR:HG23	1.66	0.78
1:A:83:ASN:ND2	1:B:80:LYS:HA	1.97	0.77
1:B:237:PHE:CE2	1:D:178:ARG:NH2	2.53	0.77
1:B:633:ILE:HG23	1:B:638:ASP:HB3	1.65	0.77
1:B:214:HIS:HE1	1:D:212:GLY:CA	1.98	0.77
1:B:595:SER:HA	1:B:599:ARG:HB2	1.65	0.77
1:C:506:LYS:HE3	1:C:721:MET:HB2	0.78	0.77
1:D:512:PRO:HB3	1:D:516:SER:HB2	1.64	0.77
1:B:512:PRO:HB2	1:B:516:SER:CB	1.90	0.77
1:B:215:VAL:HG11	1:D:215:VAL:HG11	1.68	0.76
1:D:355:ASN:N	1:D:376:GLU:OE2	2.19	0.76
1:B:619:ASN:ND2	1:C:787:LEU:HG	2.00	0.76
1:C:775:ALA:C	1:C:777:ASP:N	2.35	0.76
1:A:77:TYR:HE2	1:A:98:THR:HG21	1.49	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:ILE:CD1	1:B:645:ILE:HD12	2.16	0.75
1:C:504:ILE:HD11	1:C:723:VAL:HG11	1.66	0.75
1:B:247:ILE:HG23	1:B:248:VAL:HG23	1.67	0.75
1:D:392:GLN:NE2	1:D:437:GLY:O	2.20	0.75
1:A:504:ILE:HD12	1:A:723:VAL:HG22	1.68	0.75
1:A:742:LEU:O	1:A:745:PRO:HD2	1.87	0.75
1:D:633:ILE:HD13	1:D:645:ILE:HD13	1.69	0.75
1:B:392:GLN:NE2	1:B:437:GLY:O	2.20	0.74
1:A:729:SER:OG	1:D:729:SER:HB3	1.87	0.74
1:D:634:GLU:O	1:D:635:SER:CB	2.35	0.74
1:A:80:LYS:HA	1:B:83:ASN:ND2	2.02	0.74
1:A:513:GLY:O	1:A:514:VAL:CB	2.36	0.74
1:B:77:TYR:OH	1:B:101:PHE:O	2.06	0.74
1:C:80:LYS:HA	1:D:83:ASN:ND2	2.01	0.74
1:C:506:LYS:CG	1:C:721:MET:HB2	2.18	0.74
1:D:721:MET:HG3	1:D:776:LYS:HE2	1.69	0.74
1:B:503:MET:HB2	1:B:709:ASN:OD1	1.88	0.74
1:C:16:GLY:H	1:C:65:GLN:HE22	1.33	0.74
1:D:523:TYR:HA	1:D:526:TRP:HD1	1.52	0.73
1:C:513:GLY:O	1:C:514:VAL:CB	2.36	0.73
1:C:83:ASN:ND2	1:D:80:LYS:HA	2.02	0.73
1:D:744:THR:N	1:D:745:PRO:HD2	2.03	0.73
1:C:88:PHE:CE1	1:D:56:PHE:HD1	2.06	0.73
1:A:729:SER:CB	1:D:729:SER:HB3	2.18	0.73
1:A:14:ILE:HD13	1:A:43:LEU:HD23	1.70	0.73
1:C:372:GLY:HA2	1:C:383:THR:OG1	1.89	0.73
1:D:308:ARG:NH2	1:D:325:GLN:OE1	2.22	0.73
1:B:744:THR:N	1:B:745:PRO:HD2	2.03	0.73
1:C:77:TYR:HE2	1:C:98:THR:HG21	1.51	0.72
1:A:594:ARG:HD3	1:B:575:ASN:HB2	1.71	0.72
1:B:729:SER:HB3	1:C:729:SER:HB3	1.69	0.72
1:D:77:TYR:OH	1:D:101:PHE:O	2.08	0.72
1:D:101:PHE:HA	1:D:114:ARG:HD2	1.72	0.72
1:A:599:ARG:HH22	1:B:581:LEU:HB3	1.53	0.72
1:C:14:ILE:HD13	1:C:43:LEU:HD23	1.69	0.72
1:D:633:ILE:CG2	1:D:638:ASP:HB3	2.18	0.72
1:D:505:LYS:O	1:D:506:LYS:O	2.08	0.72
1:A:706:SER:O	1:A:710:GLU:HG2	1.90	0.71
1:B:706:SER:O	1:B:710:GLU:HG2	1.90	0.71
1:C:744:THR:N	1:C:745:PRO:HD2	2.03	0.71
1:D:512:PRO:CA	1:D:516:SER:HB3	2.20	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:ILE:HG12	1:B:221:ILE:HB	1.73	0.71
1:B:209:ILE:HA	1:B:214:HIS:HD2	1.55	0.71
1:D:247:ILE:HG23	1:D:248:VAL:HG23	1.71	0.71
1:B:246:GLN:HE21	1:B:248:VAL:H	1.37	0.71
1:C:633:ILE:O	1:C:633:ILE:HG13	1.90	0.70
1:B:523:TYR:HA	1:B:526:TRP:HD1	1.56	0.70
1:C:789:LEU:HG	1:C:793:ALA:HB2	1.73	0.70
1:B:505:LYS:O	1:B:506:LYS:O	2.08	0.70
1:B:633:ILE:CD1	1:B:645:ILE:HD13	2.20	0.70
1:A:595:SER:H	1:A:599:ARG:HE	1.39	0.70
1:C:706:SER:O	1:C:710:GLU:HG2	1.90	0.70
1:F:98:CYS:HA	1:F:109:CYS:HA	1.74	0.70
1:A:633:ILE:HG13	1:A:633:ILE:O	1.90	0.70
1:D:193:ILE:HG12	1:D:221:ILE:HB	1.72	0.70
1:D:512:PRO:CB	1:D:516:SER:OG	2.26	0.70
1:D:706:SER:O	1:D:710:GLU:HG2	1.90	0.70
1:A:88:PHE:CE1	1:B:56:PHE:HD1	2.09	0.70
1:C:91:THR:HG21	1:D:56:PHE:CE2	2.27	0.70
1:C:718:CYS:CB	1:C:773:CYS:HG	2.03	0.70
1:D:663:LYS:HA	1:D:663:LYS:CE	2.00	0.70
1:A:684:ARG:NH2	1:A:684:ARG:HB2	2.07	0.69
1:B:101:PHE:HA	1:B:114:ARG:HD2	1.73	0.69
1:B:263:SER:O	1:B:274:HIS:ND1	2.25	0.69
1:B:376:GLU:HG2	1:B:377:VAL:HG13	1.73	0.69
1:B:375:SER:HB3	1:B:378:ASP:HB2	1.74	0.69
1:C:504:ILE:HD13	1:C:504:ILE:N	2.05	0.69
1:A:506:LYS:HE3	1:A:721:MET:HB2	0.70	0.69
1:E:98:CYS:HA	1:E:109:CYS:HA	1.75	0.69
1:A:637:GLU:HG2	1:A:641:LYS:HE3	1.74	0.69
1:C:344:ASN:HD21	1:C:346:LYS:HE3	1.58	0.69
1:C:393:LYS:O	1:C:393:LYS:HG2	1.92	0.69
1:B:13:GLN:HA	1:B:44:THR:HB	1.74	0.69
1:B:209:ILE:HA	1:B:214:HIS:CD2	2.27	0.69
1:D:393:LYS:HG2	1:D:394:THR:H	1.57	0.69
1:D:631:SER:CB	1:D:632:PRO:CD	2.40	0.69
1:B:214:HIS:CE1	1:D:212:GLY:CA	2.76	0.68
1:D:637:GLU:HG2	1:D:641:LYS:HE3	1.74	0.68
1:A:393:LYS:O	1:A:393:LYS:HG2	1.92	0.68
1:A:586:GLN:HA	1:D:587:GLN:HE21	1.57	0.68
1:B:637:GLU:HG2	1:B:641:LYS:HE3	1.74	0.68
1:D:590:ASP:O	1:D:592:SER:N	2.24	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ARG:O	1:A:453:ARG:HG2	1.93	0.68
1:B:24:GLN:HE21	1:B:278:ILE:HG13	1.58	0.68
1:D:13:GLN:HA	1:D:44:THR:HB	1.76	0.68
1:D:24:GLN:HE21	1:D:278:ILE:HG13	1.58	0.68
1:C:637:GLU:HG2	1:C:641:LYS:HE3	1.74	0.68
1:D:309:ARG:HG2	1:D:311:ASN:H	1.58	0.68
1:A:375:SER:HB3	1:A:378:ASP:HB2	1.75	0.67
1:B:790:SER:OG	1:E:185:GLN:NE2	2.25	0.67
1:B:16:GLY:H	1:B:65:GLN:HE22	1.40	0.67
1:D:785:SER:O	1:D:786:ALA:HB3	1.95	0.67
1:C:520:PRO:O	1:C:619:ASN:ND2	2.28	0.67
1:A:56:PHE:HD1	1:B:88:PHE:CD2	2.12	0.67
1:A:634:GLU:O	1:A:634:GLU:HG2	1.93	0.67
1:B:619:ASN:HD21	1:C:786:ALA:HB1	1.58	0.67
1:C:718:CYS:HG	1:C:773:CYS:HG	1.36	0.67
1:A:729:SER:HB3	1:D:729:SER:HB3	1.77	0.67
1:B:309:ARG:HG2	1:B:311:ASN:H	1.60	0.67
1:B:453:ARG:HD2	1:B:460:TRP:CZ2	2.26	0.67
1:B:346:LYS:HD3	1:B:355:ASN:HD22	1.60	0.67
1:D:246:GLN:HE21	1:D:248:VAL:H	1.40	0.67
1:B:785:SER:O	1:B:786:ALA:HB3	1.95	0.66
1:C:375:SER:HB3	1:C:378:ASP:HB2	1.75	0.66
1:A:91:THR:HG21	1:B:56:PHE:CD2	2.30	0.66
1:C:56:PHE:CD2	1:D:91:THR:HG21	2.31	0.66
1:A:91:THR:HG21	1:B:56:PHE:CE2	2.30	0.66
1:A:506:LYS:HE2	1:A:721:MET:HB2	1.38	0.66
1:A:523:TYR:HA	1:A:526:TRP:HD1	1.61	0.66
1:B:209:ILE:CG2	1:D:209:ILE:CG2	2.73	0.66
1:B:757:GLY:HA3	1:C:663:LYS:HG3	1.78	0.66
1:C:91:THR:HG21	1:D:56:PHE:CD2	2.31	0.66
1:C:246:GLN:HE21	1:C:248:VAL:H	1.41	0.66
1:D:592:SER:O	1:D:599:ARG:NH2	2.29	0.66
1:A:236:GLN:NE2	1:A:365:THR:O	2.29	0.66
1:B:178:ARG:NE	1:D:237:PHE:CE1	2.63	0.66
1:B:520:PRO:O	1:B:619:ASN:ND2	2.29	0.66
1:C:80:LYS:HA	1:D:83:ASN:HD22	1.61	0.66
1:C:634:GLU:HG3	1:C:723:VAL:CB	2.24	0.66
1:A:206:ASP:HA	1:A:209:ILE:HD12	1.77	0.65
1:B:619:ASN:HD22	1:C:787:LEU:HG	1.59	0.65
1:B:628:ARG:HG3	1:B:628:ARG:O	1.95	0.65
1:D:375:SER:HB3	1:D:378:ASP:HB2	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:592:SER:HB3	1:D:599:ARG:HB2	1.78	0.65
1:A:504:ILE:HD13	1:A:504:ILE:N	2.11	0.65
1:D:51:GLU:HG3	1:D:53:ALA:H	1.61	0.65
1:B:721:MET:HG3	1:B:776:LYS:HE2	1.78	0.65
1:C:523:TYR:HA	1:C:526:TRP:HD1	1.61	0.65
1:D:348:ASP:OD1	1:D:352:LYS:N	2.30	0.65
1:A:56:PHE:N	1:B:87:SER:OG	2.29	0.65
1:C:742:LEU:O	1:C:745:PRO:HD2	1.97	0.65
1:A:246:GLN:HE21	1:A:248:VAL:H	1.44	0.65
1:A:504:ILE:HD13	1:A:504:ILE:H	1.62	0.65
1:C:13:GLN:HA	1:C:44:THR:HB	1.79	0.65
1:C:502:ILE:HG12	1:C:703:LEU:CD2	2.26	0.65
1:A:506:LYS:CG	1:A:721:MET:HB2	2.26	0.65
1:B:156:LYS:O	1:B:157:LYS:HG3	1.96	0.65
1:C:307:SER:O	1:C:308:ARG:NH1	2.25	0.65
1:D:209:ILE:HA	1:D:214:HIS:CD2	2.32	0.65
1:B:393:LYS:CG	1:B:394:THR:H	2.10	0.65
1:A:247:ILE:HG23	1:A:248:VAL:HG23	1.79	0.64
1:B:305:GLU:O	1:B:325:GLN:NE2	2.29	0.64
1:C:88:PHE:CE1	1:D:56:PHE:CD1	2.83	0.64
1:B:579:PHE:HZ	1:B:590:ASP:H	1.45	0.64
1:A:504:ILE:HD13	1:A:721:MET:O	1.97	0.64
1:D:16:GLY:H	1:D:65:GLN:HE22	1.45	0.64
1:C:663:LYS:HE2	1:C:663:LYS:CA	2.19	0.64
1:D:78:ASP:OD1	1:D:79:LYS:N	2.30	0.64
1:D:263:SER:O	1:D:274:HIS:ND1	2.31	0.64
1:D:161:THR:OG1	1:D:187:LYS:NZ	2.28	0.64
1:A:513:GLY:C	1:A:514:VAL:HG23	2.18	0.64
1:B:348:ASP:OD1	1:B:352:LYS:N	2.31	0.64
1:B:742:LEU:O	1:B:745:PRO:HD2	1.97	0.64
1:D:742:LEU:O	1:D:745:PRO:HD2	1.97	0.64
1:C:742:LEU:O	1:C:745:PRO:CD	2.46	0.64
1:A:775:ALA:C	1:A:777:ASP:N	2.35	0.63
1:C:11:SER:OG	1:C:44:THR:OG1	2.15	0.63
1:C:337:GLN:HG3	1:C:346:LYS:HG2	1.81	0.63
1:A:88:PHE:CE1	1:B:56:PHE:CD1	2.87	0.63
1:B:178:ARG:NE	1:D:237:PHE:CD1	2.67	0.63
1:D:513:GLY:O	1:D:514:VAL:HB	1.99	0.63
1:D:633:ILE:CD1	1:D:645:ILE:HD13	2.24	0.63
1:A:130:TRP:CD2	1:A:191:ARG:HD3	2.34	0.63
1:A:633:ILE:HA	1:A:638:ASP:OD2	1.97	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:513:GLY:C	1:C:514:VAL:HG23	2.18	0.63
1:A:628:ARG:NH1	1:D:622:ALA:O	2.32	0.63
1:B:78:ASP:OD1	1:B:79:LYS:N	2.31	0.63
1:D:742:LEU:O	1:D:745:PRO:CD	2.47	0.63
1:A:11:SER:OG	1:A:44:THR:OG1	2.16	0.62
1:A:520:PRO:O	1:A:619:ASN:ND2	2.32	0.62
1:C:56:PHE:HD1	1:D:88:PHE:CE2	2.17	0.62
1:C:633:ILE:HA	1:C:638:ASP:OD2	1.98	0.62
1:A:455:ALA:O	1:A:456:ASP:HB3	1.99	0.62
1:A:391:GLU:OE2	1:A:391:GLU:HA	1.99	0.62
1:B:161:THR:OG1	1:B:187:LYS:NZ	2.33	0.62
1:C:504:ILE:HD12	1:C:723:VAL:HG22	1.81	0.62
1:C:513:GLY:O	1:C:514:VAL:HB	1.99	0.62
1:C:78:ASP:OD1	1:C:79:LYS:N	2.32	0.62
1:B:742:LEU:O	1:B:745:PRO:CD	2.47	0.62
1:C:718:CYS:HB3	1:C:773:CYS:SG	2.40	0.62
1:B:393:LYS:HG2	1:B:394:THR:H	1.57	0.62
1:E:37:ARG:HD2	1:E:87:LEU:HD22	1.82	0.62
1:A:78:ASP:OD1	1:A:79:LYS:N	2.33	0.61
1:C:334:LYS:HD3	1:C:349:GLN:HA	1.82	0.61
1:A:786:ALA:HB1	1:D:619:ASN:HD21	1.66	0.61
1:A:13:GLN:HA	1:A:44:THR:HB	1.81	0.61
1:B:623:PHE:CZ	1:C:786:ALA:HB2	2.35	0.61
1:F:31:TRP:N	1:F:92:THR:O	2.32	0.61
1:A:513:GLY:O	1:A:514:VAL:HB	1.99	0.61
1:C:259:ILE:HA	1:C:262:TRP:HB3	1.82	0.61
1:C:595:SER:N	1:C:599:ARG:HE	1.96	0.61
1:D:752:LYS:O	1:D:756:GLN:HG3	2.01	0.61
1:B:164:ASN:OD1	1:B:165:VAL:N	2.34	0.61
1:B:178:ARG:CZ	1:D:237:PHE:CE2	2.83	0.61
1:C:752:LYS:O	1:C:756:GLN:HG3	2.01	0.61
1:B:334:LYS:NZ	1:B:349:GLN:O	2.26	0.61
1:B:752:LYS:O	1:B:756:GLN:HG3	2.01	0.61
1:A:525:ILE:CG1	1:B:789:LEU:HB2	2.25	0.60
1:A:594:ARG:HB3	1:B:578:TRP:HE3	1.66	0.60
1:B:661:ARG:HG3	1:B:661:ARG:O	2.00	0.60
1:E:31:TRP:N	1:E:92:THR:O	2.32	0.60
1:C:744:THR:OG1	1:C:745:PRO:HD3	2.01	0.60
1:D:630:VAL:HG22	1:D:630:VAL:O	2.00	0.60
1:A:30:ARG:NH1	1:A:269:GLU:O	2.35	0.60
1:B:744:THR:OG1	1:B:745:PRO:HD3	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:744:THR:OG1	1:D:745:PRO:HD3	2.01	0.60
1:D:583:ALA:HA	1:D:589:CYS:H	1.67	0.60
1:F:37:ARG:HD2	1:F:87:LEU:HD22	1.81	0.60
1:B:633:ILE:CG2	1:B:638:ASP:HB3	2.32	0.60
1:D:393:LYS:CG	1:D:394:THR:H	2.10	0.60
1:A:80:LYS:HA	1:B:83:ASN:HD22	1.67	0.60
1:A:752:LYS:O	1:A:756:GLN:HG3	2.01	0.59
1:B:214:HIS:CE1	1:D:212:GLY:HA2	2.37	0.59
1:B:513:GLY:O	1:B:514:VAL:HB	2.02	0.59
1:C:130:TRP:CD2	1:C:191:ARG:HD3	2.36	0.59
1:C:262:TRP:CZ2	1:C:273:ALA:HA	2.37	0.59
1:A:514:VAL:HA	1:A:794:GLY:HA3	1.83	0.59
1:B:178:ARG:NE	1:D:237:PHE:CZ	2.70	0.59
1:F:18:ALA:HA	1:F:21:PHE:HD2	1.67	0.59
1:A:78:ASP:N	1:A:81:SER:OG	2.34	0.59
1:B:372:GLY:HA2	1:B:383:THR:HG23	1.84	0.59
1:D:579:PHE:HZ	1:D:590:ASP:H	1.50	0.59
1:A:663:LYS:HA	1:A:663:LYS:CE	2.10	0.59
1:B:77:TYR:HE2	1:B:98:THR:HG21	1.67	0.59
1:B:502:ILE:HG12	1:B:703:LEU:CD2	2.33	0.59
1:A:718:CYS:CB	1:A:773:CYS:SG	2.91	0.59
1:D:477:ALA:HB1	1:D:478:PRO:HD2	1.85	0.59
1:D:586:GLN:O	1:D:588:GLY:N	2.36	0.59
1:A:56:PHE:HD1	1:B:88:PHE:CE2	2.20	0.59
1:A:308:ARG:HB3	1:A:311:ASN:HD22	1.67	0.59
1:B:477:ALA:HB1	1:B:478:PRO:HD2	1.85	0.59
1:C:477:ALA:HB1	1:C:478:PRO:HD2	1.85	0.59
1:D:663:LYS:HE2	1:D:663:LYS:CA	2.21	0.59
1:A:787:LEU:HD12	1:D:521:LEU:HA	1.85	0.59
1:C:38:THR:HG21	1:C:297:ARG:HH21	1.67	0.59
1:A:595:SER:N	1:A:599:ARG:HE	2.01	0.58
1:B:35:GLN:OE1	1:B:261:ARG:NH2	2.36	0.58
1:C:23:ASP:HB3	1:C:271:PRO:HG2	1.84	0.58
1:C:236:GLN:NE2	1:C:365:THR:O	2.35	0.58
1:C:590:ASP:O	1:C:592:SER:N	2.30	0.58
1:D:594:ARG:O	1:D:596:LEU:N	2.36	0.58
1:C:387:THR:C	1:C:389:GLY:H	2.07	0.58
1:C:416:GLU:OE1	1:C:417:GLY:N	2.30	0.58
1:D:597:SER:O	1:D:600:ILE:HG12	2.02	0.58
1:B:328:GLU:OE2	1:B:331:ARG:NH1	2.34	0.58
1:D:785:SER:O	1:D:786:ALA:CB	2.52	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:ALA:HB1	1:A:478:PRO:HD2	1.85	0.58
1:B:630:VAL:O	1:B:630:VAL:HG13	2.03	0.58
1:A:30:ARG:NH2	1:A:269:GLU:OE2	2.35	0.58
1:C:502:ILE:HG12	1:C:703:LEU:HD23	1.84	0.58
1:A:684:ARG:HB2	1:A:684:ARG:CZ	2.33	0.58
1:A:783:LYS:HG2	1:A:783:LYS:O	2.04	0.58
1:C:783:LYS:O	1:C:783:LYS:HG2	2.04	0.58
1:D:657:GLU:OE2	1:D:661:ARG:CZ	2.51	0.58
1:B:625:THR:HG21	1:C:625:THR:HG23	1.84	0.58
1:E:18:ALA:HA	1:E:21:PHE:HD2	1.69	0.58
1:B:178:ARG:HD3	1:D:237:PHE:CD1	2.39	0.57
1:B:250:TYR:HA	1:B:255:VAL:HG11	1.87	0.57
1:C:504:ILE:HD12	1:C:723:VAL:CG2	2.34	0.57
1:C:13:GLN:HB3	1:C:70:VAL:HG12	1.86	0.57
1:C:520:PRO:HB2	1:C:616:TYR:CE1	2.40	0.57
1:A:50:LEU:HD23	1:A:57:ALA:HB1	1.87	0.57
1:B:214:HIS:CE1	1:D:212:GLY:HA3	2.39	0.57
1:B:684:ARG:NH1	1:B:688:GLU:OE1	2.37	0.57
1:D:25:GLU:HG2	1:D:76:PHE:HZ	1.69	0.57
1:F:195:PRO:HD2	1:F:199:ARG:HB3	1.87	0.57
1:B:25:GLU:HG2	1:B:76:PHE:HZ	1.68	0.57
1:B:785:SER:O	1:B:786:ALA:CB	2.52	0.57
1:A:387:THR:C	1:A:389:GLY:H	2.07	0.57
1:C:308:ARG:HB3	1:C:311:ASN:HD22	1.68	0.57
1:B:209:ILE:CG2	1:D:209:ILE:HG22	2.34	0.57
1:E:37:ARG:HA	1:E:87:LEU:HA	1.85	0.57
1:C:503:MET:CB	1:C:709:ASN:OD1	2.44	0.56
1:C:347:PHE:HE1	1:C:353:ARG:HG2	1.70	0.56
1:A:266:GLU:HG2	1:A:268:LYS:H	1.70	0.56
1:B:586:GLN:O	1:B:588:GLY:N	2.38	0.56
1:B:587:GLN:HE21	1:C:586:GLN:HA	1.69	0.56
1:B:630:VAL:O	1:B:631:SER:C	2.44	0.56
1:C:345:ILE:HG12	1:C:353:ARG:NH2	2.21	0.56
1:C:503:MET:HA	1:C:721:MET:O	2.04	0.56
1:C:594:ARG:HB3	1:D:578:TRP:HE3	1.69	0.56
1:A:262:TRP:CZ2	1:A:273:ALA:HA	2.41	0.56
1:B:215:VAL:HG11	1:D:215:VAL:CG1	2.33	0.56
1:C:684:ARG:HG3	1:C:684:ARG:NH2	2.19	0.56
1:B:520:PRO:O	1:C:787:LEU:HD12	2.06	0.56
1:C:594:ARG:HD3	1:D:575:ASN:HB2	1.87	0.56
1:D:236:GLN:NE2	1:D:364:LYS:O	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ALA:HB3	1:A:192:VAL:HG22	1.85	0.56
1:A:334:LYS:HD3	1:A:349:GLN:HA	1.86	0.56
1:C:371:ILE:O	1:C:383:THR:N	2.31	0.56
1:B:308:ARG:HH21	1:B:325:GLN:H	1.53	0.56
1:C:25:GLU:OE1	1:C:25:GLU:N	2.34	0.56
1:A:13:GLN:HB3	1:A:70:VAL:HG12	1.87	0.56
1:A:307:SER:O	1:A:308:ARG:NH1	2.39	0.56
1:F:37:ARG:HA	1:F:87:LEU:HA	1.86	0.56
1:A:77:TYR:OH	1:A:101:PHE:O	2.13	0.56
1:A:628:ARG:HH21	1:D:628:ARG:HG2	1.70	0.56
1:B:600:ILE:HG22	1:C:581:LEU:HD11	1.87	0.56
1:E:36:GLN:NE2	1:E:197:ASP:O	2.35	0.56
1:A:578:TRP:CG	1:D:595:SER:HB3	2.41	0.55
1:C:50:LEU:HD23	1:C:57:ALA:HB1	1.88	0.55
1:C:504:ILE:CD1	1:C:723:VAL:HG22	2.36	0.55
1:C:634:GLU:HG2	1:C:634:GLU:O	2.06	0.55
1:D:633:ILE:HD13	1:D:645:ILE:HD12	1.83	0.55
1:E:122:GLY:HA2	1:E:125:TRP:HD1	1.71	0.55
1:F:13:ALA:HA	1:F:16:LEU:HD12	1.89	0.55
1:A:587:GLN:NE2	1:B:587:GLN:OE1	2.40	0.55
1:C:525:ILE:HG12	1:D:789:LEU:HD13	1.89	0.55
1:C:390:LEU:HD12	1:C:391:GLU:HG3	1.89	0.55
1:C:742:LEU:C	1:C:745:PRO:HD2	2.27	0.55
1:B:742:LEU:C	1:B:745:PRO:HD2	2.27	0.55
1:C:504:ILE:CD1	1:C:723:VAL:CG2	2.85	0.55
1:A:25:GLU:N	1:A:25:GLU:OE1	2.36	0.55
1:A:66:PHE:CZ	1:A:312:ALA:HB1	2.42	0.55
1:C:586:GLN:O	1:C:588:GLY:N	2.39	0.55
1:F:122:GLY:HA2	1:F:125:TRP:HD1	1.72	0.55
1:A:177:TYR:CD2	1:A:207:GLN:HG3	2.42	0.55
1:A:584:PHE:CZ	1:D:606:TRP:HZ3	2.25	0.55
1:C:78:ASP:N	1:C:81:SER:OG	2.39	0.55
1:C:587:GLN:NE2	1:D:587:GLN:OE1	2.40	0.55
1:E:195:PRO:HD2	1:E:199:ARG:HB3	1.88	0.55
1:A:393:LYS:O	1:A:394:THR:HB	2.07	0.55
1:E:191:VAL:HA	1:E:195:PRO:HG3	1.89	0.55
1:C:744:THR:N	1:C:745:PRO:CD	2.70	0.55
1:D:742:LEU:C	1:D:745:PRO:HD2	2.27	0.55
1:C:504:ILE:H	1:C:504:ILE:CD1	2.13	0.54
1:B:744:THR:N	1:B:745:PRO:CD	2.70	0.54
1:C:170:ASN:HA	1:C:173:LYS:HB2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:LEU:HD22	1:D:247:ILE:HB	1.89	0.54
1:B:178:ARG:CZ	1:D:237:PHE:CZ	2.90	0.54
1:B:608:PHE:CZ	1:B:612:ILE:HD11	2.43	0.54
1:C:393:LYS:O	1:C:394:THR:HB	2.07	0.54
1:B:209:ILE:HG22	1:D:209:ILE:CG2	2.36	0.54
1:C:316:LEU:HD22	1:D:60:ASN:HA	1.89	0.54
1:A:625:THR:HG23	1:D:625:THR:HG21	1.89	0.54
1:B:219:HIS:HD2	1:B:241:GLU:HB2	1.73	0.54
1:C:789:LEU:O	1:C:793:ALA:HB2	2.08	0.54
1:A:586:GLN:O	1:A:588:GLY:N	2.41	0.54
1:A:590:ASP:OD1	1:A:591:ILE:N	2.37	0.54
1:B:177:TYR:CD2	1:B:207:GLN:HG3	2.42	0.54
1:C:718:CYS:HB3	1:C:773:CYS:HG	1.72	0.54
1:D:76:PHE:HE1	1:D:99:PRO:HG2	1.73	0.54
1:D:744:THR:N	1:D:745:PRO:CD	2.70	0.54
1:B:610:LEU:HD21	1:C:613:ILE:HG21	1.89	0.54
1:B:619:ASN:ND2	1:C:786:ALA:HB1	2.22	0.54
1:C:66:PHE:CZ	1:C:312:ALA:HB1	2.43	0.54
1:C:211:ILE:HG13	1:C:213:LYS:H	1.73	0.54
1:B:512:PRO:HA	1:B:516:SER:HB3	1.87	0.53
1:B:627:GLU:HG2	1:B:629:MET:CE	2.38	0.53
1:D:800:VAL:HA	1:D:803:LEU:HD12	1.89	0.53
1:B:592:SER:O	1:B:599:ARG:NH2	2.41	0.53
1:B:661:ARG:HB2	1:B:661:ARG:CZ	2.38	0.53
1:E:133:LEU:HD23	1:E:136:LEU:HD12	1.91	0.53
1:C:112:GLN:HE21	1:C:352:LYS:HA	1.74	0.53
1:C:247:ILE:HG23	1:C:248:VAL:HG23	1.91	0.53
1:D:227:PHE:CD1	1:D:244:GLY:HA3	2.42	0.53
1:E:13:ALA:HA	1:E:16:LEU:HD12	1.91	0.53
1:A:79:LYS:NZ	1:A:140:ASP:HA	2.24	0.53
1:A:263:SER:O	1:A:274:HIS:ND1	2.42	0.53
1:A:455:ALA:O	1:A:456:ASP:HB2	2.07	0.53
1:E:29:THR:HG23	1:E:30:TYR:CD1	2.44	0.53
1:B:76:PHE:HE1	1:B:99:PRO:HG2	1.73	0.53
1:C:134:ALA:HB3	1:C:192:VAL:HG22	1.89	0.53
1:F:29:THR:HG23	1:F:30:TYR:CD1	2.44	0.53
1:B:453:ARG:CG	1:B:460:TRP:CE2	2.91	0.53
1:D:644:GLU:HG2	1:D:645:ILE:HG13	1.90	0.53
1:C:138:ASP:OD1	1:C:139:SER:N	2.41	0.53
1:D:161:THR:HG1	1:D:187:LYS:HZ2	1.56	0.53
1:B:225:LEU:HD22	1:B:247:ILE:HB	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:GLY:O	1:F:90:PHE:N	2.42	0.53
1:A:718:CYS:HB2	1:A:773:CYS:SG	2.49	0.52
1:B:237:PHE:CD1	1:D:178:ARG:NE	2.77	0.52
1:D:512:PRO:HA	1:D:516:SER:HB3	1.89	0.52
1:E:34:GLY:O	1:E:90:PHE:N	2.42	0.52
1:B:237:PHE:CE2	1:D:178:ARG:CZ	2.93	0.52
1:A:786:ALA:CB	1:D:619:ASN:HD21	2.23	0.52
1:C:77:TYR:CE2	1:C:100:SER:HB2	2.45	0.52
1:C:316:LEU:HD11	1:D:63:CYS:SG	2.50	0.52
1:F:36:GLN:NE2	1:F:197:ASP:O	2.38	0.52
1:F:39:PRO:O	1:F:85:PHE:N	2.42	0.52
1:A:80:LYS:HG2	1:B:83:ASN:ND2	2.24	0.52
1:A:685:THR:OG1	1:A:688:GLU:HG3	2.09	0.52
1:B:237:PHE:CE1	1:D:178:ARG:NE	2.78	0.52
1:B:590:ASP:O	1:B:599:ARG:NE	2.43	0.52
1:C:590:ASP:CG	1:C:591:ILE:H	2.13	0.52
1:D:77:TYR:HE2	1:D:98:THR:HG21	1.74	0.52
1:D:721:MET:HG3	1:D:776:LYS:CE	2.37	0.52
1:B:236:GLN:HA	1:B:363:LEU:HD21	1.91	0.52
1:B:532:ALA:O	1:B:536:VAL:HG23	2.10	0.52
1:C:600:ILE:HA	1:D:581:LEU:HD21	1.91	0.52
1:D:330:GLU:HA	1:D:333:LEU:HD12	1.91	0.52
1:B:502:ILE:HG12	1:B:703:LEU:HD23	1.91	0.52
1:B:579:PHE:CZ	1:B:591:ILE:HG22	2.44	0.52
1:D:791:ASN:OD1	1:D:792:VAL:HG23	2.09	0.52
1:E:39:PRO:O	1:E:85:PHE:N	2.43	0.52
1:F:127:SER:O	1:F:130:SER:OG	2.23	0.52
1:A:56:PHE:CD1	1:B:88:PHE:CD2	2.97	0.52
1:A:786:ALA:O	1:A:787:LEU:CB	2.55	0.52
1:B:261:ARG:O	1:B:264:THR:OG1	2.21	0.52
1:C:363:LEU:HA	1:C:368:PRO:HA	1.91	0.52
1:D:219:HIS:CD2	1:D:241:GLU:HB2	2.45	0.52
1:C:56:PHE:HD1	1:D:88:PHE:CD2	2.27	0.52
1:C:453:ARG:HD2	1:C:460:TRP:CH2	2.45	0.52
1:A:581:LEU:HD21	1:D:600:ILE:HA	1.92	0.51
1:B:594:ARG:O	1:B:596:LEU:N	2.42	0.51
1:A:259:ILE:HA	1:A:262:TRP:HB3	1.93	0.51
1:A:746:VAL:HG12	1:A:746:VAL:O	2.10	0.51
1:B:219:HIS:CD2	1:B:241:GLU:HB2	2.45	0.51
1:B:606:TRP:HZ3	1:C:584:PHE:CZ	2.28	0.51
1:C:387:THR:O	1:C:389:GLY:N	2.38	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:346:LYS:HD3	1:D:355:ASN:HD22	1.76	0.51
1:A:539:VAL:HA	1:A:542:LEU:HD12	1.93	0.51
1:D:261:ARG:O	1:D:264:THR:OG1	2.18	0.51
1:A:317:ALA:O	1:A:320:ALA:N	2.44	0.51
1:A:355:ASN:N	1:A:376:GLU:OE2	2.22	0.51
1:E:127:SER:O	1:E:130:SER:OG	2.22	0.51
1:A:504:ILE:CD1	1:A:723:VAL:HG22	2.38	0.51
1:A:721:MET:HE2	1:A:723:VAL:HG12	1.93	0.51
1:B:178:ARG:CD	1:D:237:PHE:CE1	2.93	0.51
1:C:121:LEU:HA	1:C:245:PHE:CZ	2.45	0.51
1:D:130:TRP:CD2	1:D:191:ARG:HD3	2.46	0.51
1:D:219:HIS:HD2	1:D:241:GLU:HB2	1.76	0.51
1:D:348:ASP:OD1	1:D:351:GLY:N	2.43	0.51
1:D:388:SER:OG	1:D:389:GLY:N	2.43	0.51
1:A:581:LEU:HD11	1:D:600:ILE:HG22	1.93	0.51
1:C:263:SER:O	1:C:274:HIS:ND1	2.44	0.51
1:D:608:PHE:CZ	1:D:612:ILE:HD11	2.45	0.51
1:E:177:MET:O	1:E:181:MET:HG2	2.11	0.51
1:D:794:GLY:HA2	1:D:797:TYR:CD2	2.45	0.51
1:B:130:TRP:CE2	1:B:191:ARG:HD3	2.46	0.51
1:C:504:ILE:N	1:C:504:ILE:CD1	2.73	0.51
1:D:309:ARG:HD3	1:D:311:ASN:HB2	1.94	0.51
1:A:387:THR:O	1:A:389:GLY:N	2.38	0.50
1:B:174:ASP:CG	1:B:178:ARG:HH12	2.14	0.50
1:B:348:ASP:OD1	1:B:351:GLY:N	2.45	0.50
1:C:718:CYS:CB	1:C:773:CYS:SG	2.98	0.50
1:E:157:ASP:HB3	1:E:160:LYS:HB2	1.93	0.50
1:A:763:LYS:O	1:A:767:TRP:HB2	2.11	0.50
1:B:130:TRP:CD2	1:B:191:ARG:HD3	2.45	0.50
1:B:190:ARG:HD3	1:B:218:TYR:CE1	2.46	0.50
1:C:178:ARG:NH1	1:C:211:ILE:HG22	2.27	0.50
1:C:619:ASN:ND2	1:D:787:LEU:HB2	2.26	0.50
1:D:99:PRO:HA	1:D:113:MET:HB2	1.93	0.50
1:A:347:PHE:HE1	1:A:353:ARG:HG2	1.77	0.50
1:C:211:ILE:HD12	1:C:213:LYS:HD2	1.94	0.50
1:C:763:LYS:O	1:C:767:TRP:HB2	2.12	0.50
1:A:77:TYR:CE2	1:A:100:SER:HB2	2.47	0.50
1:B:453:ARG:HG3	1:B:460:TRP:CG	2.47	0.50
1:D:130:TRP:CE2	1:D:191:ARG:HD3	2.46	0.50
1:A:17:LEU:HB2	1:A:75:GLY:HA3	1.93	0.50
1:B:789:LEU:O	1:B:789:LEU:HG	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:GLN:C	1:C:394:THR:H	2.15	0.50
1:D:763:LYS:O	1:D:767:TRP:HB2	2.11	0.50
1:F:157:ASP:HB3	1:F:160:LYS:HB2	1.94	0.50
1:A:584:PHE:HD1	1:A:605:TRP:HZ2	1.59	0.50
1:B:326:GLY:HA2	1:B:329:ILE:HD12	1.93	0.50
1:D:595:SER:HA	1:D:599:ARG:CB	2.35	0.50
1:B:132:LYS:NZ	1:B:189:GLU:OE2	2.44	0.50
1:C:521:LEU:O	1:C:526:TRP:NE1	2.44	0.50
1:D:190:ARG:HD3	1:D:218:TYR:CE1	2.47	0.50
1:B:178:ARG:NE	1:D:237:PHE:CE2	2.80	0.49
1:B:453:ARG:HG3	1:B:460:TRP:CD1	2.47	0.49
1:B:763:LYS:O	1:B:767:TRP:HB2	2.11	0.49
1:C:644:GLU:HG2	1:C:645:ILE:HG13	1.93	0.49
1:D:77:TYR:CE2	1:D:100:SER:HB2	2.47	0.49
1:D:392:GLN:CD	1:D:437:GLY:O	2.50	0.49
1:D:593:PRO:HD2	1:D:596:LEU:HD23	1.93	0.49
1:D:595:SER:O	1:D:597:SER:N	2.44	0.49
1:F:133:LEU:HD23	1:F:136:LEU:HD12	1.92	0.49
1:A:101:PHE:HA	1:A:114:ARG:HH11	1.78	0.49
1:C:597:SER:O	1:C:600:ILE:HG12	2.13	0.49
1:D:803:LEU:O	1:D:807:MET:HG2	2.12	0.49
1:A:135:TYR:HH	1:A:145:THR:HG1	1.59	0.49
1:A:744:THR:CB	1:A:745:PRO:HD3	2.42	0.49
1:C:115:PRO:HB3	1:C:356:TYR:CG	2.48	0.49
1:C:267:GLU:HG3	1:C:271:PRO:HA	1.94	0.49
1:D:627:GLU:HG2	1:D:629:MET:HE2	1.93	0.49
1:A:130:TRP:CZ3	1:A:191:ARG:HB3	2.47	0.49
1:A:392:GLN:C	1:A:394:THR:H	2.15	0.49
1:B:77:TYR:CE2	1:B:100:SER:HB2	2.48	0.49
1:A:77:TYR:CE2	1:A:98:THR:HG21	2.40	0.49
1:B:627:GLU:HG2	1:B:629:MET:HE3	1.94	0.49
1:D:177:TYR:CD2	1:D:207:GLN:HG3	2.47	0.49
1:D:337:GLN:OE1	1:D:346:LYS:NZ	2.33	0.49
1:D:532:ALA:O	1:D:536:VAL:HG23	2.12	0.49
1:A:124:LEU:HD11	1:A:128:TYR:HE1	1.77	0.49
1:C:504:ILE:CD1	1:C:723:VAL:HG13	2.36	0.49
1:C:786:ALA:O	1:C:787:LEU:CB	2.55	0.49
1:D:246:GLN:HE21	1:D:248:VAL:N	2.09	0.49
1:D:627:GLU:HG2	1:D:629:MET:CE	2.43	0.49
1:A:316:LEU:HD11	1:B:63:CYS:SG	2.53	0.49
1:B:24:GLN:NE2	1:B:278:ILE:HG13	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:PHE:CD1	1:B:244:GLY:HA3	2.48	0.49
1:C:607:PHE:O	1:C:611:ILE:HG12	2.12	0.49
1:F:170:VAL:O	1:F:174:LEU:HG	2.13	0.49
1:A:97:ILE:HG13	1:A:111:ILE:HB	1.93	0.49
1:A:247:ILE:HG13	1:A:342:SER:HB2	1.93	0.49
1:A:785:SER:O	1:A:786:ALA:HB2	2.13	0.49
1:C:619:ASN:HD21	1:D:787:LEU:HB2	1.78	0.49
1:D:243:SER:OG	1:D:362:GLU:HG2	2.13	0.49
1:A:640:SER:O	1:A:669:LYS:HE3	2.13	0.49
1:B:794:GLY:HA2	1:B:797:TYR:CD2	2.48	0.49
1:D:174:ASP:CG	1:D:178:ARG:HH12	2.16	0.49
1:D:209:ILE:HA	1:D:214:HIS:HD2	1.77	0.49
1:D:782:GLU:O	1:D:783:LYS:HG3	2.13	0.49
1:A:138:ASP:OD1	1:A:139:SER:N	2.46	0.48
1:B:329:ILE:O	1:B:333:LEU:HG	2.13	0.48
1:C:525:ILE:HG12	1:D:789:LEU:HB2	1.94	0.48
1:C:785:SER:O	1:C:786:ALA:HB2	2.13	0.48
1:D:640:SER:O	1:D:669:LYS:HE3	2.13	0.48
1:A:316:LEU:HD22	1:B:60:ASN:HA	1.95	0.48
1:B:178:ARG:CD	1:D:237:PHE:CD1	2.96	0.48
1:C:337:GLN:NE2	1:C:346:LYS:HE2	2.23	0.48
1:D:25:GLU:OE1	1:D:25:GLU:N	2.44	0.48
1:B:35:GLN:HG2	1:B:286:TYR:OH	2.13	0.48
1:C:291:VAL:HG13	1:C:336:VAL:HG11	1.95	0.48
1:C:97:ILE:HG13	1:C:111:ILE:HB	1.96	0.48
1:C:514:VAL:HA	1:C:794:GLY:HA3	1.96	0.48
1:C:789:LEU:O	1:C:793:ALA:CB	2.62	0.48
1:D:326:GLY:HA2	1:D:329:ILE:HD12	1.95	0.48
1:F:159:LEU:HD12	1:F:229:SER:HB3	1.95	0.48
1:A:23:ASP:HB3	1:A:271:PRO:HG2	1.95	0.48
1:D:250:TYR:HA	1:D:255:VAL:HG11	1.94	0.48
1:F:36:GLN:NE2	1:F:199:ARG:H	2.12	0.48
1:A:14:ILE:HG13	1:A:45:PRO:HA	1.95	0.48
1:B:161:THR:HG1	1:B:187:LYS:HZ2	1.62	0.48
1:B:237:PHE:CD1	1:D:178:ARG:HD3	2.49	0.48
1:B:417:GLY:HA2	1:B:441:LYS:NZ	2.29	0.48
1:B:789:LEU:HD21	1:E:181:MET:CE	2.44	0.48
1:F:7:ARG:HH21	1:F:224:VAL:HG13	1.79	0.48
1:A:417:GLY:HA2	1:A:441:LYS:NZ	2.29	0.48
1:A:633:ILE:HD13	1:A:645:ILE:CD1	2.43	0.48
1:D:592:SER:OG	1:D:596:LEU:HB3	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:640:SER:O	1:B:669:LYS:HE3	2.13	0.48
1:C:640:SER:O	1:C:669:LYS:HE3	2.13	0.48
1:F:28:THR:HG23	1:F:207:TRP:CD1	2.48	0.48
1:A:348:ASP:OD1	1:A:352:LYS:N	2.46	0.48
1:C:77:TYR:OH	1:C:101:PHE:O	2.16	0.48
1:A:255:VAL:O	1:A:259:ILE:HG12	2.13	0.48
1:A:784:THR:O	1:A:786:ALA:N	2.47	0.48
1:B:309:ARG:HD3	1:B:311:ASN:HB2	1.96	0.48
1:B:800:VAL:HA	1:B:803:LEU:HD12	1.94	0.48
1:A:256:SER:O	1:A:260:GLU:HG3	2.14	0.47
1:A:744:THR:CB	1:A:745:PRO:CD	2.91	0.47
1:B:25:GLU:OE1	1:B:25:GLU:N	2.45	0.47
1:C:364:LYS:HG3	1:C:369:ARG:NH2	2.29	0.47
1:B:306:ILE:HA	1:B:325:GLN:HE21	1.78	0.47
1:C:634:GLU:HG2	1:C:723:VAL:CB	2.28	0.47
1:E:28:THR:HG23	1:E:207:TRP:CD1	2.49	0.47
1:A:236:GLN:HA	1:A:363:LEU:HD21	1.97	0.47
1:B:78:ASP:N	1:B:81:SER:OG	2.48	0.47
1:B:243:SER:OG	1:B:362:GLU:HG2	2.14	0.47
1:B:579:PHE:CE1	1:B:591:ILE:HG22	2.49	0.47
1:C:299:LEU:O	1:C:303:ARG:N	2.45	0.47
1:C:633:ILE:HD13	1:C:645:ILE:CD1	2.45	0.47
1:C:657:GLU:OE2	1:C:661:ARG:CZ	2.62	0.47
1:C:784:THR:O	1:C:786:ALA:N	2.47	0.47
1:D:24:GLN:HE22	1:D:279:LYS:H	1.62	0.47
1:D:35:GLN:HG2	1:D:286:TYR:OH	2.14	0.47
1:D:417:GLY:HA2	1:D:441:LYS:NZ	2.29	0.47
1:A:522:ALA:H	1:A:525:ILE:HD12	1.79	0.47
1:C:14:ILE:HG13	1:C:45:PRO:HA	1.96	0.47
1:C:56:PHE:CD1	1:D:88:PHE:CE2	3.02	0.47
1:C:308:ARG:HB3	1:C:311:ASN:ND2	2.29	0.47
1:D:592:SER:OG	1:D:595:SER:O	2.26	0.47
1:D:633:ILE:CG2	1:D:638:ASP:CB	2.92	0.47
1:E:227:LEU:O	1:E:231:THR:HG23	2.14	0.47
1:A:607:PHE:O	1:A:611:ILE:HG12	2.14	0.47
1:D:512:PRO:HB3	1:D:516:SER:HB3	1.67	0.47
1:A:585:MET:HG3	1:D:603:GLY:HA2	1.97	0.47
1:A:629:MET:O	1:A:630:VAL:O	2.33	0.47
1:A:634:GLU:HG2	1:A:723:VAL:HB	1.93	0.47
1:B:506:LYS:CG	1:B:507:PRO:HD2	2.45	0.47
1:B:782:GLU:O	1:B:783:LYS:HG3	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:GLY:HA2	1:C:441:LYS:NZ	2.29	0.47
1:E:36:GLN:NE2	1:E:199:ARG:H	2.13	0.47
1:E:159:LEU:HD12	1:E:229:SER:HB3	1.95	0.47
1:A:506:LYS:NZ	1:A:721:MET:HG3	2.30	0.47
1:A:613:ILE:HG21	1:D:610:LEU:HD21	1.95	0.47
1:B:95:SER:HA	1:B:109:PHE:HB3	1.97	0.47
1:B:663:LYS:HE2	1:B:663:LYS:CA	2.33	0.47
1:D:534:ILE:O	1:D:537:SER:OG	2.27	0.47
1:E:7:ARG:HH21	1:E:224:VAL:HG13	1.80	0.47
1:B:24:GLN:HE22	1:B:279:LYS:H	1.61	0.47
1:A:87:SER:OG	1:B:54:ASN:OD1	2.32	0.47
1:D:790:SER:OG	1:F:185:GLN:NE2	2.39	0.47
1:E:38:VAL:HG11	1:E:85:PHE:HD2	1.79	0.47
1:F:187:PHE:HE2	1:F:203:TRP:CD1	2.32	0.47
1:C:122:LEU:HA	1:C:125:ILE:HD12	1.97	0.47
1:C:776:LYS:HD2	1:C:776:LYS:HA	1.52	0.47
1:F:141:GLY:O	1:F:145:MET:HG3	2.15	0.47
1:A:526:TRP:HA	1:A:529:ILE:HG22	1.98	0.46
1:B:24:GLN:NE2	1:B:279:LYS:H	2.13	0.46
1:B:330:GLU:HA	1:B:333:LEU:HD12	1.98	0.46
1:D:197:GLU:O	1:D:201:VAL:HG23	2.15	0.46
1:F:38:VAL:HG11	1:F:85:PHE:HD2	1.79	0.46
1:A:541:PHE:HE2	1:E:226:THR:HG23	1.80	0.46
1:A:594:ARG:O	1:A:596:LEU:N	2.49	0.46
1:B:595:SER:HB3	1:C:578:TRP:CG	2.51	0.46
1:F:189:VAL:O	1:F:193:LEU:HD13	2.15	0.46
1:D:215:VAL:HA	1:D:238:GLY:O	2.16	0.46
1:E:187:PHE:HE2	1:E:203:TRP:CD1	2.33	0.46
1:B:526:TRP:HA	1:B:529:ILE:HG22	1.97	0.46
1:D:506:LYS:HA	1:D:507:PRO:HD3	1.44	0.46
1:E:94:ILE:HG12	1:E:95:TRP:CD1	2.51	0.46
1:C:83:ASN:ND2	1:D:80:LYS:CA	2.75	0.46
1:C:323:TRP:CE3	1:C:325:GLN:HB2	2.50	0.46
1:A:597:SER:O	1:A:600:ILE:HG12	2.16	0.46
1:A:721:MET:CE	1:A:723:VAL:HG12	2.46	0.46
1:B:308:ARG:NH2	1:B:325:GLN:HG2	2.29	0.46
1:C:721:MET:CE	1:C:723:VAL:HG12	2.46	0.46
1:D:124:LEU:HD11	1:D:128:TYR:HE1	1.81	0.46
1:B:178:ARG:NE	1:D:237:PHE:CD2	2.83	0.46
1:B:309:ARG:HG2	1:B:311:ASN:N	2.30	0.46
1:C:132:LYS:HD3	1:C:159:GLN:OE1	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:506:LYS:CG	1:D:507:PRO:HD2	2.45	0.46
1:D:529:ILE:HD12	1:D:612:ILE:HD13	1.97	0.46
1:D:721:MET:CE	1:D:723:VAL:HG12	2.46	0.46
1:F:94:ILE:HG12	1:F:95:TRP:CD1	2.51	0.46
1:D:592:SER:N	1:D:599:ARG:HH21	2.14	0.46
1:A:246:GLN:HE21	1:A:248:VAL:N	2.12	0.46
1:C:80:LYS:HG2	1:D:83:ASN:ND2	2.31	0.46
1:D:95:SER:HA	1:D:109:PHE:HB3	1.97	0.46
1:E:204:ASP:OD1	1:E:205:TYR:N	2.49	0.46
1:F:195:PRO:O	1:F:197:ASP:N	2.49	0.46
1:A:330:GLU:HG2	1:A:334:LYS:HE3	1.98	0.46
1:A:786:ALA:HB1	1:D:619:ASN:ND2	2.29	0.46
1:C:112:GLN:NE2	1:C:352:LYS:HG2	2.31	0.46
1:D:329:ILE:O	1:D:333:LEU:HG	2.16	0.46
1:D:513:GLY:O	1:D:514:VAL:CB	2.64	0.46
1:E:196:GLU:OE1	1:E:198:TRP:NE1	2.48	0.46
1:A:113:MET:HB3	1:A:284:LEU:HD22	1.98	0.45
1:A:188:LYS:HD2	1:A:190:ARG:NH2	2.22	0.45
1:A:261:ARG:O	1:A:265:LEU:HG	2.16	0.45
1:A:628:ARG:NH1	1:D:623:PHE:HA	2.31	0.45
1:B:146:LEU:HA	1:B:149:VAL:HG22	1.98	0.45
1:B:250:TYR:OH	1:B:277:THR:HB	2.16	0.45
1:B:345:ILE:HG12	1:B:353:ARG:NH2	2.31	0.45
1:C:813:GLU:O	1:C:817:LYS:HG3	2.16	0.45
1:D:371:ILE:HB	1:D:386:ASP:OD2	2.15	0.45
1:E:170:VAL:O	1:E:174:LEU:HG	2.15	0.45
1:F:213:TRP:O	1:F:216:PHE:HB3	2.16	0.45
1:A:130:TRP:CE2	1:A:191:ARG:HD3	2.51	0.45
1:B:453:ARG:HG3	1:B:460:TRP:CD2	2.51	0.45
1:B:721:MET:CE	1:B:723:VAL:HG12	2.46	0.45
1:C:346:LYS:HD2	1:C:355:ASN:HD22	1.81	0.45
1:F:178:VAL:O	1:F:181:MET:HB2	2.16	0.45
1:A:227:PHE:CD1	1:A:244:GLY:HA3	2.51	0.45
1:A:326:GLY:HA2	1:A:329:ILE:HD12	1.97	0.45
1:A:521:LEU:O	1:A:526:TRP:NE1	2.49	0.45
1:B:417:GLY:HA2	1:B:441:LYS:HZ2	1.81	0.45
1:C:255:VAL:O	1:C:259:ILE:HG12	2.16	0.45
1:D:345:ILE:HG12	1:D:353:ARG:NH2	2.31	0.45
1:E:34:GLY:HA3	1:E:90:PHE:HB2	1.99	0.45
1:F:195:PRO:HB2	1:F:198:TRP:O	2.16	0.45
1:A:80:LYS:CA	1:B:83:ASN:ND2	2.77	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:GLY:O	1:A:601:VAL:HB	2.16	0.45
1:B:236:GLN:NE2	1:B:364:LYS:O	2.47	0.45
1:B:347:PHE:HE1	1:B:353:ARG:HG2	1.82	0.45
1:C:177:TYR:HE1	1:C:204:ILE:HG12	1.82	0.45
1:D:607:PHE:O	1:D:611:ILE:HG12	2.16	0.45
1:F:117:PRO:O	1:F:119:SER:N	2.49	0.45
1:B:607:PHE:O	1:B:611:ILE:HG12	2.16	0.45
1:D:122:LEU:O	1:D:126:GLU:HG3	2.16	0.45
1:D:526:TRP:HA	1:D:529:ILE:HG22	1.98	0.45
1:E:141:GLY:O	1:E:145:MET:HG3	2.16	0.45
1:E:195:PRO:HB2	1:E:198:TRP:O	2.16	0.45
1:C:18:PHE:O	1:C:49:ASN:HA	2.16	0.45
1:C:197:GLU:O	1:C:201:VAL:HG23	2.16	0.45
1:C:684:ARG:NH2	1:C:684:ARG:CG	2.75	0.45
1:D:204:ILE:O	1:D:208:VAL:HG23	2.16	0.45
1:D:598:GLY:O	1:D:601:VAL:HB	2.17	0.45
1:A:504:ILE:N	1:A:504:ILE:CD1	2.77	0.45
1:C:121:LEU:HA	1:C:245:PHE:HZ	1.81	0.45
1:C:169:ASN:HD21	1:C:172:LYS:HE3	1.82	0.45
1:C:185:GLU:HA	1:C:188:LYS:HA	1.97	0.45
1:C:506:LYS:NZ	1:C:721:MET:HG3	2.31	0.45
1:A:684:ARG:NH2	1:A:684:ARG:CB	2.79	0.45
1:A:742:LEU:O	1:A:745:PRO:CD	2.61	0.45
1:B:122:LEU:O	1:B:126:GLU:HG3	2.17	0.45
1:B:131:ASP:OD1	1:B:132:LYS:N	2.50	0.45
1:B:506:LYS:HA	1:B:507:PRO:HD3	1.44	0.45
1:C:76:PHE:CD1	1:C:99:PRO:HD2	2.52	0.45
1:C:124:LEU:HD11	1:C:128:TYR:HE1	1.82	0.45
1:C:348:ASP:OD1	1:C:352:LYS:N	2.50	0.45
1:E:213:TRP:O	1:E:216:PHE:HB3	2.17	0.45
1:A:392:GLN:C	1:A:394:THR:N	2.70	0.45
1:A:534:ILE:O	1:A:537:SER:OG	2.24	0.45
1:B:540:LEU:HD12	1:B:580:SER:HB3	1.99	0.45
1:A:541:PHE:CZ	1:E:227:LEU:HD13	2.52	0.45
1:B:595:SER:H	1:B:599:ARG:HG3	1.81	0.45
1:C:517:PHE:O	1:C:520:PRO:HD2	2.17	0.45
1:C:594:ARG:O	1:C:596:LEU:N	2.48	0.45
1:E:178:VAL:O	1:E:182:MET:HG2	2.17	0.45
1:A:18:PHE:O	1:A:49:ASN:HA	2.17	0.44
1:A:629:MET:O	1:A:630:VAL:C	2.55	0.44
1:B:124:LEU:HD11	1:B:128:TYR:HE1	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:598:GLY:O	1:C:601:VAL:HB	2.16	0.44
1:C:789:LEU:O	1:C:793:ALA:N	2.47	0.44
1:D:116:ASP:OD1	1:D:118:LYS:HG2	2.17	0.44
1:F:31:TRP:CE2	1:F:183:TYR:HE2	2.36	0.44
1:A:384:GLU:O	1:A:386:ASP:N	2.50	0.44
1:B:237:PHE:CZ	1:D:178:ARG:NE	2.85	0.44
1:C:267:GLU:CG	1:C:271:PRO:HA	2.48	0.44
1:C:809:VAL:HA	1:C:812:ILE:HG12	1.99	0.44
1:D:325:GLN:O	1:D:329:ILE:HG13	2.16	0.44
1:D:391:GLU:O	1:D:392:GLN:HG3	2.17	0.44
1:E:8:ALA:O	1:E:12:VAL:HG23	2.16	0.44
1:A:107:HIS:HA	1:A:108:PRO:HD3	1.84	0.44
1:A:172:LYS:O	1:A:174:ASP:N	2.48	0.44
1:A:663:LYS:O	1:A:663:LYS:HD3	2.18	0.44
1:B:198:ARG:CZ	1:B:230:GLY:HA2	2.47	0.44
1:B:503:MET:HA	1:B:721:MET:O	2.17	0.44
1:C:130:TRP:CZ3	1:C:191:ARG:HB3	2.53	0.44
1:A:190:ARG:HD3	1:A:218:TYR:CE1	2.53	0.44
1:B:68:ARG:HB3	1:B:70:VAL:HG13	1.99	0.44
1:B:112:GLN:HE21	1:B:352:LYS:HA	1.82	0.44
1:B:204:ILE:O	1:B:208:VAL:HG23	2.18	0.44
1:B:391:GLU:O	1:B:392:GLN:HG3	2.17	0.44
1:C:250:TYR:HA	1:C:255:VAL:HG11	1.99	0.44
1:C:599:ARG:HH22	1:D:581:LEU:HB3	1.83	0.44
1:A:595:SER:HB2	1:B:578:TRP:CG	2.53	0.44
1:A:781:LYS:O	1:A:784:THR:HG23	2.17	0.44
1:B:99:PRO:HA	1:B:113:MET:HB2	1.99	0.44
1:B:237:PHE:CZ	1:D:178:ARG:CZ	3.01	0.44
1:C:306:ILE:HA	1:C:325:GLN:HE21	1.82	0.44
1:C:314:ASP:OD1	1:C:315:CYS:N	2.51	0.44
1:C:392:GLN:C	1:C:394:THR:N	2.70	0.44
1:D:24:GLN:NE2	1:D:279:LYS:H	2.16	0.44
1:F:196:GLU:OE1	1:F:198:TRP:NE1	2.50	0.44
1:B:27:SER:O	1:B:31:VAL:HG23	2.18	0.44
1:B:323:TRP:CE3	1:B:325:GLN:HB2	2.53	0.44
1:B:388:SER:OG	1:B:389:GLY:N	2.43	0.44
1:C:17:LEU:HB2	1:C:75:GLY:HA3	1.99	0.44
1:C:521:LEU:HA	1:D:787:LEU:HD23	2.00	0.44
1:D:99:PRO:O	1:D:114:ARG:HB2	2.18	0.44
1:E:189:VAL:O	1:E:193:LEU:HD13	2.17	0.44
1:F:177:MET:HE3	1:F:212:ALA:HA	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:VAL:O	1:A:205:VAL:HG23	2.18	0.44
1:A:504:ILE:HD12	1:A:723:VAL:CG2	2.43	0.44
1:C:522:ALA:H	1:C:525:ILE:HD12	1.83	0.44
1:C:814:PHE:HA	1:C:817:LYS:HD2	2.00	0.44
1:F:204:ASP:OD1	1:F:205:TYR:N	2.50	0.44
1:A:79:LYS:O	1:A:82:VAL:HG12	2.18	0.44
1:A:174:ASP:OD2	1:A:178:ARG:NH2	2.45	0.44
1:B:57:ALA:HA	1:B:60:ASN:ND2	2.33	0.44
1:B:619:ASN:HD22	1:C:787:LEU:CD1	2.31	0.44
1:C:54:ASN:O	1:C:58:VAL:HG23	2.18	0.44
1:C:100:SER:C	1:C:114:ARG:HD3	2.37	0.44
1:C:227:PHE:CD1	1:C:244:GLY:HA3	2.53	0.44
1:D:309:ARG:HG2	1:D:311:ASN:N	2.31	0.44
1:A:628:ARG:NH2	1:D:628:ARG:H	2.16	0.44
1:C:384:GLU:O	1:C:386:ASP:N	2.50	0.44
1:C:453:ARG:NH2	1:C:484:VAL:HB	2.32	0.44
1:C:526:TRP:HA	1:C:529:ILE:HG22	1.99	0.44
1:C:592:SER:HA	1:C:593:PRO:HD3	1.85	0.44
1:C:629:MET:O	1:C:630:VAL:C	2.56	0.44
1:D:50:LEU:HD22	1:D:61:ALA:HB2	1.98	0.44
1:E:37:ARG:HG2	1:E:88:ARG:H	1.83	0.44
1:B:506:LYS:CG	1:B:507:PRO:CD	2.96	0.43
1:C:519:ASP:N	1:C:520:PRO:CD	2.81	0.43
1:C:781:LYS:O	1:C:784:THR:HG23	2.17	0.43
1:A:314:ASP:OD1	1:A:315:CYS:N	2.50	0.43
1:A:505:LYS:O	1:A:506:LYS:HG3	2.18	0.43
1:A:800:VAL:HA	1:A:803:LEU:HD12	2.01	0.43
1:C:56:PHE:CZ	1:D:91:THR:HG21	2.53	0.43
1:C:506:LYS:HG2	1:C:721:MET:SD	2.57	0.43
1:D:27:SER:O	1:D:31:VAL:HG23	2.18	0.43
1:F:34:GLY:HA3	1:F:90:PHE:HB2	2.00	0.43
1:F:195:PRO:O	1:F:198:TRP:N	2.51	0.43
1:A:56:PHE:CD1	1:B:88:PHE:CE2	3.03	0.43
1:B:100:SER:HA	1:B:114:ARG:NH2	2.33	0.43
1:B:266:GLU:HG2	1:B:268:LYS:H	1.83	0.43
1:B:308:ARG:NE	1:B:323:TRP:HB2	2.33	0.43
1:B:541:PHE:CD1	1:B:573:ILE:HA	2.53	0.43
1:C:629:MET:O	1:C:630:VAL:O	2.36	0.43
1:D:332:ALA:O	1:D:336:VAL:HG23	2.19	0.43
1:D:540:LEU:HD12	1:D:580:SER:HB3	2.00	0.43
1:D:541:PHE:CD1	1:D:573:ILE:HA	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:PRO:O	1:E:119:SER:N	2.51	0.43
1:F:227:LEU:O	1:F:231:THR:HG23	2.18	0.43
1:B:619:ASN:HD22	1:C:787:LEU:CG	2.27	0.43
1:C:113:MET:O	1:C:115:PRO:HD3	2.19	0.43
1:C:505:LYS:O	1:C:506:LYS:HG3	2.18	0.43
1:D:135:TYR:O	1:D:162:ALA:HA	2.18	0.43
1:D:372:GLY:CA	1:D:383:THR:HG23	2.42	0.43
1:D:374:TRP:CH2	1:D:376:GLU:HA	2.54	0.43
1:E:38:VAL:HB	1:E:85:PHE:HB2	2.00	0.43
1:F:8:ALA:O	1:F:12:VAL:HG23	2.17	0.43
1:A:813:GLU:O	1:A:817:LYS:HG3	2.19	0.43
1:B:197:GLU:O	1:B:201:VAL:HG23	2.17	0.43
1:E:167:VAL:O	1:E:171:LEU:HG	2.18	0.43
1:F:37:ARG:HG2	1:F:88:ARG:H	1.82	0.43
1:A:24:GLN:HE22	1:A:278:ILE:HA	1.84	0.43
1:A:101:PHE:HA	1:A:102:PRO:HD3	1.80	0.43
1:A:117:LEU:HD11	1:A:245:PHE:CG	2.53	0.43
1:A:595:SER:HA	1:A:599:ARG:HE	1.84	0.43
1:C:24:GLN:HE22	1:C:278:ILE:HA	1.83	0.43
1:D:506:LYS:CG	1:D:507:PRO:CD	2.96	0.43
1:A:153:ALA:HA	1:A:158:TRP:HB2	2.00	0.43
1:B:619:ASN:OD1	1:C:786:ALA:HB1	2.18	0.43
1:B:630:VAL:O	1:B:630:VAL:HG22	2.19	0.43
1:D:137:TYR:CE1	1:D:164:ASN:HB2	2.54	0.43
1:A:776:LYS:HA	1:A:776:LYS:HD2	1.52	0.43
1:C:316:LEU:HD13	1:D:63:CYS:CB	2.48	0.43
1:C:387:THR:C	1:C:389:GLY:N	2.72	0.43
1:C:526:TRP:O	1:C:529:ILE:HG22	2.19	0.43
1:D:201:VAL:O	1:D:205:VAL:HG23	2.19	0.43
1:E:227:LEU:O	1:E:227:LEU:HD12	2.19	0.43
1:A:101:PHE:HA	1:A:114:ARG:HD3	2.00	0.43
1:D:146:LEU:HA	1:D:149:VAL:HG22	1.99	0.43
1:A:54:ASN:O	1:A:58:VAL:HG23	2.18	0.42
1:A:387:THR:C	1:A:389:GLY:N	2.72	0.42
1:B:533:TYR:OH	1:B:581:LEU:HA	2.19	0.42
1:A:83:ASN:ND2	1:B:80:LYS:CA	2.77	0.42
1:B:105:GLY:O	1:B:107:HIS:ND1	2.52	0.42
1:B:135:TYR:O	1:B:162:ALA:HA	2.19	0.42
1:B:156:LYS:O	1:B:157:LYS:CG	2.67	0.42
1:B:592:SER:HB3	1:B:599:ARG:HG2	2.01	0.42
1:D:305:GLU:OE2	1:D:307:SER:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:223:SER:HA	1:E:226:THR:HG22	2.01	0.42
1:B:98:THR:HA	1:B:99:PRO:HD3	1.79	0.42
1:C:220:TYR:HB2	1:C:242:VAL:HG22	2.01	0.42
1:C:348:ASP:OD2	1:C:350:ASN:HB2	2.19	0.42
1:C:410:LYS:H	1:C:410:LYS:HD2	1.84	0.42
1:C:599:ARG:NH1	1:D:578:TRP:O	2.52	0.42
1:D:505:LYS:C	1:D:506:LYS:O	2.58	0.42
1:D:744:THR:OG1	1:D:745:PRO:CD	2.68	0.42
1:E:182:MET:O	1:E:185:GLN:HB3	2.20	0.42
1:A:267:GLU:HB2	1:A:274:HIS:HB3	2.02	0.42
1:A:595:SER:CA	1:A:599:ARG:HE	2.32	0.42
1:B:198:ARG:NH2	1:B:229:ASP:O	2.52	0.42
1:B:600:ILE:HA	1:C:581:LEU:HD21	2.01	0.42
1:C:115:PRO:HB3	1:C:356:TYR:CD1	2.54	0.42
1:E:3:SER:O	1:E:7:ARG:HG2	2.20	0.42
1:A:93:HIS:ND1	1:A:322:PRO:HG2	2.34	0.42
1:A:308:ARG:HB3	1:A:311:ASN:ND2	2.33	0.42
1:A:318:ASN:HA	1:A:319:PRO:HA	1.96	0.42
1:A:434:LYS:HE2	1:A:434:LYS:HB3	1.53	0.42
1:B:262:TRP:CZ2	1:B:273:ALA:HA	2.54	0.42
1:B:348:ASP:OD2	1:B:350:ASN:HB2	2.20	0.42
1:C:83:ASN:HD21	1:D:80:LYS:HA	1.81	0.42
1:C:323:TRP:CZ3	1:C:325:GLN:HB2	2.55	0.42
1:C:364:LYS:HG3	1:C:369:ARG:HH21	1.84	0.42
1:C:506:LYS:HE3	1:C:721:MET:N	2.33	0.42
1:D:24:GLN:NE2	1:D:278:ILE:HG13	2.28	0.42
1:D:131:ASP:OD1	1:D:132:LYS:N	2.53	0.42
1:A:113:MET:O	1:A:115:PRO:HD3	2.20	0.42
1:B:141:ARG:HH22	1:B:196:CYS:N	2.18	0.42
1:B:308:ARG:HE	1:B:323:TRP:HE3	1.67	0.42
1:D:299:LEU:HD23	1:D:306:ILE:HG21	2.01	0.42
1:E:134:TYR:O	1:E:138:LEU:HG	2.20	0.42
1:C:502:ILE:HG12	1:C:703:LEU:HD21	2.00	0.42
1:D:498:LEU:C	1:D:498:LEU:HD22	2.40	0.42
1:A:41:PHE:CE2	1:A:297:ARG:HD2	2.55	0.42
1:A:198:ARG:HA	1:A:201:VAL:HB	2.01	0.42
1:A:464:VAL:O	1:A:468:VAL:HG23	2.20	0.42
1:B:505:LYS:C	1:B:506:LYS:O	2.58	0.42
1:C:498:LEU:C	1:C:498:LEU:HD22	2.40	0.42
1:C:503:MET:O	1:C:503:MET:HG2	2.17	0.42
1:D:334:LYS:HA	1:D:347:PHE:HD2	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:LEU:C	1:A:745:PRO:HD2	2.38	0.42
1:B:212:GLY:CA	1:D:214:HIS:HE1	2.33	0.42
1:B:754:SER:HB3	1:B:759:LEU:HD12	2.02	0.42
1:C:26:TYR:CE2	1:C:30:ARG:HD2	2.54	0.42
1:E:10:LEU:O	1:E:14:LEU:HG	2.20	0.42
1:E:34:GLY:HA2	1:E:202:SER:HB2	2.02	0.42
1:A:197:GLU:O	1:A:201:VAL:HG23	2.20	0.42
1:A:634:GLU:HG3	1:A:723:VAL:CB	2.31	0.42
1:B:392:GLN:CD	1:B:437:GLY:O	2.58	0.42
1:B:464:VAL:O	1:B:468:VAL:HG23	2.20	0.42
1:B:518:LEU:HD22	1:B:526:TRP:CE2	2.55	0.42
1:C:30:ARG:NH2	1:C:269:GLU:OE2	2.53	0.42
1:E:195:PRO:O	1:E:198:TRP:N	2.52	0.42
1:F:117:PRO:HG3	1:F:193:LEU:HD21	2.01	0.42
1:B:619:ASN:HD21	1:C:786:ALA:CB	2.28	0.41
1:B:721:MET:HG3	1:B:776:LYS:CE	2.46	0.41
1:C:383:THR:HG22	1:C:385:ASP:H	1.85	0.41
1:C:666:VAL:HG13	1:C:667:PHE:N	2.36	0.41
1:D:347:PHE:HE1	1:D:353:ARG:HG2	1.85	0.41
1:E:31:TRP:CE2	1:E:183:TYR:HE2	2.37	0.41
1:E:194:GLY:O	1:E:196:GLU:N	2.53	0.41
1:F:178:VAL:O	1:F:182:MET:HG2	2.19	0.41
1:A:345:ILE:HG12	1:A:353:ARG:NH2	2.35	0.41
1:B:198:ARG:HG2	1:B:279:LYS:NZ	2.33	0.41
1:C:340:GLY:N	1:C:343:GLY:O	2.43	0.41
1:C:595:SER:H	1:C:599:ARG:NE	2.05	0.41
1:C:644:GLU:CG	1:C:645:ILE:HG13	2.49	0.41
1:E:21:PHE:HB3	1:E:211:LEU:HA	2.02	0.41
1:E:190:THR:O	1:E:195:PRO:HG3	2.20	0.41
1:F:34:GLY:HA2	1:F:202:SER:HB2	2.02	0.41
1:F:182:MET:O	1:F:185:GLN:HB3	2.20	0.41
1:F:223:SER:HA	1:F:226:THR:HG22	2.01	0.41
1:A:348:ASP:OD1	1:A:351:GLY:N	2.53	0.41
1:A:666:VAL:HG13	1:A:667:PHE:N	2.35	0.41
1:B:76:PHE:CE1	1:B:99:PRO:HG2	2.54	0.41
1:B:498:LEU:C	1:B:498:LEU:HD22	2.40	0.41
1:C:575:ASN:O	1:C:578:TRP:HB2	2.20	0.41
1:D:323:TRP:CZ3	1:D:325:GLN:HB2	2.55	0.41
1:D:464:VAL:O	1:D:468:VAL:HG23	2.20	0.41
1:D:666:VAL:HG13	1:D:667:PHE:N	2.35	0.41
1:D:721:MET:HE2	1:D:723:VAL:HG12	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:LEU:C	1:A:498:LEU:HD22	2.40	0.41
1:A:502:ILE:HG22	1:A:504:ILE:HG23	2.03	0.41
1:B:127:TYR:HB2	1:B:380:MET:SD	2.60	0.41
1:B:212:GLY:CA	1:D:214:HIS:CE1	3.04	0.41
1:B:215:VAL:CG1	1:D:215:VAL:HG11	2.46	0.41
1:B:591:ILE:HG23	1:B:591:ILE:O	2.21	0.41
1:D:250:TYR:OH	1:D:277:THR:HB	2.21	0.41
1:E:195:PRO:O	1:E:197:ASP:N	2.53	0.41
1:A:76:PHE:CD1	1:A:99:PRO:HD2	2.56	0.41
1:A:209:ILE:HA	1:A:214:HIS:HD2	1.86	0.41
1:A:383:THR:HG22	1:A:385:ASP:H	1.85	0.41
1:A:592:SER:HA	1:A:593:PRO:HD3	1.88	0.41
1:A:678:GLU:HA	1:A:679:PRO:C	2.41	0.41
1:A:754:SER:HB3	1:A:759:LEU:HD12	2.02	0.41
1:B:287:ASP:CG	1:B:341:LEU:H	2.24	0.41
1:B:453:ARG:HG3	1:B:460:TRP:CE2	2.55	0.41
1:C:344:ASN:HD21	1:C:346:LYS:CE	2.30	0.41
1:D:100:SER:HA	1:D:114:ARG:NH2	2.35	0.41
1:A:220:TYR:HB2	1:A:242:VAL:HG22	2.01	0.41
1:B:115:PRO:HG3	1:B:353:ARG:CZ	2.51	0.41
1:B:185:GLU:OE2	1:B:213:LYS:NZ	2.38	0.41
1:B:666:VAL:HG13	1:B:667:PHE:N	2.36	0.41
1:C:306:ILE:HD12	1:C:329:ILE:HD11	2.03	0.41
1:C:330:GLU:HG2	1:C:334:LYS:HE3	2.02	0.41
1:C:577:LEU:O	1:C:580:SER:OG	2.30	0.41
1:D:10:ASN:N	1:D:41:PHE:HA	2.35	0.41
1:F:99:GLU:OE2	1:F:108:LYS:HD2	2.21	0.41
1:A:87:SER:OG	1:B:56:PHE:N	2.38	0.41
1:A:362:GLU:O	1:A:369:ARG:N	2.50	0.41
1:A:575:ASN:O	1:A:578:TRP:HB2	2.20	0.41
1:B:228:THR:OG1	1:B:246:GLN:OE1	2.20	0.41
1:B:678:GLU:HA	1:B:679:PRO:C	2.41	0.41
1:C:464:VAL:O	1:C:468:VAL:HG23	2.20	0.41
1:C:754:SER:HB3	1:C:759:LEU:HD12	2.02	0.41
1:E:159:LEU:CD1	1:E:229:SER:HB3	2.51	0.41
1:F:116:ALA:HA	1:F:117:PRO:HA	1.80	0.41
1:A:39:SER:HA	1:A:42:ARG:NH2	2.36	0.41
1:A:718:CYS:SG	1:A:718:CYS:O	2.79	0.41
1:B:99:PRO:O	1:B:114:ARG:HB2	2.20	0.41
1:B:744:THR:OG1	1:B:745:PRO:CD	2.67	0.41
1:C:744:THR:OG1	1:C:745:PRO:CD	2.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:LYS:HB3	1:A:101:PHE:HZ	1.85	0.41
1:A:359:ASN:HA	1:A:373:TYR:HA	2.03	0.41
1:A:372:GLY:HA2	1:A:383:THR:OG1	2.20	0.41
1:A:708:MET:O	1:A:712:ILE:HG12	2.21	0.41
1:B:207:GLN:O	1:B:211:ILE:HG12	2.21	0.41
1:B:325:GLN:O	1:B:329:ILE:HG13	2.21	0.41
1:B:708:MET:O	1:B:712:ILE:HG12	2.21	0.41
1:C:56:PHE:N	1:D:87:SER:OG	2.46	0.41
1:C:332:ALA:O	1:C:336:VAL:HG23	2.20	0.41
1:C:453:ARG:HH21	1:C:484:VAL:HB	1.86	0.41
1:C:503:MET:HB2	1:C:709:ASN:CG	2.36	0.41
1:C:506:LYS:CG	1:C:721:MET:CB	2.95	0.41
1:C:634:GLU:HA	1:C:723:VAL:HG21	2.02	0.41
1:D:57:ALA:HA	1:D:60:ASN:ND2	2.35	0.41
1:D:512:PRO:HB2	1:D:516:SER:HG	1.70	0.41
1:E:99:GLU:OE2	1:E:108:LYS:HD2	2.21	0.41
1:F:134:TYR:O	1:F:138:LEU:HG	2.21	0.41
1:B:27:SER:HB3	1:B:270:TYR:HB3	2.03	0.41
1:B:172:LYS:O	1:B:174:ASP:N	2.54	0.41
1:B:523:TYR:HA	1:B:526:TRP:CD1	2.46	0.41
1:E:174:LEU:O	1:E:178:VAL:HG23	2.21	0.41
1:A:175:GLU:HA	1:A:178:ARG:HH11	1.86	0.40
1:A:246:GLN:HB2	1:A:361:MET:HG3	2.03	0.40
1:A:392:GLN:O	1:A:394:THR:N	2.54	0.40
1:A:425:CYS:SG	1:A:477:ALA:HA	2.61	0.40
1:B:128:TYR:HB3	1:B:130:TRP:NE1	2.36	0.40
1:B:190:ARG:HA	1:B:218:TYR:CD1	2.56	0.40
1:C:93:HIS:HB3	1:C:327:VAL:HG22	2.03	0.40
1:C:209:ILE:HA	1:C:214:HIS:HD2	1.86	0.40
1:C:348:ASP:OD1	1:C:351:GLY:N	2.55	0.40
1:C:540:LEU:HD12	1:C:580:SER:HB3	2.02	0.40
1:D:231:ASP:HB3	1:D:234:LYS:HE3	2.02	0.40
1:D:371:ILE:O	1:D:383:THR:OG1	2.25	0.40
1:D:743:GLY:C	1:D:745:PRO:HD2	2.41	0.40
1:D:754:SER:HB3	1:D:759:LEU:HD12	2.02	0.40
1:F:167:VAL:O	1:F:171:LEU:HG	2.21	0.40
1:A:112:GLN:NE2	1:A:352:LYS:HG2	2.36	0.40
1:A:247:ILE:HD13	1:A:358:ILE:HG12	2.02	0.40
1:A:577:LEU:O	1:A:580:SER:OG	2.32	0.40
1:B:50:LEU:HD23	1:B:57:ALA:HB1	2.03	0.40
1:B:118:LYS:NZ	1:B:144:SER:OG	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:CYS:HB3	1:B:200:LYS:HB2	2.04	0.40
1:C:79:LYS:O	1:C:82:VAL:HG12	2.21	0.40
1:D:425:CYS:SG	1:D:477:ALA:HA	2.62	0.40
1:D:678:GLU:HA	1:D:679:PRO:C	2.41	0.40
1:E:116:ALA:HA	1:E:117:PRO:HA	1.81	0.40
1:F:38:VAL:HB	1:F:85:PHE:HB2	2.03	0.40
1:F:187:PHE:O	1:F:190:THR:OG1	2.26	0.40
1:A:26:TYR:CE2	1:A:30:ARG:HD2	2.56	0.40
1:B:215:VAL:HA	1:B:238:GLY:O	2.22	0.40
1:B:489:ILE:HD12	1:B:735:ALA:HB1	2.03	0.40
1:B:521:LEU:HA	1:C:787:LEU:HD12	2.03	0.40
1:C:116:ASP:OD1	1:C:118:LYS:HG2	2.21	0.40
1:C:425:CYS:SG	1:C:477:ALA:HA	2.62	0.40
1:C:489:ILE:HD12	1:C:735:ALA:HB1	2.03	0.40
1:C:678:GLU:HA	1:C:679:PRO:C	2.41	0.40
1:D:489:ILE:HD12	1:D:735:ALA:HB1	2.03	0.40
1:D:799:LEU:O	1:D:803:LEU:HG	2.21	0.40
1:F:3:SER:O	1:F:7:ARG:HG2	2.21	0.40
1:A:532:ALA:O	1:A:536:VAL:HG23	2.21	0.40
1:A:803:LEU:O	1:A:807:MET:HG2	2.21	0.40
1:D:16:GLY:H	1:D:65:GLN:NE2	2.14	0.40
1:D:416:GLU:OE1	1:D:417:GLY:N	2.39	0.40
1:D:708:MET:O	1:D:712:ILE:HG12	2.21	0.40
1:A:671:TRP:O	1:A:675:ARG:HG2	2.22	0.40
1:B:743:GLY:C	1:B:745:PRO:HD2	2.42	0.40
1:C:708:MET:O	1:C:712:ILE:HG12	2.21	0.40
1:F:25:ALA:HB3	1:F:211:LEU:HD22	2.03	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	779/1057 (74%)	716 (92%)	47 (6%)	16 (2%)	5	30
1	B	776/1057 (73%)	723 (93%)	39 (5%)	14 (2%)	7	35
1	C	779/1057 (74%)	716 (92%)	45 (6%)	18 (2%)	5	28
1	D	776/1057 (73%)	723 (93%)	35 (4%)	18 (2%)	5	28
1	E	171/1057 (16%)	156 (91%)	7 (4%)	8 (5%)	2	16
1	F	171/1057 (16%)	156 (91%)	7 (4%)	8 (5%)	2	16
All	All	3452/6342 (54%)	3190 (92%)	180 (5%)	82 (2%)	7	27

All (82) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	385	ASP
1	A	456	ASP
1	A	514	VAL
1	A	630	VAL
1	A	776	LYS
1	B	456	ASP
1	B	506	LYS
1	B	507	PRO
1	B	512	PRO
1	B	631	SER
1	B	632	PRO
1	B	786	ALA
1	C	385	ASP
1	C	456	ASP
1	C	514	VAL
1	C	591	ILE
1	C	630	VAL
1	C	776	LYS
1	D	456	ASP
1	D	506	LYS
1	D	507	PRO
1	D	512	PRO
1	D	590	ASP
1	D	591	ILE
1	D	631	SER
1	D	632	PRO
1	D	635	SER
1	A	591	ILE
1	A	633	ILE
1	A	785	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	587	GLN
1	B	595	SER
1	B	630	VAL
1	C	174	ASP
1	C	587	GLN
1	C	633	ILE
1	C	785	SER
1	D	520	PRO
1	D	587	GLN
1	D	595	SER
1	D	596	LEU
1	E	111	SER
1	E	117	PRO
1	E	118	ALA
1	E	196	GLU
1	E	203	TRP
1	F	111	SER
1	F	118	ALA
1	F	196	GLU
1	F	203	TRP
1	A	587	GLN
1	A	594	ARG
1	A	595	SER
1	A	786	ALA
1	A	787	LEU
1	B	173	LYS
1	B	174	ASP
1	B	590	ASP
1	C	173	LYS
1	C	594	ARG
1	C	595	SER
1	C	786	ALA
1	C	787	LEU
1	D	786	ALA
1	F	117	PRO
1	A	174	ASP
1	A	775	ALA
1	C	590	ASP
1	C	775	ALA
1	D	594	ARG
1	A	394	THR
1	C	394	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	112	PHE
1	B	594	ARG
1	E	112	PHE
1	E	194	GLY
1	D	630	VAL
1	F	194	GLY
1	E	195	PRO
1	F	195	PRO
1	D	514	VAL
1	D	593	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	666/888 (75%)	648 (97%)	18 (3%)	40	58
1	B	664/888 (75%)	645 (97%)	19 (3%)	37	56
1	C	666/888 (75%)	648 (97%)	18 (3%)	40	58
1	D	664/888 (75%)	652 (98%)	12 (2%)	54	71
1	E	152/888 (17%)	151 (99%)	1 (1%)	81	87
1	F	152/888 (17%)	152 (100%)	0	100	100
All	All	2964/5328 (56%)	2896 (98%)	68 (2%)	46	64

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	369	ARG
1	A	388	SER
1	A	390	LEU
1	A	391	GLU
1	A	404	PRO
1	A	416	GLU
1	A	434	LYS
1	A	453	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	498	LEU
1	A	504	ILE
1	A	505	LYS
1	A	509	LYS
1	A	511	LYS
1	A	630	VAL
1	A	661	ARG
1	A	663	LYS
1	A	708	MET
1	A	773	CYS
1	B	384	GLU
1	B	385	ASP
1	B	393	LYS
1	B	404	PRO
1	B	416	GLU
1	B	434	LYS
1	B	453	ARG
1	B	498	LEU
1	B	503	MET
1	B	508	GLN
1	B	628	ARG
1	B	629	MET
1	B	633	ILE
1	B	634	GLU
1	B	661	ARG
1	B	663	LYS
1	B	684	ARG
1	B	708	MET
1	B	789	LEU
1	C	388	SER
1	C	390	LEU
1	C	404	PRO
1	C	410	LYS
1	C	416	GLU
1	C	434	LYS
1	C	498	LEU
1	C	503	MET
1	C	504	ILE
1	C	505	LYS
1	C	509	LYS
1	C	511	LYS
1	C	630	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	644	GLU
1	C	663	LYS
1	C	684	ARG
1	C	708	MET
1	C	773	CYS
1	D	384	GLU
1	D	385	ASP
1	D	393	LYS
1	D	404	PRO
1	D	416	GLU
1	D	434	LYS
1	D	498	LEU
1	D	508	GLN
1	D	633	ILE
1	D	644	GLU
1	D	663	LYS
1	D	708	MET
1	E	227	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	46	HIS
1	A	65	GLN
1	A	83	ASN
1	A	246	GLN
1	A	311	ASN
1	A	412	HIS
1	A	435	HIS
1	A	587	GLN
1	A	619	ASN
1	B	24	GLN
1	B	65	GLN
1	B	83	ASN
1	B	214	HIS
1	B	325	GLN
1	B	355	ASN
1	B	392	GLN
1	B	412	HIS
1	B	435	HIS
1	B	587	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	619	ASN
1	C	24	GLN
1	C	46	HIS
1	C	65	GLN
1	C	83	ASN
1	C	112	GLN
1	C	246	GLN
1	C	311	ASN
1	C	325	GLN
1	C	337	GLN
1	C	344	ASN
1	C	355	ASN
1	C	412	HIS
1	C	435	HIS
1	C	587	GLN
1	C	619	ASN
1	D	24	GLN
1	D	65	GLN
1	D	83	ASN
1	D	214	HIS
1	D	355	ASN
1	D	392	GLN
1	D	412	HIS
1	D	435	HIS
1	D	587	GLN
1	E	15	ASN
1	E	180	HIS
1	F	15	ASN
1	F	180	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	QUS	D	1101	-	6,13,13	1.28	0	1,18,18	0.29	0
2	QUS	B	1101	-	6,13,13	1.28	0	1,18,18	0.31	0
2	QUS	A	1101	-	6,13,13	1.28	0	1,18,18	0.29	0
2	QUS	C	1101	-	6,13,13	1.28	0	1,18,18	0.29	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	QUS	D	1101	-	-	2/6/8/8	0/1/1/1
2	QUS	B	1101	-	-	2/6/8/8	0/1/1/1
2	QUS	A	1101	-	-	2/6/8/8	0/1/1/1
2	QUS	C	1101	-	-	2/6/8/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	QUS	C01-C02-C03-N14
2	B	1101	QUS	C01-C02-C03-N14
2	C	1101	QUS	C01-C02-C03-N14
2	D	1101	QUS	C01-C02-C03-N14
2	A	1101	QUS	NP3-C02-C03-N14
2	B	1101	QUS	NP3-C02-C03-N14
2	C	1101	QUS	NP3-C02-C03-N14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	1101	QUS	NP3-C02-C03-N14

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	786:ALA	C	787:LEU	N	1.07

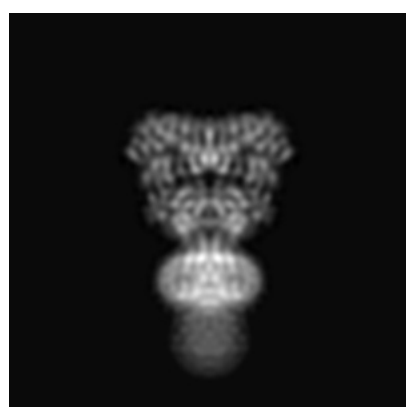
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8688. 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](#)

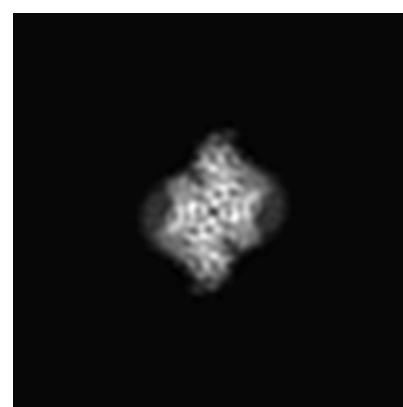
6.1.1 Primary map



X



Y



Z

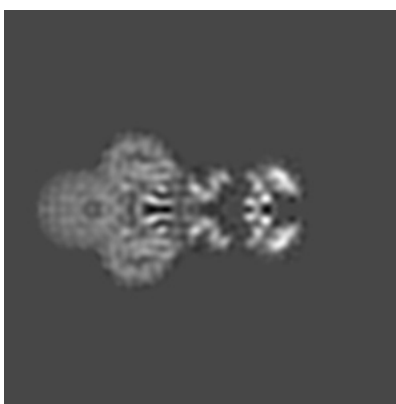
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 180



Y Index: 180



Z Index: 180

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: 180



Y Index: 189

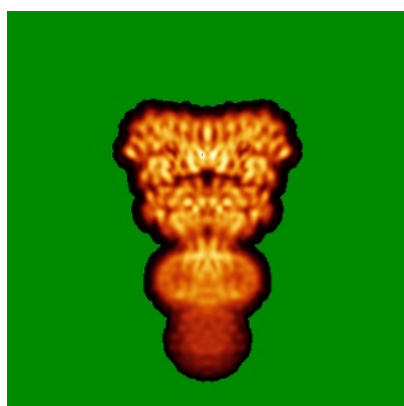


Z Index: 227

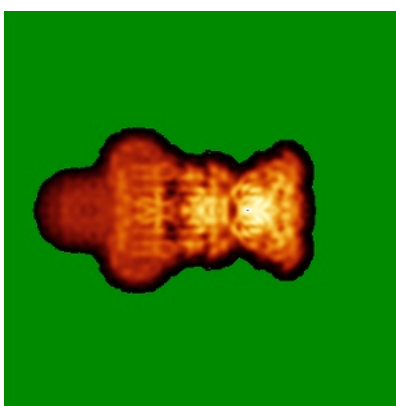
The images above show the largest variance slices of the map in three orthogonal directions.

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

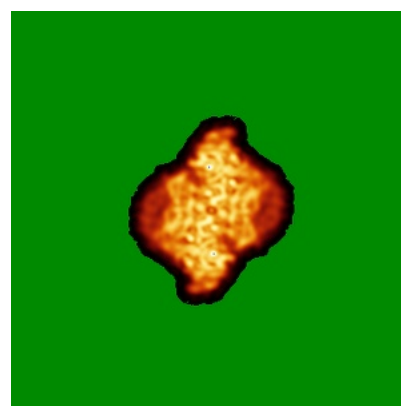
6.4.1 Primary map



X



Y

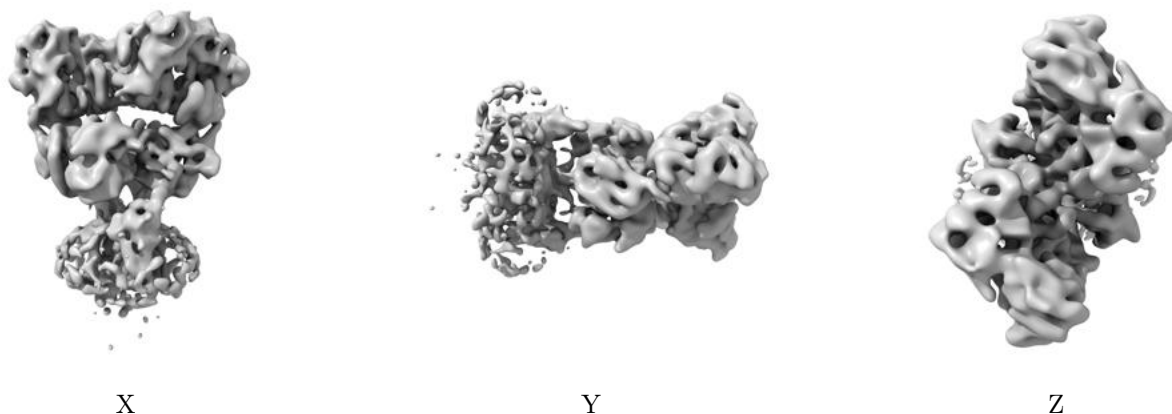


Z

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

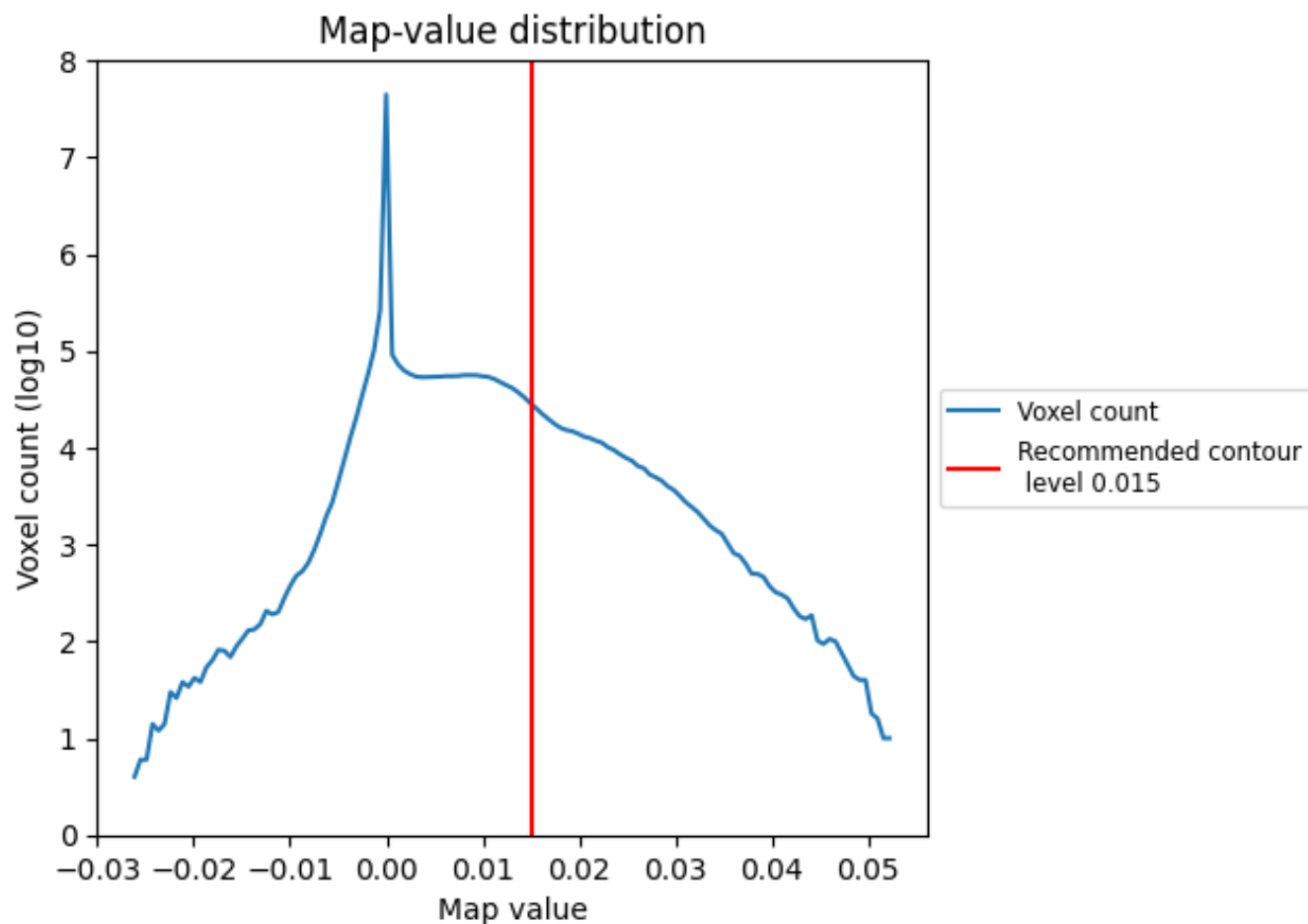
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

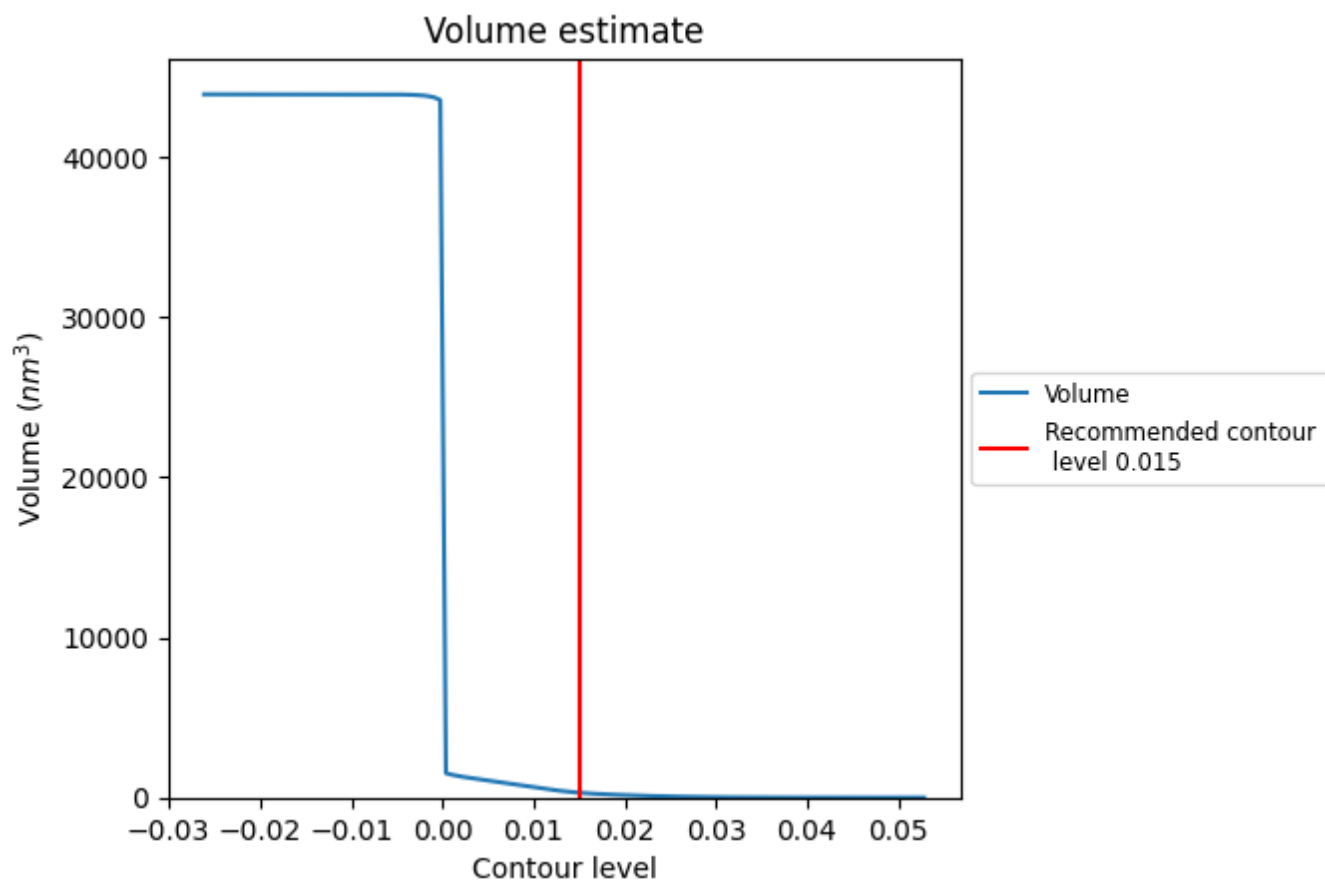
This section contains the results of statistical analysis of the map.

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.

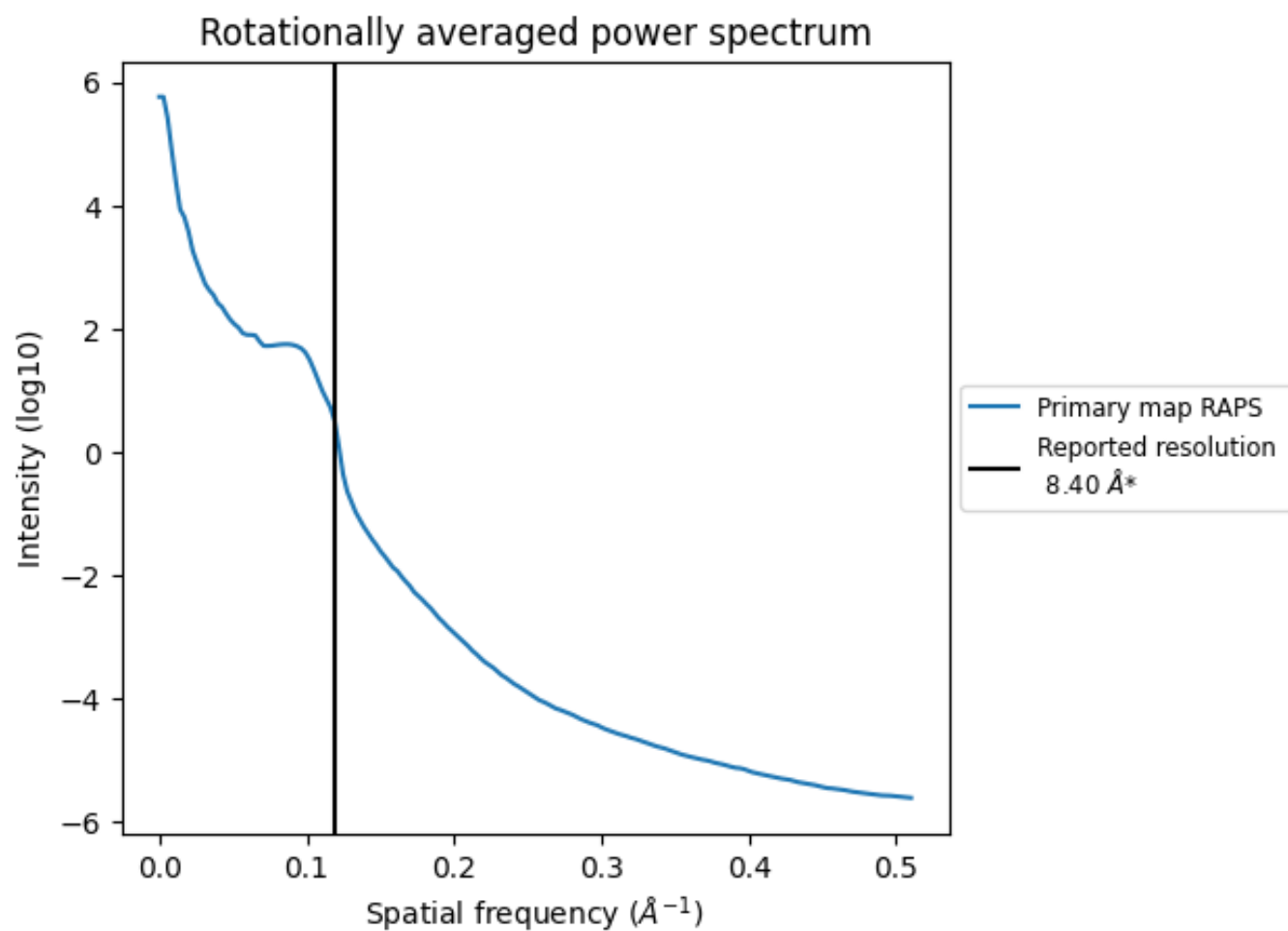
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 303 nm³; this corresponds to an approximate mass of 274 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 0.119 Å⁻¹

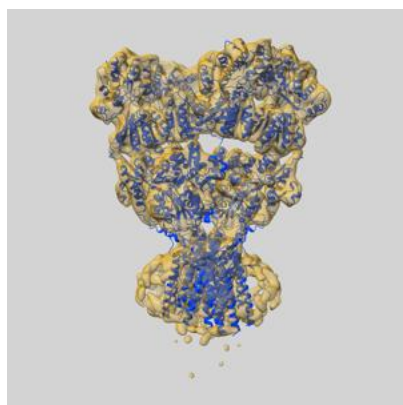
8 Fourier-Shell correlation ⓘ

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

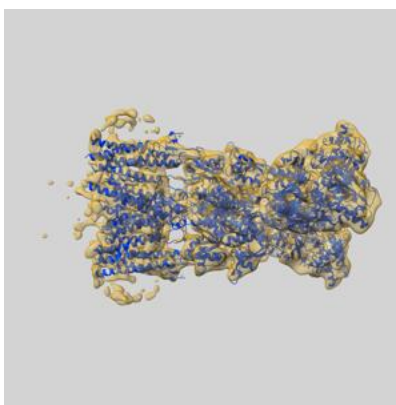
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8688 and PDB model 5VHZ. Per-residue inclusion information can be found in section 3 on page 7.

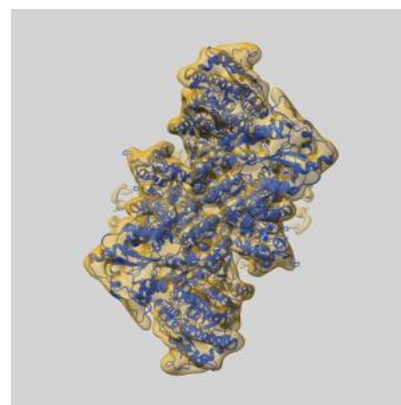
9.1 Map-model overlay [i](#)



X



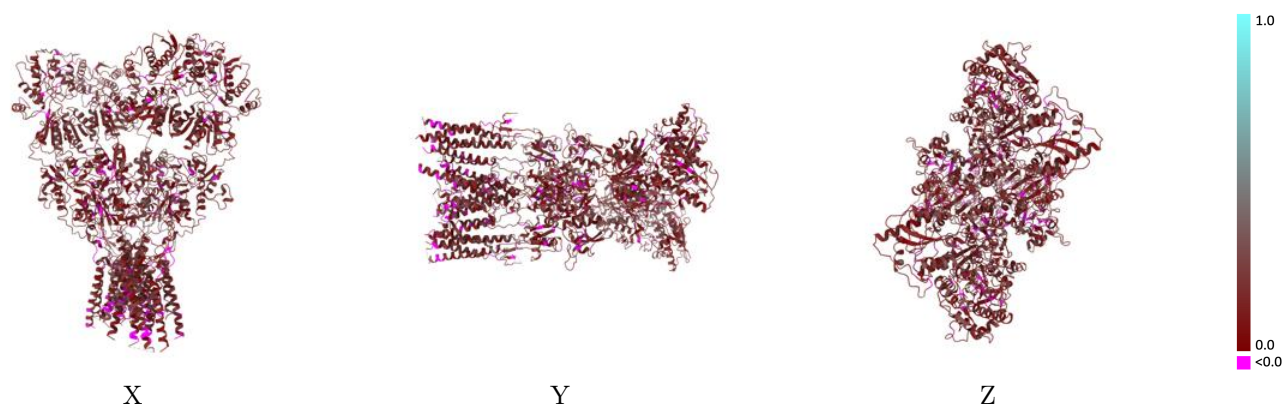
Y



Z

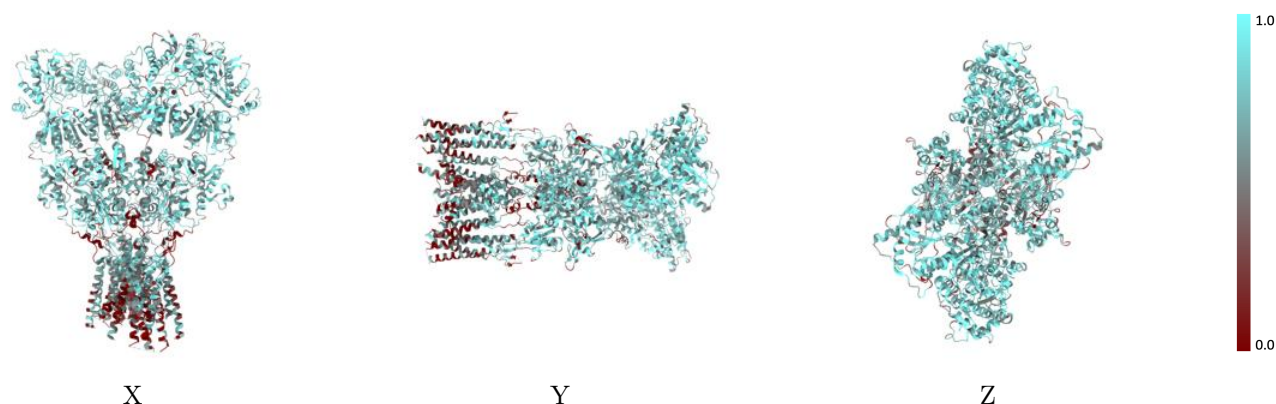
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



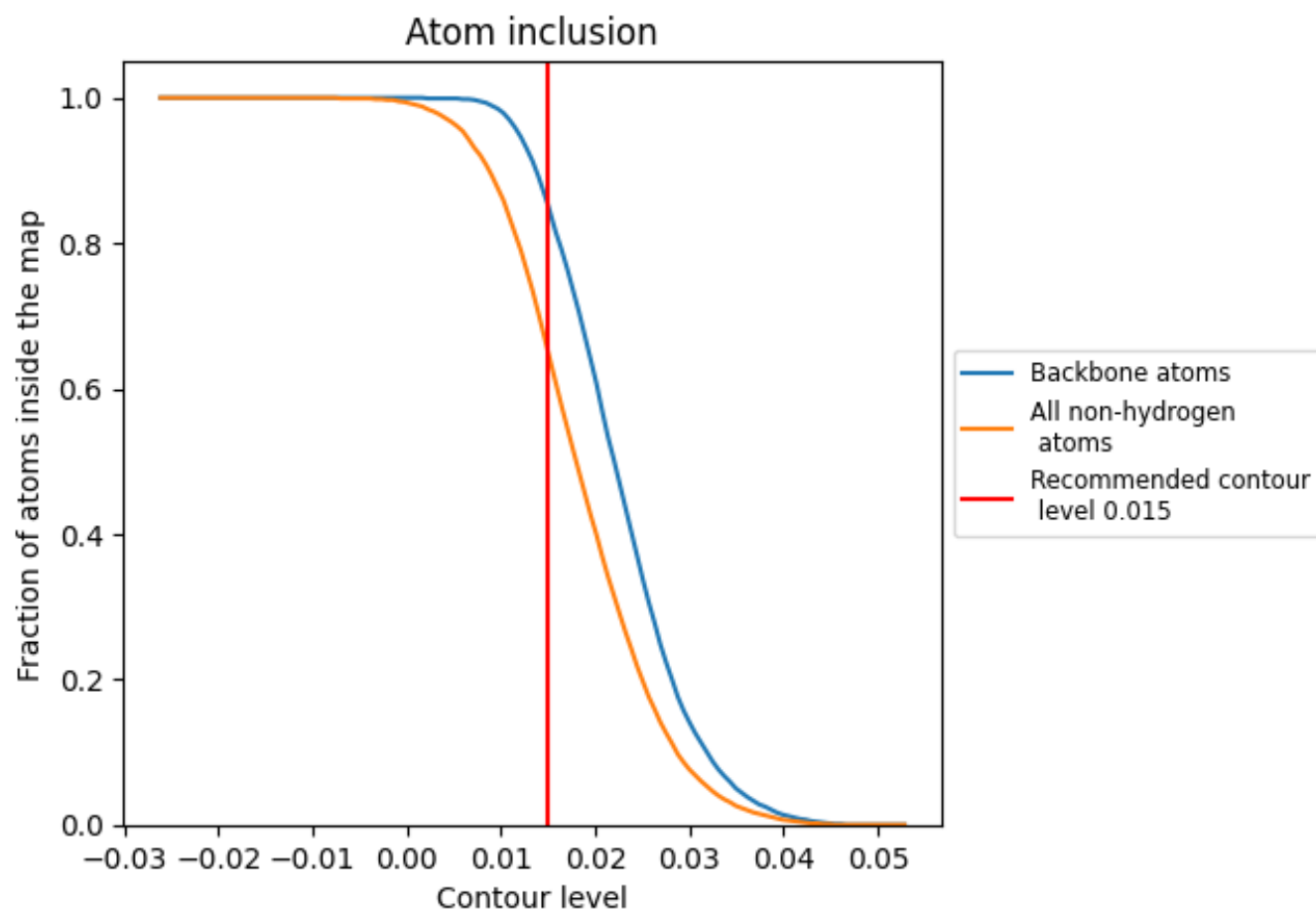
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 65% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6500	<div></div> 0.1510
A	<div></div> 0.6830	<div></div> 0.1530
B	<div></div> 0.6580	<div></div> 0.1530
C	<div></div> 0.6810	<div></div> 0.1530
D	<div></div> 0.6530	<div></div> 0.1500
E	<div></div> 0.4870	<div></div> 0.1390
F	<div></div> 0.4920	<div></div> 0.1400

