Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 03:43 pm GMT

PDB ID	:	2XFC
EMDB ID	:	EMD-1015
Title	:	CHIKUNGUNYA E1 E2 ENVELOPE GLYCOPROTEINS FITTED IN SEMLIKI FOREST VIRUS cryo-EM MAP
Authors	:	Voss, J.E.; Vaney, M.C.; Duquerroy, S.; Rey, F.A.
Deposited on	:	2010-05-21
Resolution	:	9.00 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 (i) 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 (i)) were used in the production of this report:

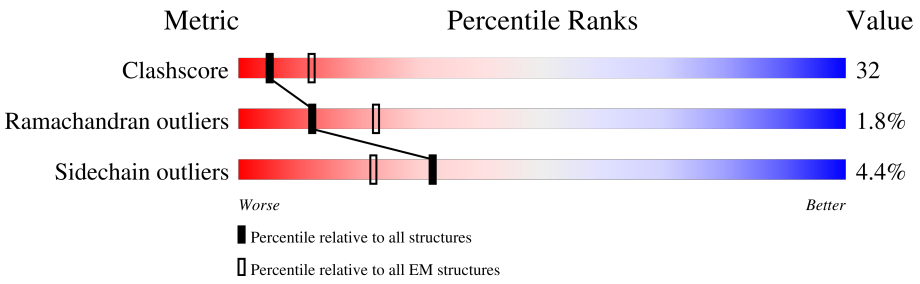
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 9.00 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	439	38% 67% 20% • • 11%
1	D	439	40% 68% 18% • 11%
1	F	439	41% 66% 21% • 11%
1	H	439	46% 67% 20% • 11%
2	B	423	29% 63% 15% • 21%
2	E	423	32% 62% 16% • 21%
2	G	423	29% 59% 18% • 21%
2	I	423	34% 61% 17% • 21%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 22420 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 E1 ENVELOPE GLYCOPROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	391	2975	1881	499	571	24	0	1
1	D	391	2975	1881	499	571	24	0	1
1	F	391	2975	1881	499	571	24	0	1
1	H	391	2975	1881	499	571	24	0	1

- Molecule 2 is a protein called E2 ENVELOPE GLYCOPROTEIN.

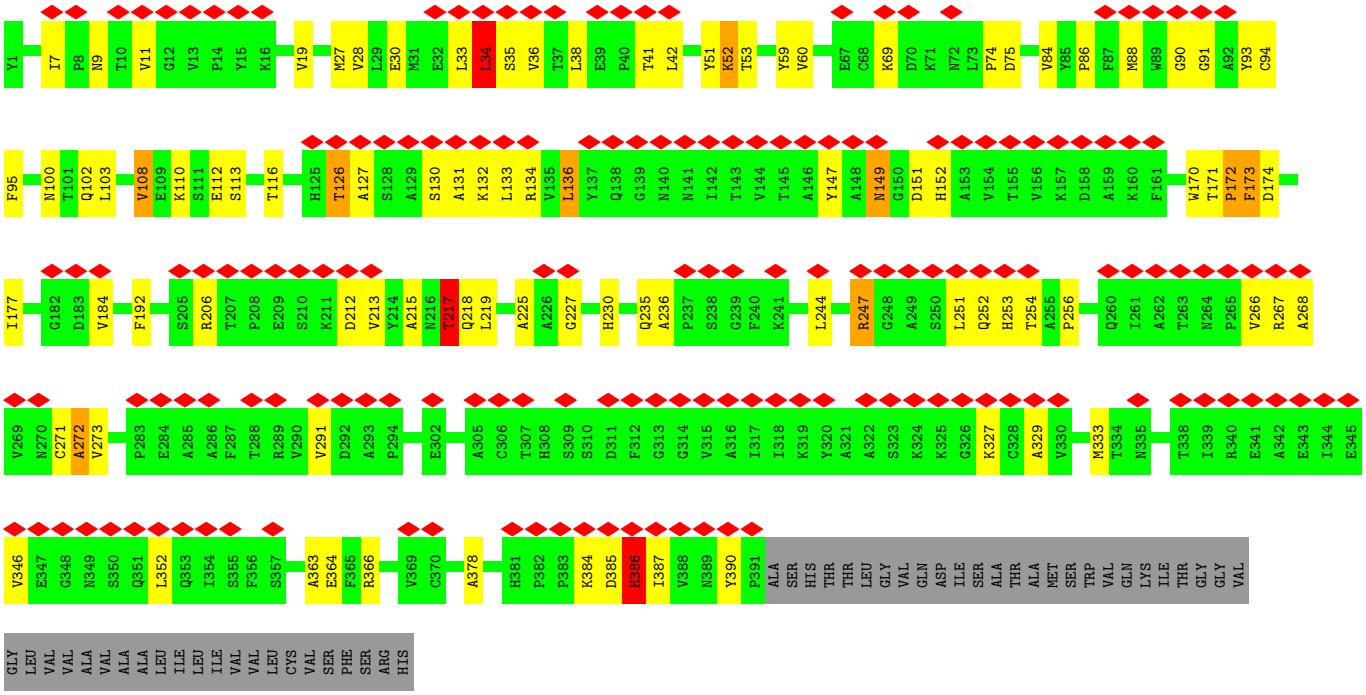
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	335	2630	1641	476	494	19	0	1
2	E	335	2630	1641	476	494	19	0	1
2	G	335	2630	1641	476	494	19	0	1
2	I	335	2630	1641	476	494	19	0	1

3 Residue-property plots (i)

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

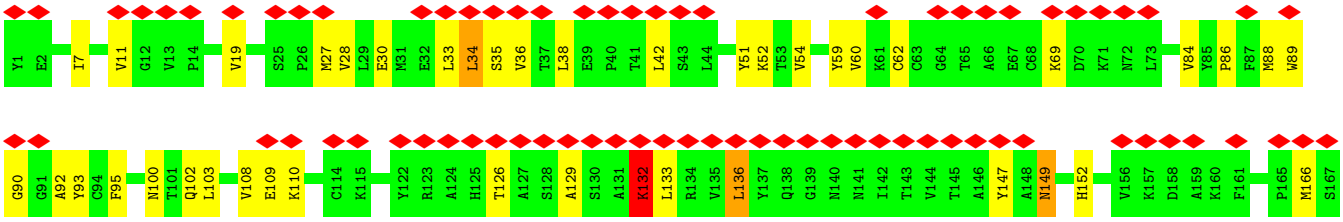
• Molecule 1: E1 ENVELOPE GLYCOPROTEIN

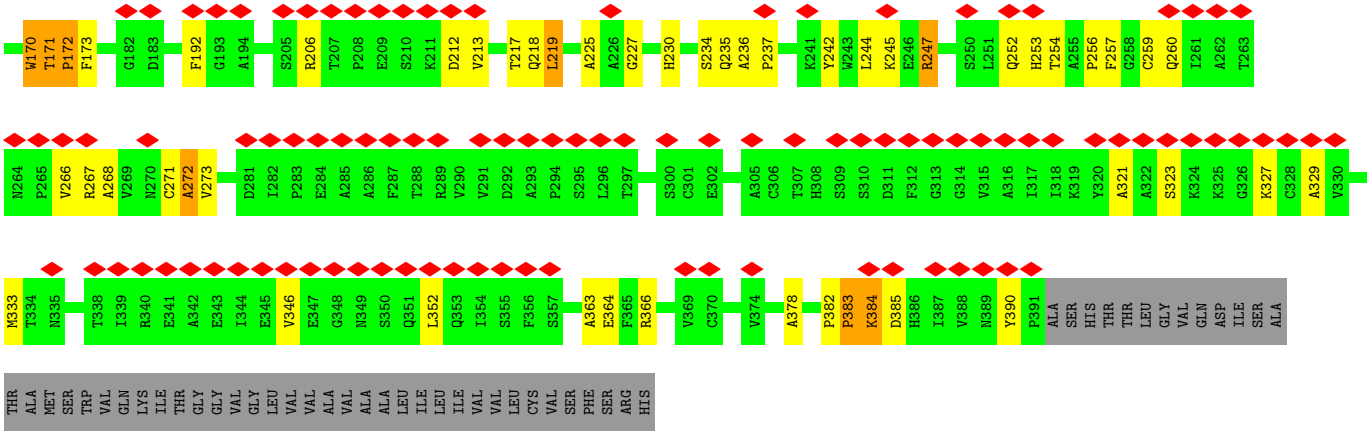
Chain A:



• Molecule 1: E1 ENVELOPE GLYCOPROTEIN

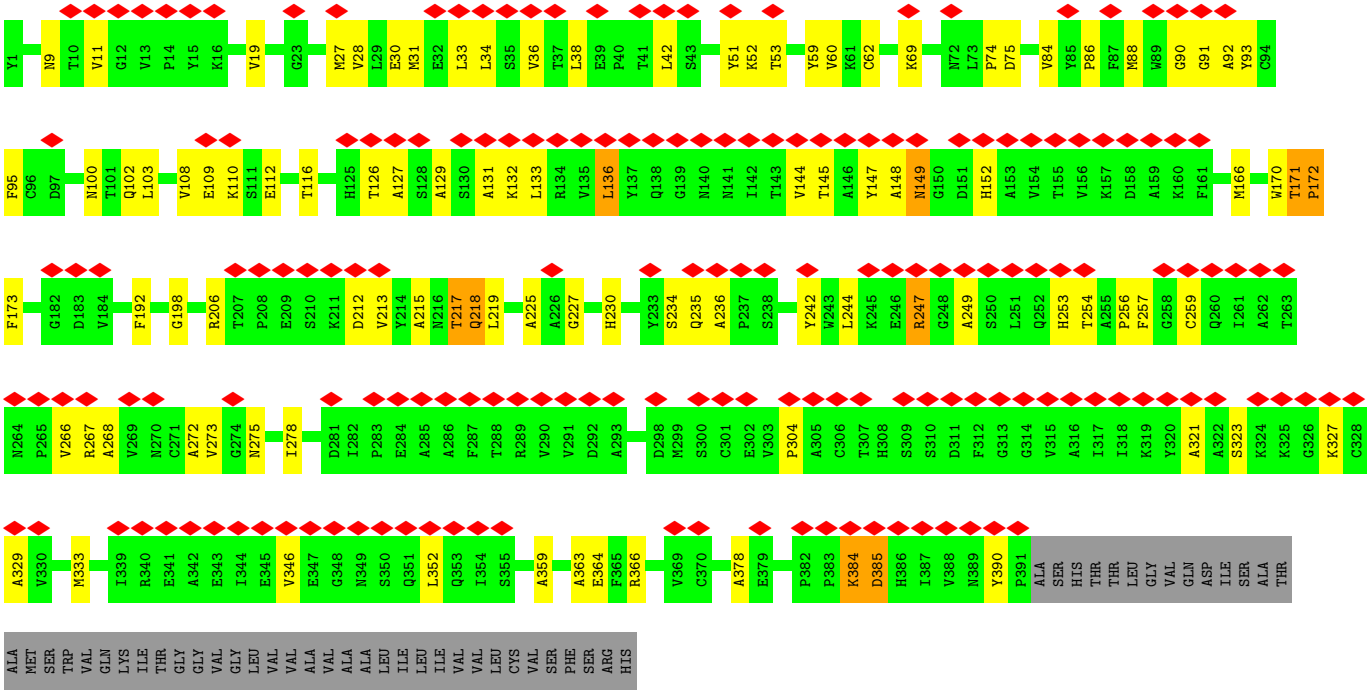
Chain D:





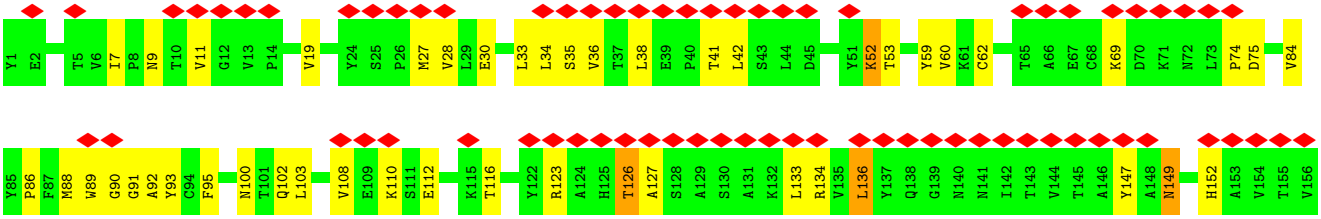
- Molecule 1: E1 ENVELOPE GLYCOPROTEIN

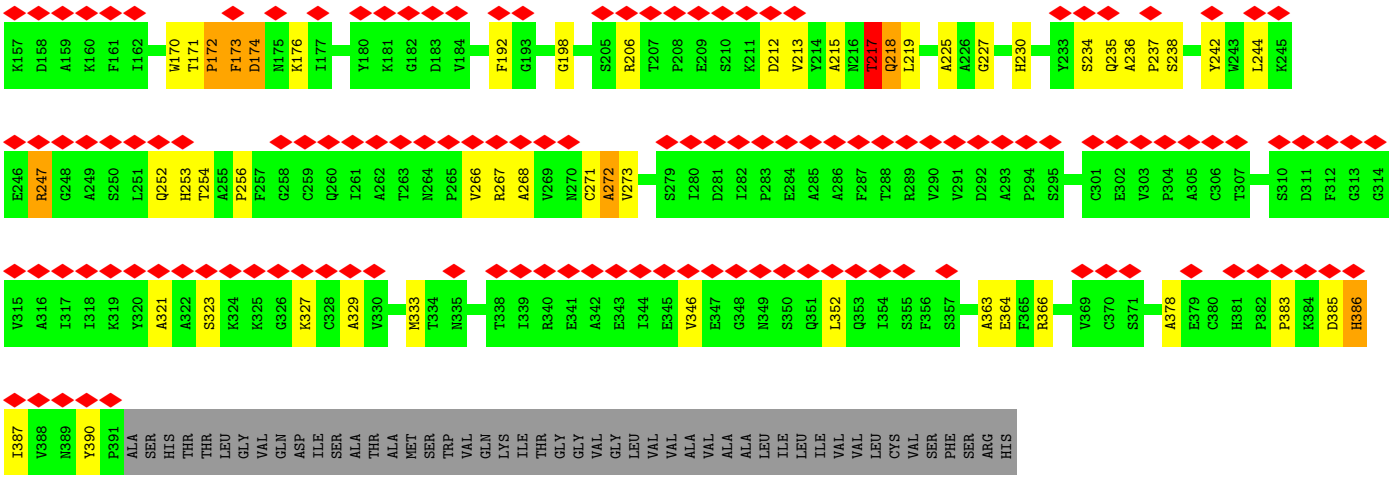
Chain F:



- Molecule 1: E1 ENVELOPE GLYCOPROTEIN

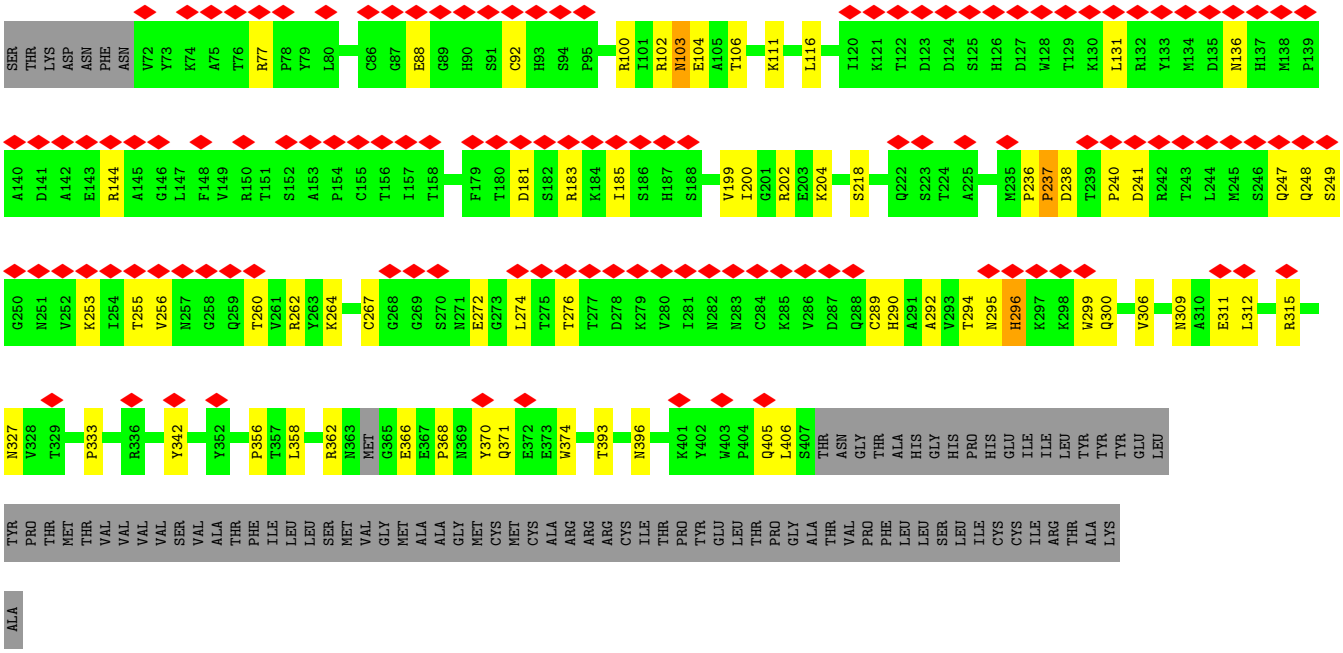
Chain H:





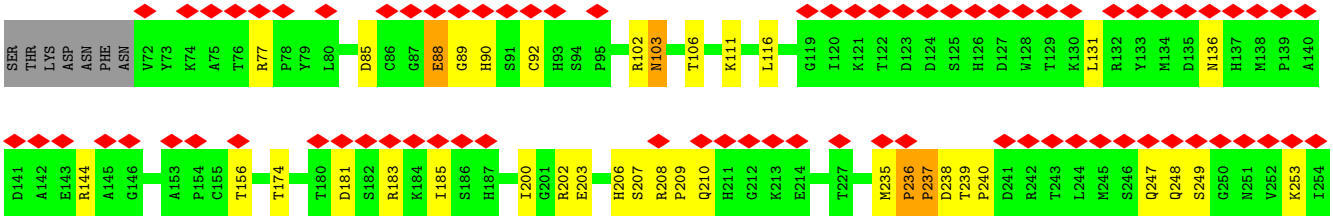
- Molecule 2: E2 ENVELOPE GLYCOPROTEIN

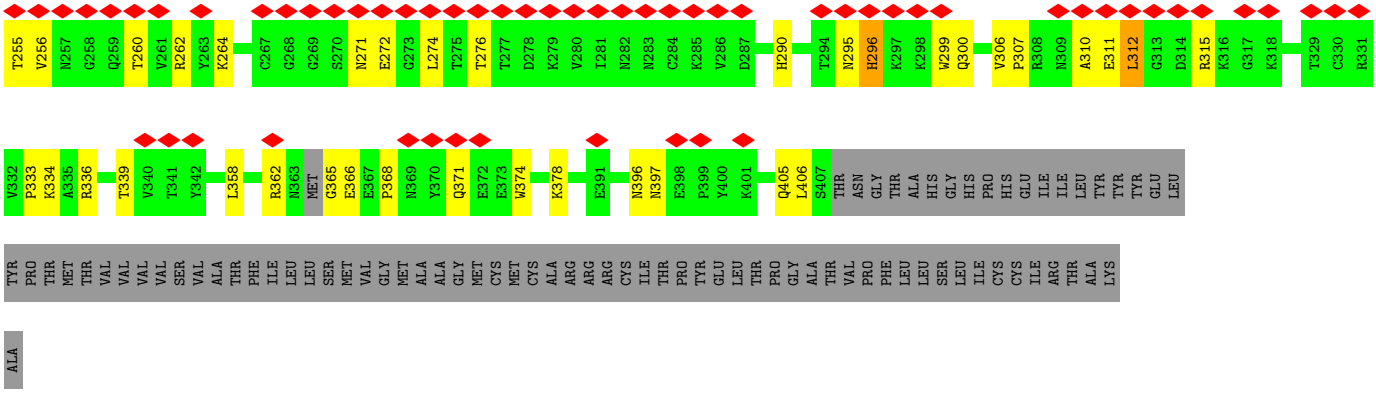
Chain B:



- Molecule 2: E2 ENVELOPE GLYCOPROTEIN

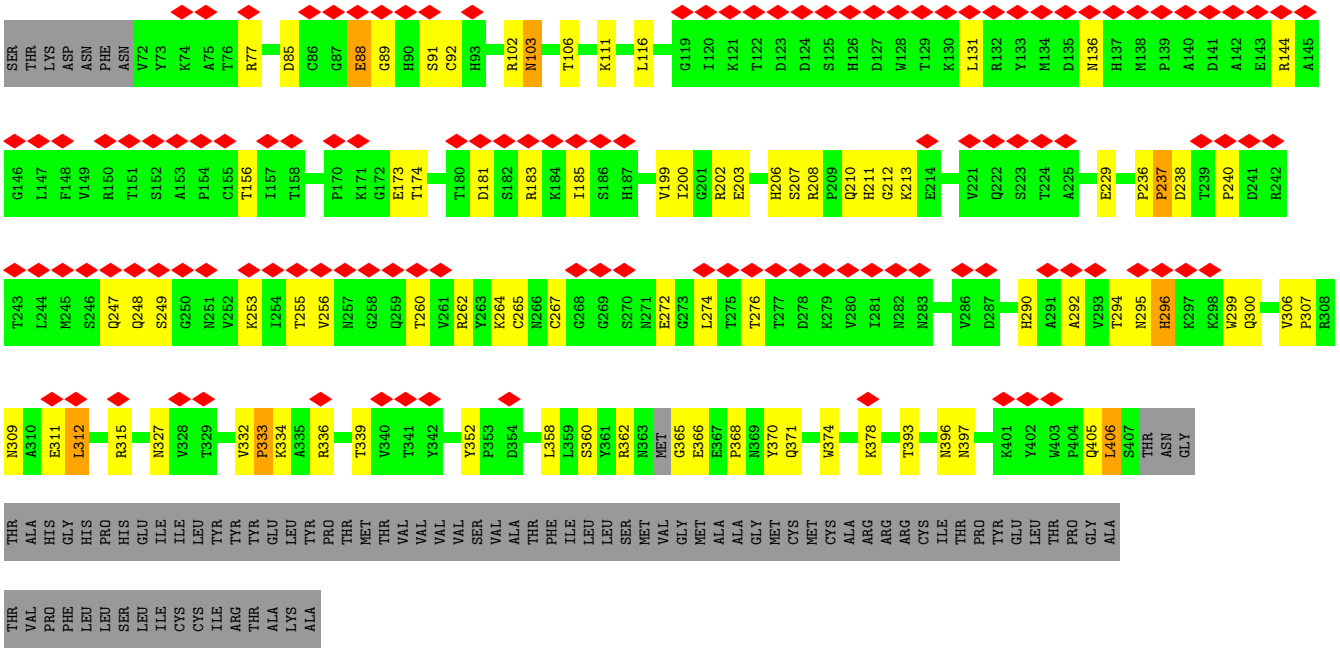
Chain E:





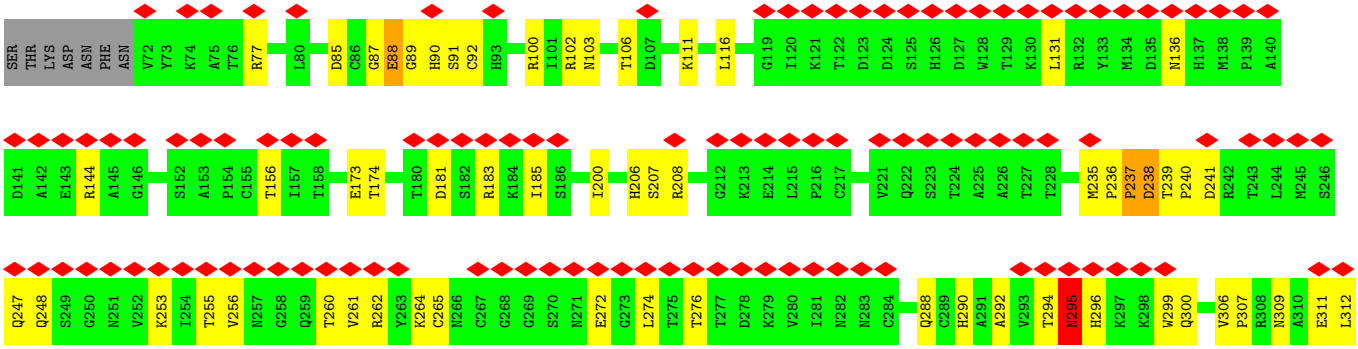
- Molecule 2: E2 ENVELOPE GLYCOPROTEIN

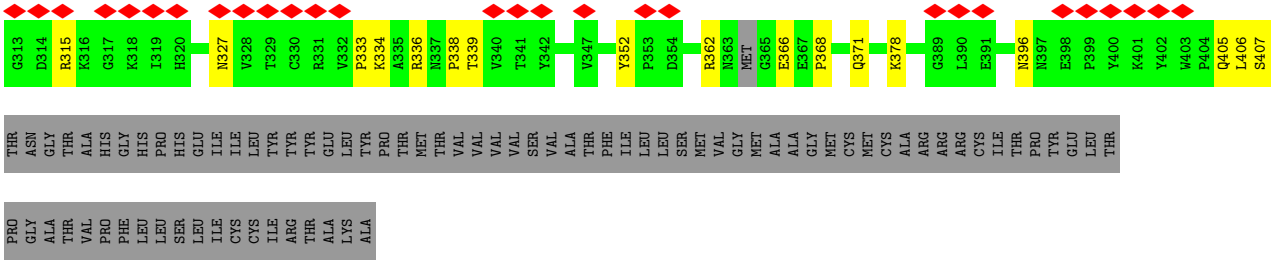
Chain G:



- Molecule 2: E2 ENVELOPE GLYCOPROTEIN

Chain I:




G313 D314 R315 K316 G317 K318 I319 H320 N327 V328 T329 C330 R331 V332 P333 K334 A335 R336 N337 P338 T339 V340 T341 Y342 V347 Y352 P353 D354 R362 N363 MET G365 E366 E367 P368 Q371 K378 G389 L390 E391 N396 N397 E398 P399 Y400 K401 Y402 W403 P404 Q405 L406 S407
THR ASN GLY THR ALA HIS GLY HIS PRO HIS GLU ILE ILE LEU TYR TYR TYR GLU LEU TYR PRO THR MET THR VAL VAL VAL VAL SER VAL ALA THR PHE ILE LEU LEU SER MET VAL GLY MET ALA ALA GLY MET CYS MET CYS ALA ARG ARG ARG CYS ILE THR PRO TYR GLU LEU THR
PRO GLY ALA THR VAL PRO PHE LEU LEU SER LEU ILE CYS CYS ILE ARG THR ALA LYS ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	6000	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI/PHILIPS CM200FEG/ST	Depositor
Voltage (kV)	100	Depositor
Electron dose ($e^-/Å^2$)	8	Depositor
Minimum defocus (nm)	975	Depositor
Maximum defocus (nm)	7628	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	25955.000	Depositor
Minimum map value	-25432.000	Depositor
Average map value	-39.429	Depositor
Map value standard deviation	4659.710	Depositor
Recommended contour level	9460.0	Depositor
Map size (Å)	758.52, 758.52, 758.52	wwPDB
Map dimensions	301, 301, 301	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	2.52, 2.52, 2.52	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	0.52	2/3046 (0.1%)	1.09	5/4147 (0.1%)
1	D	0.37	0/3047	0.59	2/4150 (0.0%)
1	F	0.58	1/3048 (0.0%)	0.77	5/4153 (0.1%)
1	H	0.61	3/3050 (0.1%)	0.83	7/4159 (0.2%)
2	B	0.37	0/2697	0.62	0/3668
2	E	0.40	0/2698	0.63	0/3671
2	G	0.37	0/2698	0.62	0/3671
2	I	0.37	0/2699	0.61	0/3674
All	All	0.46	6/22983 (0.0%)	0.74	19/31293 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
1	F	0	1
1	H	0	2
All	All	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	217	THR	C-N	24.85	1.91	1.34
1	H	217	THR	C-N	-16.38	0.96	1.34
1	A	52	LYS	C-N	15.38	1.69	1.34
1	H	52	LYS	C-N	15.20	1.69	1.34
1	A	108	VAL	C-N	14.51	1.67	1.34
1	H	108	VAL	C-N	14.41	1.67	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	217	THR	O-C-N	-56.87	31.71	122.70
1	H	217	THR	O-C-N	-27.84	78.15	122.70
1	F	217	THR	O-C-N	-26.85	79.73	122.70
1	H	217	THR	CA-C-N	16.72	153.99	117.20
1	H	217	THR	C-N-CA	14.46	157.85	121.70
1	F	217	THR	CA-C-N	12.59	144.90	117.20
1	F	217	THR	C-N-CA	10.04	146.80	121.70
1	A	108	VAL	O-C-N	-9.48	107.52	122.70
1	A	108	VAL	C-N-CA	9.10	144.45	121.70
1	A	217	THR	CA-C-N	9.02	137.04	117.20
1	H	52	LYS	O-C-N	-7.40	110.86	122.70
1	D	323	SER	C-N-CA	7.19	139.66	121.70
1	F	323	SER	C-N-CA	7.17	139.62	121.70
1	H	323	SER	C-N-CA	7.15	139.56	121.70
1	A	108	VAL	CA-C-N	6.52	131.54	117.20
1	F	323	SER	O-C-N	-5.66	113.64	122.70
1	D	323	SER	O-C-N	-5.65	113.66	122.70
1	H	323	SER	O-C-N	-5.59	113.75	122.70
1	H	52	LYS	CA-C-N	5.15	128.54	117.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	217	THR	Mainchain
1	D	321	ALA	Mainchain
1	F	321	ALA	Mainchain
1	H	217	THR	Mainchain
1	H	321	ALA	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2975	0	2877	286	0
1	D	2975	0	2875	274	0
1	F	2975	0	2876	270	0
1	H	2975	0	2877	259	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2630	0	2550	179	0
2	E	2630	0	2546	252	0
2	G	2630	0	2546	302	0
2	I	2630	0	2544	314	0
All	All	22420	0	21691	1424	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 32.

All (1424) 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)
2:I:274:LEU:HD21	2:I:296:HIS:CE1	1.20	1.70
1:A:34:LEU:HD12	1:A:132:LYS:CE	1.18	1.58
1:H:88:MET:HB3	2:I:240:PRO:CD	1.29	1.57
1:A:34:LEU:CD1	1:A:132:LYS:HE2	1.27	1.57
2:G:206:HIS:CG	2:I:174:THR:HG23	1.34	1.57
2:E:89:GLY:HA3	2:I:208:ARG:CG	1.35	1.56
1:D:234:SER:HB2	2:I:336:ARG:CB	1.22	1.55
1:A:256:PRO:CB	2:B:366:GLU:HG3	1.10	1.55
1:H:88:MET:CB	2:I:240:PRO:CD	1.79	1.55
2:G:206:HIS:CB	2:I:174:THR:CG2	1.84	1.54
2:G:339:THR:CG2	1:H:218:GLN:NE2	1.70	1.53
2:B:294:THR:CG2	2:B:295:ASN:N	1.70	1.52
2:E:237:PRO:HG3	2:E:306:VAL:CG1	1.35	1.51
2:G:237:PRO:HG3	2:G:306:VAL:CG1	1.40	1.51
1:D:88:MET:HE1	2:E:238:ASP:C	1.24	1.49
1:H:88:MET:HE1	2:I:238:ASP:C	1.24	1.49
2:E:336:ARG:HB3	1:F:234:SER:CB	1.42	1.48
2:G:206:HIS:CD2	2:I:174:THR:HG23	1.44	1.48
1:D:256:PRO:HB3	2:E:366:GLU:CG	1.43	1.48
2:G:336:ARG:NH2	1:H:236:ALA:CA	1.68	1.48
1:D:256:PRO:CA	2:E:366:GLU:HA	1.44	1.48
1:H:95:PHE:CB	2:I:264:LYS:HB3	1.44	1.45
1:A:385:ASP:HA	1:A:386:HIS:CB	1.42	1.45
2:I:260:THR:C	2:I:294:THR:CB	1.83	1.45
2:G:206:HIS:CG	2:I:174:THR:CG2	1.98	1.44
1:H:88:MET:CB	2:I:240:PRO:HD3	1.41	1.44
2:G:339:THR:HG23	1:H:218:GLN:CD	1.29	1.44
1:F:256:PRO:CB	2:G:366:GLU:CA	1.96	1.43
1:A:52:LYS:C	1:A:53:THR:N	1.69	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:GLN:HE21	2:B:362:ARG:CZ	1.32	1.43
2:E:334:LYS:HG3	2:E:396:ASN:CB	1.49	1.43
1:A:256:PRO:HB3	2:B:366:GLU:CG	0.97	1.42
1:D:245:LYS:CE	2:I:378:LYS:HB2	1.49	1.42
1:A:252:GLN:HE21	2:B:362:ARG:NH1	1.09	1.42
2:G:294:THR:HG22	2:G:295:ASN:N	1.27	1.42
1:H:52:LYS:C	1:H:53:THR:N	1.69	1.42
1:D:90:GLY:H	2:E:240:PRO:CG	1.29	1.41
2:G:206:HIS:NE2	2:I:173:GLU:CB	1.84	1.41
1:D:237:PRO:HG2	2:I:352:TYR:CG	1.56	1.40
1:A:93:TYR:CA	2:B:290:HIS:CE1	2.02	1.40
1:D:90:GLY:C	2:E:240:PRO:HB2	1.41	1.40
1:A:34:LEU:CD1	1:A:132:LYS:CE	1.80	1.40
1:D:89:TRP:HE1	2:E:239:THR:CG2	1.33	1.39
1:D:89:TRP:NE1	2:E:239:THR:HG23	1.12	1.39
1:A:256:PRO:CA	2:B:366:GLU:HA	1.53	1.38
2:I:237:PRO:HG3	2:I:306:VAL:CG1	1.53	1.38
1:A:291:VAL:HG21	1:F:304:PRO:C	1.39	1.38
1:D:234:SER:CB	2:I:336:ARG:CB	2.00	1.38
2:I:274:LEU:CD2	2:I:296:HIS:CE1	2.05	1.38
1:D:256:PRO:CB	2:E:366:GLU:HG3	1.53	1.37
1:A:385:ASP:HB2	2:B:405:GLN:NE2	1.38	1.37
1:D:90:GLY:N	2:E:240:PRO:HG2	1.08	1.37
1:D:256:PRO:CB	2:E:366:GLU:HA	1.54	1.37
1:A:90:GLY:CA	2:B:240:PRO:O	1.69	1.37
1:A:170:TRP:CZ3	1:A:172:PRO:HD3	1.57	1.36
1:A:291:VAL:HG21	1:F:304:PRO:CA	1.46	1.36
1:A:385:ASP:CB	2:B:405:GLN:HG3	1.06	1.36
2:B:237:PRO:HG3	2:B:306:VAL:CG1	1.55	1.36
2:E:334:LYS:CG	2:E:396:ASN:HB2	1.53	1.36
1:A:385:ASP:CB	2:B:405:GLN:CG	1.89	1.35
2:G:274:LEU:CD2	2:G:311:GLU:OE2	1.73	1.35
2:E:336:ARG:CZ	1:F:235:GLN:C	1.94	1.34
1:D:234:SER:HB2	2:I:336:ARG:CA	1.57	1.34
1:H:33:LEU:CD2	1:H:133:LEU:HD13	1.55	1.33
1:H:95:PHE:HB2	2:I:264:LYS:CB	1.58	1.33
1:F:90:GLY:CA	2:G:240:PRO:O	1.77	1.33
1:A:385:ASP:CA	1:A:386:HIS:HB2	1.50	1.32
2:G:206:HIS:HB3	2:I:174:THR:CG2	1.50	1.32
1:A:34:LEU:HD12	1:A:132:LYS:CD	1.57	1.32
2:E:274:LEU:CD2	2:E:311:GLU:HB2	1.59	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:336:ARG:CB	1:H:234:SER:HB2	1.61	1.31
1:F:74:PRO:CB	1:F:215:ALA:HB3	1.60	1.31
1:F:171:THR:O	1:F:173:PHE:N	1.62	1.31
1:F:253:HIS:O	2:G:362:ARG:CD	1.79	1.31
2:E:336:ARG:NH1	1:F:235:GLN:HA	1.43	1.30
2:G:339:THR:CG2	1:H:218:GLN:CD	1.95	1.30
1:A:252:GLN:NE2	2:B:362:ARG:HH12	1.25	1.30
1:F:75:ASP:OD2	1:F:217:THR:N	1.63	1.30
1:F:62:CYS:CB	2:G:264:LYS:HE2	1.62	1.29
2:I:260:THR:O	2:I:294:THR:N	1.62	1.29
1:A:256:PRO:HA	2:B:366:GLU:CA	1.61	1.29
2:I:260:THR:C	2:I:294:THR:HB	0.92	1.29
2:G:339:THR:HG23	1:H:218:GLN:NE2	0.95	1.28
1:A:90:GLY:N	2:B:240:PRO:HG2	1.46	1.28
1:D:237:PRO:HG2	2:I:352:TYR:CB	1.63	1.28
1:F:95:PHE:CD1	2:G:264:LYS:O	1.80	1.28
1:F:256:PRO:HG3	2:G:366:GLU:O	1.23	1.28
1:H:88:MET:SD	2:I:238:ASP:O	1.92	1.28
2:B:274:LEU:HD23	2:B:311:GLU:OE2	1.17	1.28
1:F:256:PRO:CB	2:G:366:GLU:HA	1.56	1.28
2:E:336:ARG:CB	1:F:234:SER:HB2	1.63	1.27
1:A:127:ALA:CB	1:A:171:THR:CB	2.12	1.27
1:D:256:PRO:HB3	2:E:366:GLU:CA	1.61	1.26
1:A:93:TYR:HE1	2:B:238:ASP:OD2	1.18	1.26
1:A:127:ALA:CB	1:A:171:THR:HB	1.65	1.26
2:E:89:GLY:CA	2:I:208:ARG:HG3	1.62	1.26
1:H:7:ILE:HD11	1:H:33:LEU:CD1	1.63	1.26
2:G:210:GLN:HE21	2:I:91:SER:CB	1.47	1.26
1:D:256:PRO:HB3	2:E:366:GLU:CB	1.64	1.26
1:A:93:TYR:HA	2:B:290:HIS:CE1	1.63	1.25
1:A:291:VAL:CG2	1:F:304:PRO:O	1.83	1.25
2:I:274:LEU:CD2	2:I:296:HIS:HE1	1.43	1.25
1:A:90:GLY:C	2:B:240:PRO:HB2	1.55	1.25
2:G:210:GLN:HG3	2:I:91:SER:CB	1.65	1.24
1:H:88:MET:CE	2:I:238:ASP:O	1.84	1.24
1:F:217:THR:C	1:F:218:GLN:N	1.91	1.24
1:F:253:HIS:C	2:G:362:ARG:HD3	1.55	1.24
1:F:256:PRO:CG	2:G:366:GLU:O	1.85	1.24
1:F:95:PHE:CD1	2:G:264:LYS:C	1.80	1.24
2:G:206:HIS:NE2	2:I:173:GLU:HB3	1.44	1.23
1:A:291:VAL:HG21	1:F:304:PRO:O	1.35	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:TRP:CH2	1:D:172:PRO:HD3	1.73	1.23
1:H:252:GLN:O	2:I:362:ARG:NH1	1.71	1.23
2:G:294:THR:CG2	2:G:295:ASN:N	2.02	1.23
1:A:252:GLN:NE2	2:B:362:ARG:NH1	1.79	1.22
2:B:294:THR:HG22	2:B:295:ASN:N	0.89	1.22
2:G:336:ARG:NH2	1:H:236:ALA:HA	0.91	1.22
1:F:257:PHE:H	2:G:365:GLY:CA	1.52	1.22
2:G:210:GLN:CG	2:I:91:SER:HB3	1.69	1.22
2:I:260:THR:O	2:I:294:THR:HB	1.35	1.22
2:I:260:THR:O	2:I:294:THR:CB	1.86	1.21
1:A:252:GLN:NE2	2:B:362:ARG:HH22	1.38	1.21
1:D:89:TRP:NE1	2:E:239:THR:CG2	1.96	1.20
1:H:88:MET:CE	2:I:238:ASP:C	2.06	1.20
1:H:33:LEU:HG	1:H:133:LEU:CD1	1.69	1.20
1:D:256:PRO:CB	2:E:366:GLU:CG	2.12	1.20
2:G:274:LEU:HD23	2:G:311:GLU:OE2	1.09	1.20
1:A:151:ASP:OD2	1:H:176:LYS:NZ	1.73	1.20
1:A:252:GLN:NE2	2:B:362:ARG:NH2	1.89	1.20
1:A:385:ASP:HB2	2:B:405:GLN:CD	1.61	1.20
1:F:95:PHE:CG	2:G:264:LYS:C	2.08	1.19
1:H:88:MET:CB	2:I:240:PRO:CG	2.20	1.19
2:B:237:PRO:HG3	2:B:306:VAL:HG11	1.22	1.19
1:F:95:PHE:HD1	2:G:264:LYS:O	1.10	1.19
1:A:74:PRO:CB	1:A:215:ALA:HB3	1.72	1.19
1:D:234:SER:CA	2:I:336:ARG:HB3	1.71	1.19
1:H:385:ASP:CA	1:H:386:HIS:HB2	1.73	1.19
1:F:253:HIS:O	2:G:362:ARG:HD3	1.03	1.18
1:F:11:VAL:CG2	1:F:36:VAL:HG23	1.71	1.18
2:I:260:THR:O	2:I:294:THR:CA	1.91	1.18
1:A:172:PRO:HG2	1:A:268:ALA:HB2	1.21	1.18
2:G:336:ARG:NH1	1:H:236:ALA:N	1.91	1.18
2:E:336:ARG:HH12	1:F:236:ALA:N	1.31	1.18
1:A:254:THR:HA	2:B:368:PRO:CG	1.72	1.17
1:F:256:PRO:CG	2:G:366:GLU:C	2.13	1.17
2:G:207:SER:HB2	2:I:85:ASP:CB	1.71	1.17
1:D:11:VAL:CG2	1:D:36:VAL:HG23	1.75	1.16
1:A:95:PHE:H	2:B:264:LYS:CB	1.57	1.16
1:A:172:PRO:CG	1:A:268:ALA:CB	2.23	1.16
1:H:170:TRP:CH2	1:H:172:PRO:HB3	1.80	1.16
1:H:385:ASP:HA	1:H:386:HIS:CB	1.71	1.16
1:A:384:LYS:HG3	1:A:385:ASP:H	1.10	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:385:ASP:O	2:E:405:GLN:HG3	1.44	1.16
1:D:245:LYS:HE2	2:I:378:LYS:CB	1.74	1.15
2:G:352:TYR:CD2	1:H:237:PRO:HD2	1.79	1.15
2:G:352:TYR:HB3	1:H:237:PRO:HD3	1.27	1.15
2:B:294:THR:HG22	2:B:295:ASN:CA	1.75	1.15
1:F:256:PRO:CG	2:G:366:GLU:HA	1.77	1.15
2:E:237:PRO:CG	2:E:306:VAL:CG1	2.23	1.14
1:F:235:GLN:HG2	1:F:236:ALA:N	1.61	1.14
2:G:378:LYS:HD2	1:H:242:TYR:CD1	1.82	1.14
1:H:88:MET:HB2	2:I:240:PRO:CG	1.73	1.14
2:E:339:THR:HG23	1:F:218:GLN:CD	1.68	1.14
1:A:127:ALA:HB3	1:A:171:THR:HB	1.18	1.14
2:E:336:ARG:NH1	1:F:236:ALA:N	1.71	1.13
1:A:172:PRO:HG3	1:A:268:ALA:CB	1.78	1.13
1:A:218:GLN:HB2	1:A:236:ALA:HB2	1.22	1.13
1:A:34:LEU:HD12	1:A:132:LYS:HE3	1.21	1.12
1:A:385:ASP:HB2	2:B:405:GLN:CG	1.62	1.13
1:A:291:VAL:CG2	1:F:304:PRO:CA	2.27	1.12
1:A:34:LEU:HB2	1:A:132:LYS:HB2	1.25	1.12
2:G:207:SER:HB2	2:I:85:ASP:HB2	1.18	1.12
1:H:7:ILE:HD11	1:H:33:LEU:HD11	1.31	1.12
2:G:336:ARG:HB3	1:H:234:SER:HB2	1.14	1.12
1:A:149:ASN:OD1	1:H:123:ARG:NH2	1.83	1.12
2:E:336:ARG:NH1	1:F:235:GLN:CA	2.12	1.12
2:I:237:PRO:HG3	2:I:306:VAL:HG12	1.20	1.11
1:F:256:PRO:HG3	2:G:366:GLU:C	1.66	1.11
1:A:170:TRP:CH2	1:A:172:PRO:HB3	1.86	1.11
1:H:256:PRO:HB3	2:I:366:GLU:HG3	1.11	1.10
1:A:127:ALA:HB2	1:A:171:THR:CB	1.77	1.10
1:D:89:TRP:CZ2	2:E:239:THR:HG22	1.85	1.10
1:H:93:TYR:CA	2:I:290:HIS:CE1	2.31	1.10
1:D:11:VAL:HG23	1:D:36:VAL:HG23	1.23	1.10
1:D:218:GLN:HE22	2:I:338:PRO:C	1.43	1.10
2:E:336:ARG:HD3	1:F:235:GLN:N	1.63	1.10
1:F:108:VAL:HG21	1:F:217:THR:OG1	1.51	1.10
2:E:89:GLY:CA	2:I:208:ARG:CG	2.26	1.09
1:A:93:TYR:C	2:B:290:HIS:CE1	2.24	1.09
1:D:34:LEU:CD1	1:D:132:LYS:CE	2.31	1.09
1:D:88:MET:HE2	2:E:238:ASP:O	1.48	1.09
1:D:218:GLN:NE2	2:I:339:THR:HA	1.65	1.09
1:H:93:TYR:HA	2:I:290:HIS:CE1	1.81	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:GLY:CA	2:E:240:PRO:HB2	1.83	1.09
1:F:256:PRO:CG	2:G:366:GLU:CA	2.30	1.09
1:D:259:CYS:SG	1:D:271:CYS:HB3	1.93	1.08
2:G:206:HIS:CE1	2:I:173:GLU:O	2.06	1.08
2:G:237:PRO:HG3	2:G:306:VAL:HG12	1.19	1.08
1:H:256:PRO:HB3	2:I:366:GLU:CG	1.83	1.08
1:A:95:PHE:H	2:B:264:LYS:HB2	1.16	1.08
1:H:7:ILE:HD11	1:H:33:LEU:HD12	1.36	1.08
1:A:172:PRO:CG	1:A:268:ALA:HB2	1.84	1.08
1:A:173:PHE:CE1	1:A:184:VAL:HG11	1.89	1.08
2:E:274:LEU:HD22	2:E:311:GLU:HB2	1.32	1.08
2:I:260:THR:CA	2:I:294:THR:HB	1.78	1.08
1:D:11:VAL:HG23	1:D:36:VAL:CG2	1.84	1.08
1:F:74:PRO:HB2	1:F:215:ALA:HB3	1.35	1.08
2:G:237:PRO:HG3	2:G:306:VAL:HG11	1.33	1.08
2:B:333:PRO:O	2:B:396:ASN:ND2	1.85	1.07
1:F:132:LYS:HG2	1:F:145:THR:OG1	1.55	1.07
2:E:237:PRO:CG	2:E:306:VAL:HG12	1.81	1.07
2:I:294:THR:HG22	2:I:295:ASN:H	1.15	1.07
1:F:74:PRO:HB3	1:F:215:ALA:HB3	1.32	1.07
1:F:90:GLY:C	2:G:240:PRO:HB2	1.74	1.07
1:A:172:PRO:HG3	1:A:268:ALA:HB1	1.37	1.06
1:D:234:SER:CB	2:I:336:ARG:HB3	1.76	1.06
1:A:90:GLY:C	2:B:240:PRO:CB	2.23	1.06
1:D:256:PRO:CA	2:E:366:GLU:CA	2.33	1.06
1:D:256:PRO:HA	2:E:366:GLU:HA	1.28	1.06
1:F:88:MET:CB	2:G:240:PRO:CD	2.33	1.06
1:D:34:LEU:HB2	1:D:132:LYS:HB2	1.37	1.06
1:H:95:PHE:HB3	2:I:264:LYS:HB3	1.11	1.06
1:A:95:PHE:N	2:B:264:LYS:HB2	1.70	1.06
2:G:208:ARG:NH2	2:I:90:HIS:HD2	1.19	1.06
1:F:62:CYS:HB2	2:G:264:LYS:CE	1.86	1.05
1:F:88:MET:CB	2:G:240:PRO:HD3	1.85	1.05
1:F:127:ALA:HB2	1:F:171:THR:HG21	1.38	1.05
1:D:62:CYS:HB3	2:E:264:LYS:CE	1.84	1.05
2:E:237:PRO:HG3	2:E:306:VAL:HG11	1.27	1.05
2:G:208:ARG:NH2	2:I:90:HIS:CD2	1.96	1.05
1:D:234:SER:HA	2:I:336:ARG:HB3	1.38	1.05
1:A:34:LEU:HD11	1:A:132:LYS:HE2	1.33	1.05
2:G:237:PRO:CG	2:G:306:VAL:CG1	2.35	1.05
1:H:95:PHE:CB	2:I:264:LYS:CB	2.20	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:172:PRO:HG2	1:H:268:ALA:HB2	1.39	1.05
1:D:88:MET:CE	2:E:238:ASP:C	1.90	1.04
1:D:90:GLY:N	2:E:240:PRO:CG	1.99	1.04
1:F:257:PHE:H	2:G:365:GLY:HA2	1.18	1.04
1:H:252:GLN:NE2	2:I:362:ARG:HH22	1.55	1.04
1:D:234:SER:HB2	2:I:336:ARG:HB2	1.12	1.04
1:F:93:TYR:HE1	2:G:238:ASP:OD2	1.40	1.04
1:F:256:PRO:HB2	2:G:366:GLU:HA	1.39	1.04
1:A:11:VAL:HG21	1:A:35:SER:CA	1.87	1.04
1:D:256:PRO:HA	2:E:366:GLU:CA	1.87	1.04
2:G:206:HIS:CE1	2:I:173:GLU:HB3	1.92	1.04
1:D:34:LEU:HD13	1:D:132:LYS:HE2	1.36	1.04
2:E:174:THR:HG23	2:I:206:HIS:CB	1.88	1.04
2:G:274:LEU:HD23	2:G:311:GLU:CD	1.78	1.04
1:A:93:TYR:CE1	2:B:238:ASP:OD2	2.10	1.03
1:A:256:PRO:HB3	2:B:366:GLU:HG2	1.34	1.03
1:D:90:GLY:O	2:E:240:PRO:HB2	1.55	1.03
2:G:206:HIS:CB	2:I:174:THR:HG21	1.61	1.03
1:H:116:THR:HG23	2:I:327:ASN:OD1	1.55	1.03
1:D:88:MET:SD	2:E:238:ASP:O	2.16	1.03
1:D:90:GLY:C	2:E:240:PRO:CB	2.26	1.03
2:E:208:ARG:HG3	2:G:89:GLY:O	1.57	1.03
1:H:95:PHE:CD1	2:I:264:LYS:C	2.32	1.03
2:I:294:THR:HG22	2:I:295:ASN:N	1.68	1.03
2:I:294:THR:CG2	2:I:295:ASN:H	1.70	1.03
2:G:206:HIS:CB	2:I:174:THR:HG22	1.80	1.03
2:G:206:HIS:NE2	2:I:173:GLU:HB2	1.67	1.03
2:I:274:LEU:HD21	2:I:296:HIS:NE2	1.73	1.03
1:D:256:PRO:CB	2:E:366:GLU:CA	2.25	1.02
1:H:62:CYS:HB2	2:I:264:LYS:HE2	1.41	1.02
1:A:34:LEU:HD13	1:A:132:LYS:HE2	1.34	1.02
1:F:88:MET:HB2	2:G:240:PRO:HD3	1.39	1.02
1:D:256:PRO:HB2	2:E:366:GLU:HG3	1.39	1.02
2:E:274:LEU:CD2	2:E:311:GLU:CB	2.36	1.02
1:A:93:TYR:HA	2:B:290:HIS:HE1	0.97	1.02
1:D:62:CYS:HB3	2:E:264:LYS:HE2	1.03	1.02
1:D:234:SER:CB	2:I:336:ARG:HB2	1.76	1.02
1:A:385:ASP:HB3	2:B:405:GLN:CG	1.67	1.02
1:A:127:ALA:HB2	1:A:171:THR:OG1	1.59	1.01
1:D:234:SER:HB2	2:I:336:ARG:HA	1.39	1.01
1:F:88:MET:HB3	2:G:240:PRO:CD	1.88	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:90:GLY:HA3	2:G:240:PRO:O	0.85	1.01
1:A:11:VAL:HG21	1:A:35:SER:HA	1.05	1.01
1:A:74:PRO:HB3	1:A:215:ALA:HB3	1.42	1.01
1:D:237:PRO:CG	2:I:352:TYR:CG	2.41	1.01
1:F:359:ALA:CB	2:G:406:LEU:HD12	1.90	1.01
2:G:208:ARG:NH1	2:I:90:HIS:N	2.05	1.01
2:E:237:PRO:HG3	2:E:306:VAL:HG12	1.05	1.01
2:G:210:GLN:NE2	2:I:91:SER:HB3	1.75	1.01
2:G:336:ARG:HB3	1:H:234:SER:CB	1.91	1.01
1:D:11:VAL:HG11	1:D:35:SER:HA	1.43	1.01
1:D:171:THR:O	1:D:173:PHE:N	1.92	1.01
2:G:210:GLN:NE2	2:I:91:SER:CB	2.23	1.01
1:H:33:LEU:CG	1:H:133:LEU:CD1	2.38	1.01
2:E:237:PRO:HB3	2:E:307:PRO:O	1.60	1.01
1:F:108:VAL:HG11	1:F:217:THR:HG21	1.38	1.01
1:A:170:TRP:CZ3	1:A:172:PRO:CD	2.43	1.00
1:F:108:VAL:C	1:F:109:GLU:N	2.14	1.00
2:G:210:GLN:HG3	2:I:91:SER:HB3	1.06	1.00
1:D:259:CYS:SG	1:D:271:CYS:CB	2.49	1.00
1:F:235:GLN:C	1:F:236:ALA:N	2.13	1.00
1:D:62:CYS:CB	2:E:264:LYS:HE2	1.92	1.00
1:D:89:TRP:CE2	2:E:239:THR:CG2	2.44	1.00
1:D:34:LEU:HD12	1:D:132:LYS:CE	1.92	1.00
1:D:88:MET:CE	2:E:238:ASP:O	0.70	1.00
1:H:88:MET:HB2	2:I:240:PRO:CD	1.61	1.00
1:F:257:PHE:HB3	1:F:272:ALA:HB3	1.42	1.00
1:A:385:ASP:HB3	2:B:405:GLN:HG3	1.05	0.99
1:D:88:MET:HE3	2:E:238:ASP:O	1.18	0.99
1:A:75:ASP:OD2	1:A:217:THR:N	1.88	0.99
1:D:170:TRP:CZ2	1:D:172:PRO:N	2.30	0.99
1:A:95:PHE:CD1	2:B:289:CYS:HA	1.97	0.99
1:F:90:GLY:HA3	2:G:240:PRO:C	1.82	0.99
1:H:88:MET:HB2	2:I:240:PRO:HG3	1.39	0.99
2:E:174:THR:CG2	2:I:206:HIS:HB2	1.91	0.99
1:F:74:PRO:CB	1:F:215:ALA:CB	2.41	0.99
1:A:172:PRO:HG2	1:A:268:ALA:CB	1.88	0.99
1:A:75:ASP:CG	1:A:217:THR:H	1.67	0.99
2:E:274:LEU:HD23	2:E:311:GLU:CD	1.82	0.98
1:A:90:GLY:HA3	2:B:240:PRO:C	1.81	0.98
1:A:170:TRP:CE3	1:A:172:PRO:HD3	1.97	0.98
2:G:378:LYS:NZ	1:H:242:TYR:HB2	1.77	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:GLN:O	2:B:362:ARG:NH1	1.96	0.98
1:H:88:MET:CB	2:I:240:PRO:HG3	1.90	0.98
1:A:254:THR:CA	2:B:368:PRO:HG3	1.91	0.98
2:B:274:LEU:HD21	2:B:296:HIS:NE2	1.78	0.98
1:F:171:THR:HG1	1:F:173:PHE:HD2	0.98	0.98
1:H:33:LEU:CG	1:H:133:LEU:HD13	1.93	0.98
1:D:234:SER:CA	2:I:336:ARG:CB	2.37	0.98
2:G:352:TYR:HD2	1:H:237:PRO:HD2	1.14	0.98
1:H:235:GLN:C	1:H:236:ALA:N	2.15	0.98
1:A:385:ASP:CB	2:B:405:GLN:HE21	1.76	0.98
1:A:88:MET:CB	2:B:240:PRO:HD3	1.94	0.98
2:G:210:GLN:HE21	2:I:91:SER:HB3	1.26	0.98
1:A:90:GLY:O	2:B:240:PRO:HB2	1.64	0.97
1:A:256:PRO:HB2	2:B:366:GLU:HG3	1.43	0.97
1:D:90:GLY:CA	2:E:240:PRO:HG2	1.94	0.97
1:A:11:VAL:CG2	1:A:35:SER:HA	1.94	0.97
1:D:218:GLN:NE2	2:I:338:PRO:C	2.11	0.97
1:A:254:THR:HA	2:B:368:PRO:HG2	1.45	0.97
1:F:62:CYS:HB2	2:G:264:LYS:HE2	1.00	0.97
1:H:252:GLN:HE21	2:I:362:ARG:HH22	1.07	0.97
2:G:352:TYR:HB3	1:H:237:PRO:CD	1.93	0.97
1:D:245:LYS:CE	2:I:378:LYS:CB	2.37	0.96
2:G:336:ARG:HB2	1:H:234:SER:HB2	1.44	0.96
1:H:172:PRO:CG	1:H:268:ALA:HB2	1.95	0.96
1:H:88:MET:CA	2:I:240:PRO:HG3	1.96	0.96
1:A:95:PHE:N	2:B:264:LYS:CB	2.27	0.96
1:H:88:MET:HB3	2:I:240:PRO:HD2	0.99	0.96
1:H:88:MET:C	2:I:240:PRO:HG2	1.85	0.96
1:H:170:TRP:CZ3	1:H:172:PRO:HD3	2.01	0.96
1:A:218:GLN:HB2	1:A:236:ALA:CB	1.94	0.96
1:D:34:LEU:CD1	1:D:132:LYS:HE2	1.96	0.96
1:D:34:LEU:HD12	1:D:132:LYS:HE3	1.43	0.96
1:H:93:TYR:C	2:I:290:HIS:CE1	2.37	0.96
1:D:7:ILE:HD11	1:D:33:LEU:HD11	1.47	0.96
1:D:89:TRP:CE2	2:E:239:THR:HG23	1.99	0.96
2:E:334:LYS:HD3	2:E:396:ASN:C	1.84	0.96
1:H:256:PRO:CB	2:I:366:GLU:HG3	1.96	0.96
1:H:33:LEU:CD2	1:H:133:LEU:CD1	2.43	0.95
1:H:173:PHE:O	1:H:174:ASP:O	1.82	0.95
1:A:90:GLY:HA3	2:B:240:PRO:O	0.78	0.95
2:B:274:LEU:CD2	2:B:311:GLU:OE2	2.13	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:129:ALA:HB3	1:F:166:MET:HG3	1.45	0.95
1:H:7:ILE:CD1	1:H:33:LEU:HD12	1.95	0.95
1:H:133:LEU:HG	1:H:134:ARG:H	1.30	0.95
1:F:170:TRP:CZ2	1:F:172:PRO:HA	2.01	0.95
1:H:33:LEU:HD23	1:H:133:LEU:HD13	1.46	0.95
2:E:336:ARG:HH11	1:F:235:GLN:HA	0.99	0.95
1:D:170:TRP:CG	1:D:171:THR:N	2.34	0.95
1:A:384:LYS:HG3	1:A:385:ASP:N	1.77	0.94
1:A:291:VAL:HG23	1:F:304:PRO:O	1.64	0.94
2:G:206:HIS:HB2	2:I:174:THR:HG22	1.45	0.94
1:H:95:PHE:HB2	2:I:264:LYS:HB3	1.23	0.94
1:D:95:PHE:CE2	2:E:271:ASN:ND2	2.35	0.94
1:H:88:MET:HE1	2:I:239:THR:N	1.81	0.94
1:A:173:PHE:CE1	1:A:184:VAL:CG1	2.51	0.94
1:D:234:SER:CB	2:I:336:ARG:HA	1.97	0.94
1:H:33:LEU:HD21	1:H:133:LEU:HD13	1.48	0.94
2:G:206:HIS:HB2	2:I:174:THR:CG2	1.97	0.93
1:A:252:GLN:HE22	2:B:362:ARG:HH22	1.14	0.93
1:D:95:PHE:CZ	2:E:271:ASN:HB2	2.02	0.93
1:F:93:TYR:CE1	2:G:238:ASP:OD2	2.21	0.93
1:F:385:ASP:O	2:G:405:GLN:HG3	1.67	0.93
2:G:208:ARG:HH22	2:I:90:HIS:HD2	1.13	0.93
2:G:210:GLN:NE2	2:I:91:SER:OG	2.00	0.93
1:A:254:THR:CA	2:B:368:PRO:CG	2.45	0.93
1:A:90:GLY:O	2:B:240:PRO:C	2.07	0.93
1:F:235:GLN:CG	1:F:236:ALA:N	2.32	0.93
1:F:11:VAL:HG23	1:F:36:VAL:HG23	1.49	0.93
1:H:383:PRO:CG	2:I:407:SER:N	2.32	0.93
1:A:256:PRO:CB	2:B:366:GLU:CG	1.93	0.93
1:F:129:ALA:CB	1:F:166:MET:HG3	1.97	0.93
1:F:170:TRP:CH2	1:F:172:PRO:N	2.36	0.93
1:H:170:TRP:HH2	1:H:172:PRO:HB3	1.31	0.93
1:H:88:MET:HB2	2:I:240:PRO:HD3	1.17	0.92
1:F:256:PRO:HB3	2:G:366:GLU:CA	1.56	0.92
1:A:90:GLY:H	2:B:240:PRO:HG2	1.29	0.92
1:A:291:VAL:HG21	1:F:304:PRO:HA	1.48	0.92
1:D:90:GLY:CA	2:E:240:PRO:CB	2.47	0.92
2:G:208:ARG:HH21	2:I:88:GLU:CB	1.82	0.92
2:B:294:THR:CB	2:B:295:ASN:N	2.32	0.92
1:F:88:MET:HB3	2:G:240:PRO:HD2	1.50	0.92
1:A:256:PRO:HB3	2:B:366:GLU:CB	1.99	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:TRP:CZ2	2:E:239:THR:CG2	2.52	0.92
2:G:339:THR:HG22	1:H:218:GLN:NE2	1.84	0.92
2:G:336:ARG:NH2	1:H:236:ALA:N	2.16	0.92
1:D:7:ILE:HD11	1:D:33:LEU:CD1	2.00	0.92
2:E:90:HIS:CD2	2:I:208:ARG:HH12	1.88	0.91
2:G:294:THR:CB	2:G:295:ASN:N	2.34	0.91
1:H:11:VAL:HA	1:H:33:LEU:O	1.70	0.91
1:A:90:GLY:N	2:B:240:PRO:CG	2.33	0.91
1:F:74:PRO:HB2	1:F:215:ALA:CB	1.97	0.91
1:F:90:GLY:N	2:G:240:PRO:HG2	1.85	0.91
1:H:93:TYR:HA	2:I:290:HIS:HE1	1.34	0.91
1:A:91:GLY:N	2:B:240:PRO:HB2	1.84	0.91
1:A:173:PHE:CZ	1:A:184:VAL:HG11	2.04	0.91
1:A:88:MET:HB3	2:B:240:PRO:HD3	1.52	0.91
2:B:237:PRO:CG	2:B:306:VAL:CG1	2.47	0.91
1:F:256:PRO:HG2	2:G:366:GLU:HA	1.50	0.91
1:A:291:VAL:CG2	1:F:304:PRO:HA	1.99	0.91
1:D:89:TRP:HZ2	2:E:239:THR:HG22	1.32	0.91
2:E:89:GLY:HA3	2:I:208:ARG:HG3	0.92	0.91
1:H:254:THR:HA	2:I:368:PRO:HG3	1.53	0.91
1:F:88:MET:HB2	2:G:240:PRO:CD	1.97	0.90
1:F:116:THR:HG23	2:G:327:ASN:ND2	1.85	0.90
1:A:34:LEU:CB	1:A:132:LYS:HB2	2.00	0.90
1:A:252:GLN:NE2	2:B:362:ARG:CZ	2.09	0.90
2:G:208:ARG:CZ	2:I:90:HIS:N	2.33	0.90
2:E:89:GLY:HA3	2:I:208:ARG:CD	2.00	0.90
2:E:274:LEU:HD21	2:E:311:GLU:HB2	1.53	0.90
2:G:212:GLY:HA3	2:G:332:VAL:O	1.70	0.90
1:D:245:LYS:HE2	2:I:378:LYS:HB2	0.91	0.90
1:H:252:GLN:HE21	2:I:362:ARG:NH2	1.68	0.90
1:F:74:PRO:HB3	1:F:215:ALA:CB	2.02	0.90
1:A:74:PRO:HB2	1:A:215:ALA:HB3	1.53	0.90
2:B:262:ARG:NH2	2:B:309:ASN:OD1	2.05	0.90
1:H:88:MET:CA	2:I:240:PRO:CG	2.50	0.90
1:H:127:ALA:CB	1:H:171:THR:HB	2.01	0.89
2:E:174:THR:CG2	2:I:206:HIS:CB	2.50	0.89
1:D:11:VAL:HG21	1:D:35:SER:C	1.93	0.89
2:E:89:GLY:HA3	2:I:208:ARG:HG2	1.51	0.89
2:E:334:LYS:HD3	2:E:397:ASN:N	1.88	0.89
1:A:127:ALA:CB	1:A:171:THR:OG1	2.16	0.89
2:I:261:VAL:N	2:I:294:THR:HB	1.86	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:336:ARG:CZ	1:H:236:ALA:N	2.34	0.89
1:H:88:MET:C	2:I:240:PRO:CG	2.41	0.89
2:B:262:ARG:HH22	2:B:309:ASN:CG	1.76	0.89
1:A:74:PRO:CB	1:A:215:ALA:CB	2.51	0.89
1:H:93:TYR:HE1	2:I:238:ASP:OD2	1.56	0.89
1:H:95:PHE:CD1	2:I:264:LYS:O	2.25	0.89
2:E:174:THR:HG23	2:I:206:HIS:HB2	1.50	0.88
1:F:170:TRP:CZ2	1:F:172:PRO:N	2.41	0.88
1:F:170:TRP:CD2	1:F:171:THR:N	2.41	0.88
1:H:385:ASP:HA	1:H:386:HIS:HB2	0.90	0.88
1:A:170:TRP:CH2	1:A:172:PRO:CB	2.56	0.88
1:D:170:TRP:CD2	1:D:171:THR:N	2.42	0.88
1:D:252:GLN:O	2:E:362:ARG:NH1	2.06	0.88
2:E:203:GLU:OE2	2:E:396:ASN:ND2	2.05	0.88
1:D:34:LEU:HD13	1:D:132:LYS:CE	1.99	0.88
2:E:208:ARG:HG2	2:G:89:GLY:HA3	1.56	0.88
2:I:274:LEU:HD23	2:I:296:HIS:HE1	1.36	0.88
2:E:336:ARG:NE	1:F:235:GLN:C	2.27	0.88
2:G:208:ARG:HH22	2:I:90:HIS:CD2	1.87	0.88
1:D:170:TRP:CH2	1:D:172:PRO:CD	2.55	0.88
2:I:261:VAL:C	2:I:294:THR:OG1	2.11	0.88
2:E:206:HIS:CD2	2:G:174:THR:HG23	2.09	0.88
1:H:95:PHE:HB2	2:I:264:LYS:C	1.94	0.88
1:F:127:ALA:CB	1:F:171:THR:HG21	2.03	0.87
1:F:170:TRP:CZ2	1:F:172:PRO:CA	2.57	0.87
1:A:90:GLY:CA	2:B:240:PRO:HG2	2.04	0.87
1:H:95:PHE:HD1	2:I:264:LYS:O	1.57	0.87
1:A:34:LEU:HD12	1:A:132:LYS:HD3	1.57	0.87
2:I:237:PRO:CG	2:I:306:VAL:CG1	2.49	0.87
1:F:170:TRP:CZ3	1:F:172:PRO:HD3	2.10	0.86
1:F:359:ALA:HB1	2:G:406:LEU:HD12	1.56	0.86
1:F:129:ALA:HB3	1:F:166:MET:CG	2.04	0.86
2:G:237:PRO:CG	2:G:306:VAL:HG12	2.00	0.86
2:G:378:LYS:HZ2	1:H:242:TYR:HB2	1.40	0.86
1:A:90:GLY:H	2:B:240:PRO:CG	1.86	0.86
1:A:95:PHE:H	2:B:264:LYS:HB3	1.39	0.86
1:D:95:PHE:CZ	2:E:271:ASN:CB	2.57	0.86
1:H:256:PRO:HA	2:I:366:GLU:HA	1.56	0.86
1:D:259:CYS:HG	1:D:271:CYS:CB	1.84	0.86
1:F:256:PRO:HG2	2:G:366:GLU:O	1.76	0.85
1:F:217:THR:O	1:F:218:GLN:N	2.08	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:336:ARG:HH21	1:H:236:ALA:HA	1.35	0.85
1:D:254:THR:HA	2:E:368:PRO:CG	2.05	0.85
1:A:172:PRO:O	1:A:173:PHE:CG	2.30	0.85
1:A:385:ASP:HB2	2:B:405:GLN:HE21	1.04	0.85
2:E:156:THR:OG1	2:G:88:GLU:OE2	1.75	0.85
2:G:339:THR:HG23	1:H:218:GLN:OE1	1.77	0.85
1:H:172:PRO:CG	1:H:268:ALA:CB	2.53	0.85
1:F:257:PHE:N	2:G:365:GLY:CA	2.38	0.85
1:H:172:PRO:O	1:H:173:PHE:CG	2.30	0.85
1:D:237:PRO:HG2	2:I:352:TYR:HB3	1.54	0.85
2:I:237:PRO:HG3	2:I:306:VAL:HG11	1.58	0.85
2:G:207:SER:CB	2:I:85:ASP:HB2	2.06	0.84
1:A:172:PRO:O	1:A:173:PHE:CD2	2.30	0.84
2:G:294:THR:O	2:G:295:ASN:CA	2.18	0.84
1:H:90:GLY:C	2:I:240:PRO:HB2	1.97	0.84
1:H:170:TRP:CH2	1:H:172:PRO:CB	2.60	0.84
1:D:90:GLY:CA	2:E:240:PRO:CG	2.53	0.84
1:D:245:LYS:NZ	2:I:378:LYS:HB2	1.91	0.84
2:G:294:THR:O	2:G:295:ASN:N	2.10	0.84
1:A:74:PRO:HB3	1:A:215:ALA:CB	2.07	0.84
1:D:218:GLN:NE2	2:I:338:PRO:O	2.07	0.84
1:F:359:ALA:HB2	2:G:406:LEU:HD12	1.57	0.84
2:G:210:GLN:CD	2:I:91:SER:HB3	1.97	0.84
2:E:89:GLY:C	2:I:208:ARG:NH1	2.31	0.84
1:F:11:VAL:HG22	1:F:36:VAL:HG23	1.58	0.84
1:D:237:PRO:CG	2:I:352:TYR:CB	2.55	0.84
1:D:256:PRO:HB3	2:E:366:GLU:HG2	1.56	0.84
1:H:52:LYS:HE3	2:I:100:ARG:NH1	1.92	0.84
1:D:237:PRO:HB2	2:I:352:TYR:CD2	2.12	0.84
2:G:156:THR:HG21	2:I:88:GLU:OE2	1.77	0.84
1:D:95:PHE:CE2	2:E:271:ASN:CG	2.51	0.84
2:E:202:ARG:HG2	2:E:358:LEU:HD13	1.59	0.83
1:F:171:THR:OG1	1:F:173:PHE:CD2	2.30	0.83
1:H:386:HIS:O	1:H:387:ILE:HD13	1.78	0.83
2:B:274:LEU:HD21	2:B:296:HIS:CE1	2.12	0.83
2:G:339:THR:HG21	1:H:218:GLN:CD	1.98	0.83
1:H:91:GLY:N	2:I:240:PRO:HB2	1.92	0.83
1:A:34:LEU:CD1	1:A:132:LYS:HE3	1.87	0.83
2:E:90:HIS:CG	2:I:208:ARG:HH12	1.95	0.83
1:F:90:GLY:O	2:G:240:PRO:HB2	1.78	0.83
2:G:336:ARG:CB	1:H:234:SER:CB	2.49	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:206:HIS:NE2	2:I:173:GLU:C	2.32	0.83
1:A:127:ALA:HB2	1:A:171:THR:CG2	2.09	0.83
1:F:127:ALA:HB2	1:F:171:THR:CG2	2.09	0.83
1:H:95:PHE:HB2	2:I:264:LYS:CA	2.09	0.83
2:G:208:ARG:HH21	2:I:88:GLU:HB3	1.44	0.82
1:A:34:LEU:CD1	1:A:132:LYS:HD3	2.06	0.82
2:E:208:ARG:CG	2:G:89:GLY:O	2.27	0.82
1:A:170:TRP:HZ3	1:A:271:CYS:SG	2.02	0.82
2:E:378:LYS:HD2	1:F:242:TYR:CD1	2.14	0.82
2:G:294:THR:C	2:G:295:ASN:N	2.32	0.82
2:G:262:ARG:NH2	2:G:309:ASN:OD1	2.13	0.82
1:H:172:PRO:HG3	1:H:268:ALA:CB	2.09	0.82
2:G:294:THR:HG22	2:G:295:ASN:CA	2.09	0.82
1:H:33:LEU:HG	1:H:133:LEU:HD12	1.61	0.82
1:D:254:THR:HA	2:E:368:PRO:HG2	1.62	0.82
1:F:253:HIS:CA	2:G:362:ARG:HD3	2.09	0.82
2:G:336:ARG:CZ	1:H:236:ALA:HA	2.03	0.82
1:D:34:LEU:HB2	1:D:132:LYS:CB	2.10	0.82
1:F:62:CYS:HB3	2:G:264:LYS:HE2	1.60	0.82
2:G:336:ARG:CZ	1:H:236:ALA:CA	2.58	0.82
1:H:95:PHE:CG	2:I:264:LYS:C	2.53	0.82
1:F:93:TYR:CA	2:G:290:HIS:CE1	2.63	0.81
2:G:206:HIS:CD2	2:I:174:THR:CG2	2.40	0.81
2:G:202:ARG:NH2	2:G:393:THR:O	2.13	0.81
1:D:253:HIS:O	2:E:368:PRO:CG	2.29	0.81
1:D:259:CYS:HG	1:D:271:CYS:HG	1.04	0.81
1:A:95:PHE:HD1	2:B:289:CYS:HA	1.43	0.81
1:D:218:GLN:HB2	1:D:236:ALA:HA	1.62	0.81
1:H:7:ILE:CD1	1:H:33:LEU:CD1	2.51	0.81
1:A:127:ALA:HB3	1:A:171:THR:CB	1.95	0.81
1:D:237:PRO:HG2	2:I:352:TYR:CD2	2.14	0.81
2:E:336:ARG:NH1	1:F:235:GLN:C	2.29	0.81
1:F:129:ALA:HB1	1:F:166:MET:CE	2.10	0.81
1:F:75:ASP:CG	1:F:217:THR:H	1.83	0.80
1:F:95:PHE:CG	2:G:265:CYS:N	2.25	0.80
1:F:33:LEU:HD22	1:F:131:ALA:HB1	1.64	0.80
1:D:51:TYR:CE1	1:D:108:VAL:CG2	2.63	0.80
1:D:52:LYS:HG2	1:D:54:VAL:HG23	1.63	0.80
1:H:75:ASP:OD2	1:H:217:THR:N	2.15	0.80
1:H:95:PHE:HB2	2:I:264:LYS:HB2	1.61	0.80
2:E:336:ARG:CZ	1:F:235:GLN:CA	2.55	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:VAL:HG21	1:D:36:VAL:HG23	1.63	0.80
1:D:237:PRO:HD2	2:I:352:TYR:CD1	2.15	0.80
1:D:95:PHE:CE2	2:E:271:ASN:HB2	2.16	0.80
2:E:378:LYS:HD2	1:F:242:TYR:CE1	2.17	0.80
2:G:207:SER:CB	2:I:85:ASP:CB	2.57	0.80
2:E:336:ARG:HD3	1:F:234:SER:C	2.01	0.80
1:H:90:GLY:O	2:I:241:ASP:N	2.15	0.80
1:F:256:PRO:CB	2:G:366:GLU:C	2.48	0.80
1:A:88:MET:HB3	2:B:240:PRO:CD	2.12	0.79
2:G:237:PRO:HB3	2:G:307:PRO:O	1.83	0.79
1:A:88:MET:HB2	2:B:240:PRO:HD3	1.62	0.79
1:A:384:LYS:CG	1:A:385:ASP:H	1.93	0.79
2:G:206:HIS:HB3	2:I:174:THR:HG21	0.82	0.79
2:I:261:VAL:N	2:I:294:THR:CB	2.44	0.79
1:H:383:PRO:HG2	2:I:407:SER:N	1.97	0.79
1:F:93:TYR:C	2:G:290:HIS:CE1	2.56	0.79
1:F:129:ALA:CB	1:F:166:MET:CE	2.60	0.79
1:F:257:PHE:N	2:G:365:GLY:HA2	1.96	0.79
2:E:274:LEU:HD21	2:E:311:GLU:CB	2.06	0.79
1:F:171:THR:OG1	1:F:173:PHE:HD2	1.64	0.79
2:I:261:VAL:CA	2:I:294:THR:OG1	2.31	0.79
1:D:89:TRP:CE2	2:E:239:THR:HG22	2.13	0.78
1:F:62:CYS:CB	2:G:264:LYS:CE	2.50	0.78
1:A:34:LEU:CD1	1:A:132:LYS:CD	2.35	0.78
1:F:170:TRP:CG	1:F:171:THR:N	2.47	0.78
1:A:90:GLY:H	2:B:240:PRO:CD	1.96	0.78
1:F:90:GLY:H	2:G:240:PRO:HG2	1.47	0.78
1:D:33:LEU:HD23	1:D:133:LEU:HD13	1.66	0.78
1:H:253:HIS:O	2:I:368:PRO:CB	2.31	0.78
2:I:294:THR:CG2	2:I:295:ASN:N	2.33	0.78
1:A:385:ASP:CA	1:A:386:HIS:CB	2.30	0.77
1:A:170:TRP:HH2	1:A:172:PRO:HB3	1.41	0.77
1:D:34:LEU:CD1	1:D:132:LYS:HE3	2.07	0.77
2:B:237:PRO:HG3	2:B:306:VAL:HG12	1.65	0.77
1:F:75:ASP:OD2	1:F:217:THR:CA	2.32	0.77
2:G:210:GLN:HG3	2:I:91:SER:HB2	1.60	0.77
1:H:254:THR:HA	2:I:368:PRO:CG	2.15	0.77
2:E:339:THR:HG23	1:F:218:GLN:NE2	1.99	0.77
1:F:90:GLY:C	2:G:240:PRO:CB	2.52	0.77
2:I:333:PRO:O	2:I:396:ASN:ND2	2.16	0.77
2:B:238:ASP:HB3	2:B:292:ALA:HB1	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:170:TRP:CH2	1:F:172:PRO:CD	2.67	0.77
1:F:108:VAL:HG11	1:F:217:THR:CG2	2.15	0.77
2:I:260:THR:HB	2:I:295:ASN:N	1.99	0.77
2:E:274:LEU:CD2	2:E:311:GLU:CD	2.53	0.76
1:F:11:VAL:HG23	1:F:36:VAL:CG2	2.15	0.76
1:H:88:MET:HE2	2:I:239:THR:HA	1.67	0.76
1:H:225:ALA:H	1:H:230:HIS:HE1	1.33	0.76
2:B:248:GLN:HG2	2:B:253:LYS:HB2	1.68	0.76
1:A:173:PHE:HE1	1:A:184:VAL:CG1	1.96	0.76
1:A:93:TYR:C	2:B:290:HIS:ND1	2.40	0.76
2:E:88:GLU:OE2	2:I:156:THR:HG21	1.85	0.76
1:H:172:PRO:HG3	1:H:268:ALA:HB1	1.66	0.76
1:D:257:PHE:H	2:E:366:GLU:N	1.84	0.75
1:F:93:TYR:HA	2:G:290:HIS:CE1	2.21	0.75
1:D:52:LYS:HE2	1:D:54:VAL:HG22	1.68	0.75
1:H:88:MET:N	2:I:240:PRO:HG3	2.00	0.75
1:D:253:HIS:O	2:E:368:PRO:CB	2.34	0.75
1:A:94:CYS:HA	2:B:264:LYS:HD2	1.68	0.75
1:A:385:ASP:HB3	2:B:405:GLN:HG2	1.65	0.75
2:G:210:GLN:CG	2:I:91:SER:CB	2.47	0.75
2:G:352:TYR:CE2	1:H:198:GLY:HA3	2.21	0.75
2:I:237:PRO:CG	2:I:306:VAL:HG12	2.11	0.75
1:D:385:ASP:O	2:E:405:GLN:CG	2.31	0.75
1:A:385:ASP:CB	2:B:405:GLN:NE2	2.32	0.75
1:D:225:ALA:H	1:D:230:HIS:HE1	1.34	0.75
2:G:156:THR:HG22	2:I:88:GLU:OE1	1.87	0.75
1:A:74:PRO:HB2	1:A:215:ALA:CB	2.14	0.75
1:F:256:PRO:HB3	2:G:366:GLU:C	2.06	0.74
2:I:248:GLN:HG2	2:I:253:LYS:HB2	1.68	0.74
1:A:88:MET:CB	2:B:240:PRO:CD	2.65	0.74
1:A:225:ALA:H	1:A:230:HIS:HE1	1.33	0.74
1:D:253:HIS:O	2:E:368:PRO:HB2	1.87	0.74
1:H:127:ALA:HB2	1:H:171:THR:CB	2.15	0.74
1:D:256:PRO:HA	2:E:366:GLU:C	2.08	0.74
2:E:336:ARG:HD3	1:F:235:GLN:CA	2.18	0.74
1:D:170:TRP:CZ2	1:D:172:PRO:CD	2.71	0.74
2:G:378:LYS:HZ2	1:H:242:TYR:CB	2.01	0.74
2:G:274:LEU:HD21	2:G:296:HIS:CE1	2.21	0.74
1:F:225:ALA:H	1:F:230:HIS:HE1	1.33	0.74
1:D:33:LEU:CD2	1:D:133:LEU:HD13	2.17	0.74
2:E:336:ARG:HB3	1:F:234:SER:OG	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:235:GLN:CA	1:F:236:ALA:N	2.50	0.73
1:F:254:THR:HG22	2:G:370:TYR:HB2	1.69	0.73
1:D:95:PHE:CE2	2:E:271:ASN:CB	2.72	0.73
2:E:248:GLN:HG2	2:E:253:LYS:HB2	1.68	0.73
1:F:129:ALA:HB1	1:F:166:MET:HE1	1.69	0.73
2:E:90:HIS:CD2	2:I:208:ARG:NH1	2.56	0.73
2:G:206:HIS:NE2	2:I:173:GLU:CA	2.51	0.73
1:D:62:CYS:CB	2:E:264:LYS:CE	2.57	0.73
2:E:378:LYS:HZ2	1:F:242:TYR:CB	2.01	0.73
2:E:207:SER:HB2	2:G:85:ASP:HB2	1.71	0.73
2:G:248:GLN:HG2	2:G:253:LYS:HB2	1.68	0.73
2:G:206:HIS:CG	2:I:174:THR:HG22	2.06	0.72
1:A:291:VAL:CG2	1:F:304:PRO:C	2.30	0.72
1:A:33:LEU:CD2	1:A:133:LEU:HD13	2.20	0.72
1:A:52:LYS:HE3	2:B:100:ARG:NH1	2.05	0.72
1:F:170:TRP:HZ2	1:F:172:PRO:HA	1.53	0.72
1:D:11:VAL:HA	1:D:33:LEU:O	1.90	0.72
1:D:382:PRO:O	1:D:383:PRO:O	2.08	0.72
1:D:171:THR:C	1:D:173:PHE:H	1.93	0.72
1:H:88:MET:HE1	2:I:238:ASP:CA	2.18	0.72
1:A:218:GLN:CB	1:A:236:ALA:HB2	2.12	0.72
1:A:170:TRP:CZ3	1:A:271:CYS:SG	2.83	0.71
2:E:336:ARG:CB	1:F:234:SER:CB	2.38	0.71
2:E:378:LYS:NZ	1:F:198:GLY:O	2.21	0.71
1:H:11:VAL:CG2	1:H:36:VAL:HG23	2.20	0.71
1:D:171:THR:OG1	1:D:173:PHE:HD2	1.73	0.71
2:E:334:LYS:CD	2:E:396:ASN:C	2.59	0.71
1:F:129:ALA:O	1:F:148:ALA:HB3	1.90	0.71
1:F:256:PRO:HB2	2:G:366:GLU:CA	2.02	0.71
1:D:90:GLY:HA3	2:E:240:PRO:HB2	1.73	0.71
1:F:129:ALA:CB	1:F:166:MET:CG	2.64	0.71
2:G:274:LEU:CD2	2:G:311:GLU:CD	2.49	0.71
1:F:170:TRP:C	1:F:171:THR:HG22	2.10	0.71
2:E:274:LEU:HD23	2:E:311:GLU:CG	2.19	0.71
1:H:268:ALA:HB1	1:H:271:CYS:SG	2.31	0.71
1:F:91:GLY:O	2:G:240:PRO:HG3	1.91	0.71
2:E:262:ARG:HA	2:E:274:LEU:H	1.56	0.71
1:H:88:MET:H	2:I:240:PRO:HG3	1.55	0.71
1:D:254:THR:CA	2:E:368:PRO:HG3	2.20	0.70
1:D:218:GLN:NE2	2:I:339:THR:CA	2.20	0.70
1:A:127:ALA:HB2	1:A:171:THR:HG21	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:ILE:HG21	2:B:342:TYR:CD2	2.26	0.70
1:D:52:LYS:O	1:D:108:VAL:C	2.30	0.70
2:E:336:ARG:HB3	1:F:234:SER:HB2	0.71	0.70
2:G:378:LYS:HZ1	1:H:242:TYR:HB2	1.56	0.70
1:A:90:GLY:CA	2:B:240:PRO:C	2.49	0.70
1:F:127:ALA:CB	1:F:171:THR:CG2	2.70	0.70
1:H:253:HIS:O	2:I:368:PRO:CG	2.40	0.70
1:A:90:GLY:C	2:B:240:PRO:C	2.49	0.69
2:E:207:SER:CB	2:G:85:ASP:HB2	2.22	0.69
1:H:95:PHE:CB	2:I:264:LYS:C	2.61	0.69
1:A:91:GLY:N	2:B:240:PRO:CB	2.53	0.69
1:A:256:PRO:HA	2:B:366:GLU:HA	0.75	0.69
1:D:51:TYR:OH	1:D:235:GLN:NE2	2.25	0.69
2:G:207:SER:HB2	2:I:85:ASP:CG	2.12	0.69
1:A:33:LEU:HD23	1:A:133:LEU:HD13	1.74	0.69
2:B:262:ARG:NH2	2:B:309:ASN:CG	2.42	0.69
2:B:262:ARG:HA	2:B:274:LEU:H	1.56	0.69
1:D:259:CYS:CB	1:D:271:CYS:SG	2.80	0.69
2:G:237:PRO:O	2:G:238:ASP:CG	2.30	0.69
2:G:339:THR:CG2	1:H:218:GLN:OE1	2.36	0.69
1:A:90:GLY:C	2:B:240:PRO:CG	2.60	0.69
1:A:173:PHE:HE1	1:A:184:VAL:HG12	1.56	0.69
1:D:11:VAL:CG2	1:D:36:VAL:CG2	2.54	0.69
1:D:88:MET:HB3	2:E:240:PRO:HD3	1.72	0.69
1:D:252:GLN:NE2	2:E:362:ARG:HH22	1.89	0.69
1:D:34:LEU:CB	1:D:132:LYS:HB2	2.18	0.69
1:D:254:THR:C	2:E:368:PRO:HG3	2.13	0.69
2:I:237:PRO:O	2:I:238:ASP:CG	2.30	0.69
2:I:262:ARG:NH2	2:I:309:ASN:OD1	2.25	0.69
1:H:256:PRO:CA	2:I:366:GLU:HA	2.23	0.69
1:D:170:TRP:CE2	1:D:172:PRO:N	2.61	0.69
1:D:256:PRO:CG	2:E:366:GLU:CG	2.71	0.69
2:G:156:THR:CG2	2:I:88:GLU:OE2	2.41	0.69
2:G:262:ARG:HA	2:G:274:LEU:H	1.56	0.69
1:H:127:ALA:HB3	1:H:171:THR:HB	1.74	0.69
2:I:262:ARG:HA	2:I:274:LEU:H	1.56	0.69
2:I:294:THR:O	2:I:295:ASN:CG	2.30	0.69
2:B:274:LEU:HD23	2:B:311:GLU:CD	2.10	0.69
1:H:33:LEU:HG	1:H:133:LEU:HD11	1.72	0.68
1:H:91:GLY:O	2:I:240:PRO:CB	2.41	0.68
1:H:11:VAL:HG23	1:H:36:VAL:HG23	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:SER:CB	2:I:336:ARG:CA	2.43	0.68
2:G:378:LYS:CD	1:H:242:TYR:CD1	2.71	0.68
1:A:34:LEU:HD11	1:A:132:LYS:CE	1.96	0.68
1:D:88:MET:HE1	2:E:239:THR:N	2.07	0.68
1:D:254:THR:HA	2:E:368:PRO:HG3	1.76	0.68
1:H:170:TRP:CZ3	1:H:172:PRO:CD	2.75	0.68
1:H:133:LEU:HG	1:H:134:ARG:N	2.07	0.68
1:F:88:MET:HB2	2:G:240:PRO:CG	2.22	0.68
2:G:208:ARG:H	2:I:89:GLY:HA2	1.59	0.68
1:D:242:TYR:HD1	2:I:378:LYS:HD3	1.58	0.68
2:G:208:ARG:NH2	2:I:87:GLY:O	2.26	0.68
2:I:274:LEU:CD1	2:I:294:THR:HG23	2.24	0.68
1:A:127:ALA:HB2	1:A:171:THR:HG1	1.57	0.67
1:D:90:GLY:HA3	2:E:240:PRO:O	1.93	0.67
1:D:237:PRO:CB	2:I:352:TYR:CD2	2.76	0.67
1:D:256:PRO:CG	2:E:366:GLU:HG3	2.24	0.67
2:E:174:THR:HG23	2:I:206:HIS:CG	2.30	0.67
1:H:92:ALA:HB3	2:I:290:HIS:HD2	1.59	0.67
1:H:95:PHE:CG	2:I:265:CYS:N	2.53	0.67
1:D:52:LYS:HG2	1:D:54:VAL:CG2	2.25	0.67
1:D:170:TRP:CZ3	1:D:172:PRO:HD3	2.27	0.67
1:D:237:PRO:CG	2:I:352:TYR:CD2	2.77	0.67
1:D:234:SER:C	2:I:336:ARG:HB2	2.14	0.67
1:H:33:LEU:HD23	1:H:133:LEU:CD1	2.16	0.67
2:I:261:VAL:N	2:I:294:THR:OG1	2.27	0.67
2:B:294:THR:HG22	2:B:295:ASN:CB	2.23	0.67
1:F:91:GLY:N	2:G:240:PRO:HB2	2.08	0.67
1:H:127:ALA:CB	1:H:171:THR:CB	2.73	0.67
1:A:90:GLY:C	2:B:240:PRO:HG2	2.14	0.67
1:A:91:GLY:N	2:B:240:PRO:CG	2.58	0.67
2:B:238:ASP:HB3	2:B:292:ALA:CB	2.24	0.67
1:F:11:VAL:CG2	1:F:36:VAL:CG2	2.62	0.67
2:G:208:ARG:O	2:I:89:GLY:O	2.12	0.67
1:F:9:ASN:OD1	1:F:36:VAL:HG11	1.95	0.66
1:F:257:PHE:H	2:G:365:GLY:C	1.98	0.66
1:A:127:ALA:CB	1:A:171:THR:CG2	2.70	0.66
1:D:90:GLY:HA3	2:E:240:PRO:C	2.15	0.66
1:F:75:ASP:OD2	1:F:217:THR:OG1	2.13	0.66
1:F:129:ALA:CB	1:F:166:MET:SD	2.83	0.66
1:F:256:PRO:HG2	2:G:366:GLU:CA	2.15	0.66
1:D:51:TYR:CE1	1:D:108:VAL:HG22	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:171:THR:C	1:F:173:PHE:N	2.47	0.66
2:G:206:HIS:CE1	2:I:173:GLU:C	2.69	0.66
1:D:259:CYS:CB	1:D:271:CYS:HG	2.09	0.66
2:G:274:LEU:HD21	2:G:311:GLU:OE2	1.89	0.66
1:A:172:PRO:O	1:A:173:PHE:CB	2.43	0.66
1:A:253:HIS:HB3	2:B:370:TYR:HB2	1.78	0.66
1:D:234:SER:C	2:I:336:ARG:CB	2.62	0.66
1:F:93:TYR:CE1	2:G:238:ASP:HB2	2.31	0.66
1:A:7:ILE:HD11	1:A:33:LEU:CD1	2.26	0.66
1:D:170:TRP:CZ2	1:D:172:PRO:CA	2.79	0.66
1:D:245:LYS:HE2	2:I:378:LYS:CG	2.26	0.66
1:D:271:CYS:O	1:D:272:ALA:C	2.33	0.66
1:F:235:GLN:C	1:F:236:ALA:CA	2.63	0.66
2:G:156:THR:CG2	2:I:88:GLU:OE1	2.44	0.66
2:E:339:THR:HG23	1:F:218:GLN:OE1	1.95	0.66
1:F:93:TYR:HA	2:G:290:HIS:HE1	1.60	0.65
1:F:249:ALA:HB2	2:G:370:TYR:CE2	2.32	0.65
2:B:274:LEU:CD2	2:B:296:HIS:CE1	2.79	0.65
2:G:260:THR:HB	2:G:295:ASN:N	2.12	0.65
1:A:116:THR:HG21	2:B:218:SER:HB3	1.79	0.65
1:D:88:MET:HB3	2:E:240:PRO:CD	2.26	0.65
1:H:88:MET:CG	2:I:240:PRO:HD3	2.26	0.65
2:E:274:LEU:CD2	2:E:311:GLU:CG	2.75	0.65
1:F:253:HIS:O	2:G:362:ARG:CG	2.44	0.65
1:F:172:PRO:HG3	1:F:259:CYS:SG	2.35	0.65
1:H:171:THR:O	1:H:173:PHE:N	2.30	0.65
2:I:238:ASP:HB3	2:I:292:ALA:CB	2.27	0.65
2:I:294:THR:O	2:I:295:ASN:ND2	2.30	0.65
1:D:252:GLN:NE2	2:E:362:ARG:NH2	2.45	0.65
1:H:93:TYR:O	2:I:290:HIS:CE1	2.49	0.65
1:A:268:ALA:HB1	1:A:271:CYS:SG	2.38	0.64
2:B:199:VAL:HG11	2:B:374:TRP:CZ2	2.32	0.64
1:D:252:GLN:HE21	2:E:362:ARG:NH1	1.94	0.64
1:D:384:LYS:HE3	1:D:385:ASP:HB2	1.80	0.64
1:A:271:CYS:O	1:A:272:ALA:C	2.34	0.64
1:D:218:GLN:HB2	1:D:236:ALA:CA	2.27	0.64
1:F:170:TRP:CZ3	1:F:172:PRO:CD	2.81	0.64
2:G:336:ARG:NH2	1:H:236:ALA:CB	2.57	0.64
1:H:127:ALA:HB2	1:H:171:THR:HB	1.76	0.64
2:B:204:LYS:HE3	2:B:374:TRP:CE2	2.33	0.64
1:H:271:CYS:O	1:H:272:ALA:C	2.35	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:MET:CB	2:E:240:PRO:HD3	2.27	0.64
2:G:333:PRO:O	2:G:396:ASN:HB2	1.97	0.64
1:H:254:THR:CA	2:I:368:PRO:HG3	2.26	0.64
2:E:334:LYS:CG	2:E:396:ASN:CB	2.37	0.64
1:A:91:GLY:N	2:B:240:PRO:HG2	2.13	0.64
2:E:90:HIS:N	2:I:208:ARG:NH1	2.46	0.64
2:G:294:THR:HB	2:G:295:ASN:N	2.13	0.64
1:A:94:CYS:O	2:B:290:HIS:CB	2.47	0.63
1:F:88:MET:HB2	2:G:240:PRO:HG3	1.78	0.63
1:H:95:PHE:HB3	2:I:264:LYS:CB	2.04	0.63
1:F:129:ALA:HB1	1:F:166:MET:SD	2.37	0.63
1:F:90:GLY:CA	2:G:240:PRO:C	2.56	0.63
1:F:257:PHE:HB3	1:F:272:ALA:CB	2.24	0.63
1:F:95:PHE:H	2:G:264:LYS:HD2	1.64	0.63
2:G:207:SER:CB	2:I:85:ASP:OD1	2.46	0.63
1:D:34:LEU:CD1	1:D:132:LYS:CD	2.77	0.63
2:E:260:THR:HG21	2:E:296:HIS:CE1	2.33	0.63
2:E:336:ARG:NH2	1:F:235:GLN:C	2.49	0.63
1:H:385:ASP:CA	1:H:386:HIS:CB	2.51	0.63
2:I:294:THR:C	2:I:295:ASN:CG	2.57	0.63
1:H:383:PRO:HG3	2:I:407:SER:N	2.10	0.63
1:A:90:GLY:H	2:B:240:PRO:HD2	1.62	0.63
1:A:95:PHE:N	2:B:264:LYS:HB3	2.04	0.63
1:D:95:PHE:HE2	2:E:271:ASN:ND2	1.92	0.63
1:H:253:HIS:O	2:I:368:PRO:HB2	1.99	0.63
1:A:91:GLY:CA	2:B:240:PRO:HB2	2.28	0.63
1:D:252:GLN:HE21	2:E:362:ARG:CZ	2.12	0.63
1:D:7:ILE:CD1	1:D:33:LEU:CD1	2.75	0.63
1:D:11:VAL:HG21	1:D:35:SER:CA	2.28	0.63
1:F:273:VAL:O	1:F:273:VAL:HG13	1.98	0.63
1:H:172:PRO:O	1:H:173:PHE:CD1	2.51	0.63
2:E:208:ARG:HG2	2:G:89:GLY:CA	2.28	0.62
1:F:93:TYR:CD1	2:G:238:ASP:HB2	2.34	0.62
2:G:352:TYR:CD2	1:H:237:PRO:CD	2.71	0.62
2:G:208:ARG:NH2	2:I:88:GLU:HB3	2.13	0.62
1:F:33:LEU:HD22	1:F:131:ALA:CB	2.29	0.62
1:F:52:LYS:C	1:F:53:THR:N	2.53	0.62
1:F:132:LYS:HA	1:F:144:VAL:O	1.98	0.62
1:F:170:TRP:CH2	1:F:172:PRO:CA	2.81	0.62
2:E:237:PRO:CB	2:E:306:VAL:HG12	2.29	0.62
1:D:252:GLN:HE22	2:E:362:ARG:HH22	1.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:GLY:C	2:B:240:PRO:O	2.38	0.62
1:A:90:GLY:CA	2:B:240:PRO:CG	2.78	0.62
1:D:90:GLY:HA3	2:E:240:PRO:CB	2.26	0.61
2:E:237:PRO:CG	2:E:306:VAL:HG11	2.10	0.61
2:G:208:ARG:HH21	2:I:88:GLU:CA	2.10	0.61
1:H:52:LYS:HE3	2:I:100:ARG:HH12	1.66	0.61
1:A:256:PRO:HA	2:B:366:GLU:C	2.21	0.61
1:F:92:ALA:HB3	2:G:290:HIS:CD2	2.35	0.61
1:D:252:GLN:NE2	2:E:362:ARG:HH12	1.98	0.61
2:G:378:LYS:HB2	1:H:242:TYR:CE1	2.35	0.61
2:E:206:HIS:CD2	2:G:174:THR:CG2	2.84	0.61
2:G:333:PRO:O	2:G:396:ASN:CB	2.48	0.61
1:H:90:GLY:O	2:I:240:PRO:C	2.35	0.61
1:D:237:PRO:CD	2:I:352:TYR:CD1	2.84	0.61
1:F:359:ALA:HB1	2:G:406:LEU:CD1	2.30	0.61
1:A:256:PRO:CG	2:B:366:GLU:CG	2.77	0.60
2:E:334:LYS:HG3	2:E:396:ASN:HB2	0.68	0.60
2:E:336:ARG:CD	1:F:235:GLN:CA	2.79	0.60
2:E:206:HIS:CG	2:G:174:THR:CG2	2.84	0.60
1:F:171:THR:O	1:F:172:PRO:C	2.37	0.60
1:F:253:HIS:HA	2:G:362:ARG:HD3	1.80	0.60
1:H:273:VAL:O	1:H:273:VAL:HG13	2.00	0.60
2:B:204:LYS:HB2	2:B:356:PRO:HB2	1.83	0.60
1:D:34:LEU:HD12	1:D:132:LYS:CD	2.30	0.60
1:F:88:MET:CB	2:G:240:PRO:CG	2.78	0.60
1:A:173:PHE:CE1	1:A:251:LEU:CD1	2.85	0.60
1:D:171:THR:OG1	1:D:173:PHE:CD2	2.55	0.60
1:H:173:PHE:C	1:H:174:ASP:O	2.38	0.60
1:D:88:MET:SD	2:E:238:ASP:HB2	2.41	0.60
2:E:203:GLU:CD	2:E:396:ASN:ND2	2.54	0.60
1:A:254:THR:HA	2:B:368:PRO:CD	2.32	0.60
1:A:256:PRO:CA	2:B:366:GLU:CA	2.44	0.60
2:E:210:GLN:HE21	2:G:91:SER:HB3	1.66	0.60
1:F:253:HIS:O	2:G:362:ARG:CB	2.49	0.59
1:F:257:PHE:H	2:G:365:GLY:N	1.99	0.59
1:D:245:LYS:CE	2:I:378:LYS:HD2	2.32	0.59
2:E:174:THR:HG23	2:I:206:HIS:HB3	1.82	0.59
1:H:74:PRO:CB	1:H:215:ALA:HB3	2.32	0.59
1:A:291:VAL:HG22	1:F:304:PRO:HA	1.80	0.59
2:I:238:ASP:HB3	2:I:292:ALA:HB1	1.83	0.59
2:B:236:PRO:HB3	2:B:237:PRO:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:PRO:CG	2:E:366:GLU:HG2	2.31	0.59
2:G:294:THR:O	2:G:295:ASN:HA	2.01	0.59
1:D:256:PRO:CB	2:E:366:GLU:HG2	2.19	0.59
2:E:378:LYS:HZ2	1:F:242:TYR:HB2	1.67	0.59
1:H:88:MET:CE	2:I:239:THR:N	2.50	0.59
1:F:129:ALA:HB2	1:F:166:MET:HE2	1.83	0.59
1:H:271:CYS:O	1:H:273:VAL:N	2.36	0.59
1:F:112:GLU:HB3	2:G:229:GLU:HG2	1.84	0.58
2:G:156:THR:HG21	2:I:88:GLU:CD	2.24	0.58
1:F:254:THR:HG22	2:G:370:TYR:CB	2.33	0.58
2:I:274:LEU:HD12	2:I:294:THR:HG23	1.85	0.58
1:D:34:LEU:HB3	1:D:132:LYS:HD3	1.84	0.58
1:D:234:SER:CA	2:I:336:ARG:HB2	2.21	0.58
1:F:42:LEU:HD11	1:F:266:VAL:HG22	1.85	0.58
1:H:42:LEU:HD11	1:H:266:VAL:HG22	1.85	0.58
1:A:171:THR:O	1:A:172:PRO:C	2.42	0.58
2:G:207:SER:HB2	2:I:85:ASP:OD1	2.04	0.58
1:A:172:PRO:HG3	1:A:271:CYS:SG	2.44	0.58
1:H:95:PHE:HB2	2:I:264:LYS:O	2.04	0.58
1:A:90:GLY:O	2:B:240:PRO:CB	2.41	0.57
2:G:208:ARG:CZ	2:I:90:HIS:H	2.16	0.57
1:D:256:PRO:C	2:E:366:GLU:HA	2.19	0.57
2:E:89:GLY:HA3	2:I:208:ARG:NE	2.15	0.57
2:G:333:PRO:O	2:G:396:ASN:ND2	2.37	0.57
2:I:334:LYS:HE2	2:I:396:ASN:O	2.04	0.57
1:D:42:LEU:HD11	1:D:266:VAL:HG22	1.85	0.57
1:D:252:GLN:NE2	2:E:362:ARG:NH1	2.51	0.57
1:F:171:THR:C	1:F:173:PHE:H	2.01	0.57
1:H:11:VAL:HG22	1:H:33:LEU:O	2.05	0.57
1:H:91:GLY:O	2:I:240:PRO:CG	2.52	0.57
1:H:252:GLN:HE21	2:I:362:ARG:CZ	2.17	0.57
1:A:91:GLY:O	2:B:240:PRO:HG3	2.03	0.57
2:B:294:THR:HB	2:B:295:ASN:N	2.20	0.57
1:F:253:HIS:HA	2:G:362:ARG:NE	2.20	0.57
2:G:212:GLY:CA	2:G:332:VAL:O	2.50	0.57
1:H:386:HIS:O	1:H:387:ILE:CD1	2.51	0.57
1:A:42:LEU:HD11	1:A:266:VAL:HG22	1.85	0.57
1:A:256:PRO:CB	2:B:366:GLU:HA	2.33	0.57
1:D:92:ALA:N	2:E:290:HIS:CD2	2.72	0.57
1:A:252:GLN:CD	2:B:362:ARG:HH12	2.01	0.57
1:D:51:TYR:CE1	1:D:108:VAL:HG21	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:274:LEU:HD11	2:I:294:THR:HG23	1.87	0.57
1:A:9:ASN:OD1	1:A:36:VAL:HG21	2.05	0.57
1:A:94:CYS:O	2:B:290:HIS:HB2	2.05	0.57
1:D:7:ILE:CD1	1:D:33:LEU:HD12	2.35	0.57
1:D:89:TRP:CD1	2:E:240:PRO:HD2	2.40	0.57
2:E:334:LYS:HD3	2:E:397:ASN:CA	2.34	0.57
1:F:147:TYR:H	1:F:152:HIS:HD2	1.53	0.57
1:F:170:TRP:O	1:F:171:THR:HG22	2.05	0.57
1:F:257:PHE:N	2:G:365:GLY:C	2.54	0.57
2:G:336:ARG:HH21	2:G:352:TYR:CB	2.17	0.57
2:B:237:PRO:HG3	2:B:306:VAL:HG13	1.72	0.57
1:D:245:LYS:HZ3	2:I:378:LYS:HB2	1.70	0.57
1:F:90:GLY:O	2:G:240:PRO:C	2.43	0.56
1:F:253:HIS:HA	2:G:362:ARG:CZ	2.34	0.56
2:B:199:VAL:HG11	2:B:374:TRP:HZ2	1.70	0.56
2:E:174:THR:CG2	2:I:206:HIS:HB3	2.33	0.56
1:A:385:ASP:HA	1:A:386:HIS:HB2	0.61	0.56
1:D:234:SER:HB3	2:I:336:ARG:HA	1.86	0.56
1:D:237:PRO:HB2	2:I:352:TYR:CE2	2.40	0.56
2:E:237:PRO:O	2:E:238:ASP:CG	2.44	0.56
1:F:11:VAL:HG13	1:F:34:LEU:O	2.05	0.56
2:G:213:LYS:O	2:G:332:VAL:HG22	2.06	0.56
2:G:336:ARG:HB2	1:H:234:SER:CB	2.26	0.56
1:D:237:PRO:CG	2:I:352:TYR:HB3	2.30	0.56
1:F:254:THR:HA	2:G:368:PRO:HB2	1.87	0.56
2:I:262:ARG:N	2:I:294:THR:OG1	2.38	0.56
1:A:170:TRP:CH2	1:A:172:PRO:CD	2.88	0.56
2:G:378:LYS:HD2	1:H:242:TYR:CG	2.38	0.56
1:H:172:PRO:O	1:H:173:PHE:CD2	2.59	0.56
1:F:172:PRO:CG	1:F:259:CYS:SG	2.94	0.56
1:H:92:ALA:CB	2:I:290:HIS:CD2	2.88	0.56
1:D:95:PHE:CE1	2:E:271:ASN:HB2	2.40	0.56
1:F:253:HIS:HA	2:G:362:ARG:CD	2.36	0.56
2:G:336:ARG:HH21	2:G:352:TYR:HB2	1.70	0.55
1:A:386:HIS:O	1:A:387:ILE:HD13	2.06	0.55
1:A:147:TYR:H	1:A:152:HIS:HD2	1.53	0.55
1:D:237:PRO:HD2	2:I:352:TYR:CE1	2.41	0.55
1:H:93:TYR:CE1	2:I:238:ASP:OD2	2.48	0.55
1:H:147:TYR:H	1:H:152:HIS:HD2	1.53	0.55
2:I:237:PRO:C	2:I:238:ASP:CG	2.65	0.55
2:I:237:PRO:HB3	2:I:307:PRO:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:TYR:HB2	1:A:108:VAL:CG1	2.37	0.55
1:F:92:ALA:HB3	2:G:290:HIS:HD2	1.70	0.55
2:G:211:HIS:HB3	1:H:225:ALA:HB1	1.88	0.55
2:I:260:THR:HB	2:I:294:THR:C	2.27	0.55
1:D:129:ALA:HB1	1:D:166:MET:HE1	1.89	0.55
1:D:89:TRP:HE1	2:E:239:THR:HG23	0.48	0.55
1:D:147:TYR:H	1:D:152:HIS:HD2	1.53	0.55
1:D:88:MET:SD	2:E:238:ASP:CB	2.94	0.55
1:H:88:MET:HE2	2:I:239:THR:CA	2.36	0.55
1:A:256:PRO:C	2:B:366:GLU:HA	2.25	0.55
1:D:90:GLY:O	2:E:240:PRO:CB	2.43	0.55
2:B:260:THR:HB	2:B:295:ASN:N	2.22	0.55
1:H:90:GLY:C	2:I:240:PRO:CB	2.74	0.55
1:H:253:HIS:O	2:I:368:PRO:HG3	2.07	0.55
2:E:90:HIS:HD2	2:I:208:ARG:HH22	1.55	0.54
2:E:334:LYS:HE2	2:E:396:ASN:O	2.07	0.54
1:F:33:LEU:CD2	1:F:131:ALA:HB1	2.36	0.54
2:G:352:TYR:CB	1:H:237:PRO:CD	2.78	0.54
1:A:385:ASP:HB3	1:A:387:ILE:N	2.22	0.54
1:D:11:VAL:CG1	1:D:35:SER:HA	2.29	0.54
2:E:336:ARG:CZ	1:F:235:GLN:HA	2.22	0.54
2:G:334:LYS:HD3	2:G:397:ASN:HA	1.90	0.54
2:E:262:ARG:NH1	2:E:310:ALA:HB3	2.23	0.54
2:G:156:THR:CG2	2:I:88:GLU:CD	2.75	0.54
2:G:352:TYR:CB	1:H:237:PRO:HD3	2.18	0.54
1:H:95:PHE:CE1	2:I:288:GLN:O	2.61	0.54
1:D:108:VAL:O	1:D:109:GLU:N	2.40	0.54
1:D:34:LEU:CB	1:D:132:LYS:HD3	2.37	0.54
1:D:257:PHE:H	2:E:365:GLY:C	2.10	0.54
1:D:257:PHE:N	2:E:365:GLY:C	2.61	0.54
2:E:90:HIS:CD2	2:I:208:ARG:HH22	2.25	0.54
2:G:202:ARG:NH1	2:G:360:SER:OG	2.40	0.54
1:A:112:GLU:HB2	2:B:102:ARG:NH2	2.22	0.54
2:E:206:HIS:CG	2:G:174:THR:HG23	2.42	0.54
1:A:88:MET:CE	2:B:238:ASP:H	2.21	0.54
2:E:89:GLY:C	2:I:208:ARG:HG3	2.28	0.54
1:F:384:LYS:HG3	1:F:385:ASP:N	2.23	0.54
1:H:170:TRP:CE3	1:H:172:PRO:HD3	2.43	0.54
1:A:127:ALA:CB	1:A:171:THR:HG21	2.36	0.53
1:F:88:MET:CB	2:G:240:PRO:HG3	2.39	0.53
1:A:93:TYR:O	2:B:290:HIS:CE1	2.60	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:129:ALA:HB2	1:F:166:MET:HG3	1.85	0.53
1:F:170:TRP:CE3	1:F:171:THR:N	2.77	0.53
1:H:90:GLY:N	2:I:240:PRO:HG2	2.23	0.53
1:A:38:LEU:HD13	1:A:172:PRO:CD	2.39	0.53
1:H:90:GLY:HA3	2:I:241:ASP:HA	1.90	0.53
2:I:274:LEU:CD2	2:I:311:GLU:OE2	2.56	0.53
1:D:217:THR:O	1:D:218:GLN:N	2.41	0.53
1:F:108:VAL:O	1:F:109:GLU:N	2.41	0.53
1:H:91:GLY:CA	2:I:240:PRO:HB2	2.38	0.53
2:B:294:THR:C	2:B:295:ASN:N	2.62	0.53
1:D:11:VAL:HG11	1:D:35:SER:CA	2.21	0.53
1:D:237:PRO:HG2	2:I:352:TYR:HB2	1.80	0.53
1:D:254:THR:CA	2:E:368:PRO:CG	2.79	0.53
2:E:89:GLY:CA	2:I:208:ARG:NH1	2.71	0.53
1:H:91:GLY:O	2:I:240:PRO:HG3	2.08	0.53
1:F:132:LYS:HG2	1:F:145:THR:CB	2.38	0.53
1:A:256:PRO:CB	2:B:366:GLU:HG2	2.10	0.53
1:D:171:THR:C	1:D:173:PHE:N	2.48	0.53
1:F:88:MET:HB3	2:G:240:PRO:HD3	1.65	0.53
1:D:62:CYS:CB	2:E:264:LYS:NZ	2.72	0.53
1:A:95:PHE:HA	2:B:290:HIS:HB3	1.91	0.53
2:E:85:ASP:OD1	2:I:207:SER:HB2	2.08	0.53
1:A:28:VAL:HG23	1:A:329:ALA:HB1	1.92	0.52
1:D:219:LEU:N	1:D:236:ALA:N	2.53	0.52
1:F:129:ALA:CB	1:F:166:MET:HE2	2.40	0.52
1:F:235:GLN:C	1:F:236:ALA:HA	2.29	0.52
1:H:52:LYS:HE3	2:I:100:ARG:CZ	2.40	0.52
1:A:95:PHE:CD1	2:B:289:CYS:CA	2.83	0.52
2:G:294:THR:CA	2:G:295:ASN:N	2.72	0.52
1:H:28:VAL:HG23	1:H:329:ALA:HB1	1.92	0.52
1:D:28:VAL:HG23	1:D:329:ALA:HB1	1.92	0.52
1:A:170:TRP:CZ2	1:A:172:PRO:HA	2.44	0.52
1:D:34:LEU:CD1	1:D:132:LYS:HD3	2.39	0.52
1:H:33:LEU:CG	1:H:133:LEU:HD12	2.26	0.52
2:G:237:PRO:CG	2:G:306:VAL:HG11	2.21	0.52
2:I:295:ASN:O	2:I:296:HIS:HB2	2.09	0.52
1:A:34:LEU:HB3	1:A:132:LYS:HD3	1.92	0.52
1:D:256:PRO:CA	2:E:366:GLU:O	2.58	0.52
1:A:38:LEU:HB2	1:A:268:ALA:HB3	1.92	0.51
1:A:95:PHE:HD1	2:B:289:CYS:CA	2.18	0.51
1:A:90:GLY:O	2:B:241:ASP:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:90:GLY:HA3	2:I:241:ASP:CA	2.30	0.51
1:A:38:LEU:HD13	1:A:172:PRO:HD2	1.93	0.51
1:A:385:ASP:HA	1:A:386:HIS:HB3	1.73	0.51
2:B:202:ARG:NH2	2:B:393:THR:O	2.43	0.51
1:D:38:LEU:HB2	1:D:268:ALA:HB3	1.92	0.51
1:D:245:LYS:NZ	2:I:378:LYS:O	2.40	0.51
2:G:206:HIS:CD2	2:I:173:GLU:HB2	2.43	0.51
1:H:38:LEU:HB2	1:H:268:ALA:HB3	1.92	0.51
1:H:92:ALA:CB	2:I:290:HIS:HD2	2.19	0.51
1:H:385:ASP:OD2	1:H:387:ILE:N	2.44	0.51
1:F:38:LEU:HB2	1:F:268:ALA:HB3	1.92	0.51
1:F:95:PHE:H	2:G:264:LYS:CD	2.23	0.51
1:H:173:PHE:O	1:H:174:ASP:C	2.49	0.51
2:I:237:PRO:HG3	2:I:306:VAL:HG13	1.77	0.51
1:D:88:MET:CE	2:E:238:ASP:CA	2.87	0.51
1:D:273:VAL:HG13	1:D:273:VAL:O	2.10	0.51
2:E:206:HIS:NE2	2:G:173:GLU:HB3	2.26	0.51
2:G:106:THR:HB	2:G:200:ILE:HD11	1.93	0.51
2:G:274:LEU:HD21	2:G:296:HIS:HE1	1.70	0.51
1:A:116:THR:HG23	2:B:327:ASN:OD1	2.10	0.51
2:E:106:THR:HB	2:E:200:ILE:HD11	1.93	0.51
1:F:28:VAL:HG23	1:F:329:ALA:HB1	1.91	0.51
1:F:93:TYR:HE1	2:G:238:ASP:CG	2.10	0.51
1:D:88:MET:HE3	2:E:238:ASP:C	1.94	0.51
1:F:90:GLY:H	2:G:240:PRO:CG	2.21	0.51
2:E:334:LYS:CG	2:E:396:ASN:CA	2.89	0.51
1:F:253:HIS:C	2:G:362:ARG:CD	2.49	0.51
1:A:94:CYS:C	2:B:290:HIS:HB3	2.31	0.51
1:A:130:SER:O	1:A:131:ALA:HB2	2.12	0.50
2:B:106:THR:HB	2:B:200:ILE:HD11	1.93	0.50
1:F:110:LYS:HG3	1:F:213:VAL:HG11	1.94	0.50
1:A:112:GLU:CB	2:B:102:ARG:NH2	2.74	0.50
1:D:252:GLN:HE21	2:E:362:ARG:NH2	2.08	0.50
2:G:237:PRO:CB	2:G:306:VAL:HG12	2.41	0.50
2:I:106:THR:HB	2:I:200:ILE:HD11	1.93	0.50
1:A:88:MET:C	2:B:240:PRO:HG3	2.32	0.50
1:F:11:VAL:HG21	1:F:36:VAL:H	1.77	0.50
1:A:95:PHE:HE2	2:B:267:CYS:H	1.58	0.50
2:E:89:GLY:CA	2:I:208:ARG:HG2	2.23	0.50
2:E:336:ARG:CB	1:F:234:SER:OG	2.52	0.50
1:H:172:PRO:C	1:H:173:PHE:CG	2.85	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LEU:HB2	1:A:132:LYS:CB	2.18	0.50
1:A:93:TYR:O	2:B:290:HIS:ND1	2.45	0.50
1:D:33:LEU:O	1:D:34:LEU:O	2.30	0.50
1:D:89:TRP:HZ2	2:E:239:THR:CG2	2.06	0.50
1:A:127:ALA:HB1	1:A:171:THR:OG1	2.08	0.50
1:F:170:TRP:C	1:F:171:THR:CG2	2.80	0.50
2:E:236:PRO:HG2	2:E:295:ASN:CB	2.42	0.49
2:E:237:PRO:CB	2:E:307:PRO:O	2.48	0.49
1:F:75:ASP:OD2	1:F:217:THR:CB	2.60	0.49
1:F:90:GLY:C	2:G:240:PRO:C	2.71	0.49
1:A:7:ILE:HD11	1:A:33:LEU:HD12	1.93	0.49
1:A:132:LYS:O	1:A:133:LEU:HB2	2.12	0.49
1:A:113:SER:HB3	2:B:104:GLU:HG2	1.93	0.49
1:A:254:THR:C	2:B:368:PRO:HG3	2.32	0.49
2:I:237:PRO:O	2:I:238:ASP:OD1	2.30	0.49
1:A:173:PHE:CE1	1:A:251:LEU:HD13	2.48	0.49
1:D:237:PRO:CD	2:I:352:TYR:CG	2.94	0.49
1:A:170:TRP:CZ2	1:A:172:PRO:CA	2.96	0.49
1:H:74:PRO:HB2	1:H:215:ALA:HB3	1.94	0.49
1:A:52:LYS:C	1:A:53:THR:CA	2.73	0.49
1:D:52:LYS:HE2	1:D:54:VAL:CG2	2.40	0.49
1:D:129:ALA:HB1	1:D:166:MET:CE	2.43	0.49
1:F:91:GLY:O	2:G:240:PRO:CG	2.60	0.49
2:G:203:GLU:CD	2:G:396:ASN:ND2	2.66	0.49
1:D:256:PRO:CA	2:E:366:GLU:C	2.76	0.49
2:I:238:ASP:CB	2:I:292:ALA:HB1	2.42	0.49
1:F:171:THR:O	1:F:173:PHE:CA	2.54	0.49
1:A:256:PRO:CG	2:B:366:GLU:HG2	2.43	0.49
1:D:92:ALA:N	2:E:290:HIS:NE2	2.60	0.49
1:H:19:VAL:HB	1:H:27:MET:HB3	1.95	0.49
2:I:116:LEU:HD22	2:I:131:LEU:HD21	1.94	0.49
1:D:89:TRP:HE1	2:E:239:THR:CB	2.16	0.49
1:D:245:LYS:HE2	2:I:378:LYS:HD2	1.93	0.49
2:E:378:LYS:NZ	1:F:242:TYR:HB2	2.27	0.49
2:G:116:LEU:HD22	2:G:131:LEU:HD21	1.94	0.49
1:H:171:THR:O	1:H:171:THR:HG23	2.13	0.49
2:B:202:ARG:O	2:B:358:LEU:HB2	2.13	0.48
1:H:9:ASN:OD1	1:H:36:VAL:HG21	2.12	0.48
1:H:92:ALA:HB3	2:I:290:HIS:CD2	2.42	0.48
1:A:52:LYS:HE3	2:B:100:ARG:CZ	2.42	0.48
1:A:110:LYS:HG3	1:A:213:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:TYR:CD1	2:E:238:ASP:CB	2.96	0.48
1:H:90:GLY:CA	2:I:241:ASP:HA	2.43	0.48
1:A:88:MET:HE3	2:B:238:ASP:H	1.77	0.48
1:A:173:PHE:CE1	1:A:184:VAL:HG12	2.34	0.48
1:A:173:PHE:HE1	1:A:251:LEU:HD12	1.77	0.48
1:D:171:THR:O	1:D:172:PRO:C	2.49	0.48
1:D:245:LYS:HE2	2:I:378:LYS:CD	2.44	0.48
2:E:89:GLY:CA	2:I:208:ARG:NE	2.74	0.48
2:E:116:LEU:HD22	2:E:131:LEU:HD21	1.94	0.48
2:G:208:ARG:CZ	2:I:89:GLY:C	2.81	0.48
1:H:33:LEU:CA	1:H:133:LEU:HD12	2.43	0.48
1:D:257:PHE:H	2:E:366:GLU:CA	2.26	0.48
2:I:238:ASP:HB3	2:I:292:ALA:HB3	1.95	0.48
2:B:204:LYS:HG3	2:B:374:TRP:CH2	2.49	0.48
1:D:110:LYS:HG3	1:D:213:VAL:HG11	1.95	0.48
2:I:294:THR:HG23	2:I:295:ASN:H	1.70	0.48
1:D:256:PRO:HA	2:E:366:GLU:O	2.14	0.48
1:F:62:CYS:HB3	2:G:264:LYS:CE	2.34	0.48
1:A:88:MET:HB2	2:B:240:PRO:CD	2.36	0.48
1:A:19:VAL:HB	1:A:27:MET:HB3	1.95	0.48
1:D:19:VAL:HB	1:D:27:MET:HB3	1.95	0.48
1:D:93:TYR:CD1	2:E:238:ASP:HB2	2.49	0.48
1:A:218:GLN:HB2	1:A:236:ALA:CA	2.44	0.48
2:B:116:LEU:HD22	2:B:131:LEU:HD21	1.94	0.48
2:B:237:PRO:O	2:B:238:ASP:OD1	2.32	0.48
1:D:260:GLN:HE22	2:E:362:ARG:NH2	2.12	0.48
1:F:30:GLU:HB3	1:F:136:LEU:HB2	1.96	0.48
2:G:202:ARG:HH12	2:G:360:SER:CB	2.27	0.48
1:F:19:VAL:HB	1:F:27:MET:HB3	1.95	0.47
1:H:383:PRO:CD	2:I:407:SER:N	2.77	0.47
1:H:385:ASP:OD2	1:H:387:ILE:CA	2.62	0.47
1:A:7:ILE:HD11	1:A:33:LEU:HD11	1.95	0.47
1:A:35:SER:O	1:A:131:ALA:CB	2.62	0.47
1:A:36:VAL:HA	1:A:131:ALA:HB2	1.96	0.47
2:E:262:ARG:HH12	2:E:310:ALA:HB3	1.78	0.47
2:G:208:ARG:NH1	2:I:89:GLY:C	2.66	0.47
1:F:92:ALA:CB	2:G:290:HIS:CD2	2.97	0.47
2:E:208:ARG:NE	2:G:88:GLU:O	2.47	0.47
2:G:274:LEU:HD22	2:G:311:GLU:HB2	1.96	0.47
1:D:90:GLY:C	2:E:240:PRO:CG	2.82	0.47
1:F:95:PHE:CD2	2:G:265:CYS:N	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:237:PRO:O	2:G:238:ASP:OD1	2.33	0.47
1:H:235:GLN:CA	1:H:236:ALA:N	2.77	0.47
1:A:34:LEU:HD13	1:A:132:LYS:HD3	1.96	0.47
1:D:236:ALA:HB2	2:I:339:THR:HG21	1.96	0.47
2:G:203:GLU:HB2	2:G:396:ASN:HD21	1.79	0.47
1:H:7:ILE:HD12	1:H:33:LEU:HD12	1.88	0.47
1:H:110:LYS:HG3	1:H:213:VAL:HG11	1.96	0.47
1:A:171:THR:O	1:A:171:THR:HG23	2.15	0.47
2:E:274:LEU:CD2	2:E:311:GLU:OE2	2.62	0.47
1:H:30:GLU:HB3	1:H:136:LEU:HB2	1.96	0.47
1:A:51:TYR:CE1	1:A:235:GLN:NE2	2.83	0.47
1:A:170:TRP:CH2	1:A:172:PRO:CG	2.98	0.47
1:D:257:PHE:N	2:E:366:GLU:HA	2.29	0.47
2:E:209:PRO:HG3	2:E:333:PRO:HD3	1.97	0.47
1:F:235:GLN:CB	1:F:236:ALA:N	2.77	0.47
1:A:30:GLU:HB3	1:A:136:LEU:HB2	1.96	0.46
1:F:108:VAL:CG2	1:F:217:THR:OG1	2.44	0.46
1:F:133:LEU:HD22	1:F:278:ILE:HD13	1.97	0.46
1:H:75:ASP:OD2	1:H:217:THR:OG1	2.16	0.46
1:A:7:ILE:CD1	1:A:33:LEU:HD12	2.46	0.46
1:D:11:VAL:HG21	1:D:36:VAL:N	2.28	0.46
1:H:60:VAL:HG22	1:H:102:GLN:HG3	1.97	0.46
1:A:218:GLN:HB2	1:A:236:ALA:N	2.30	0.46
1:A:60:VAL:HG22	1:A:102:GLN:HG3	1.97	0.46
1:A:133:LEU:HG	1:A:134:ARG:H	1.80	0.46
1:H:75:ASP:CG	1:H:217:THR:H	2.15	0.46
1:D:30:GLU:HB3	1:D:136:LEU:HB2	1.96	0.46
1:D:149:ASN:HD22	1:D:149:ASN:H	1.63	0.46
1:H:149:ASN:H	1:H:149:ASN:HD22	1.63	0.46
1:A:170:TRP:CZ3	1:A:172:PRO:CG	2.98	0.46
1:D:11:VAL:HG21	1:D:35:SER:HA	1.97	0.46
2:E:203:GLU:OE2	2:E:334:LYS:HA	2.15	0.46
1:A:206:ARG:HG3	1:A:206:ARG:HH11	1.80	0.46
1:D:60:VAL:HG22	1:D:102:GLN:HG3	1.97	0.46
2:E:312:LEU:HD13	2:E:315:ARG:HB2	1.98	0.46
1:F:149:ASN:HD22	1:F:149:ASN:H	1.63	0.46
2:G:352:TYR:CG	1:H:237:PRO:HD2	2.40	0.46
1:H:33:LEU:HA	1:H:133:LEU:HD12	1.97	0.46
2:B:312:LEU:HD13	2:B:315:ARG:HB2	1.98	0.46
1:D:253:HIS:O	2:E:368:PRO:HG2	2.12	0.46
2:E:334:LYS:HD3	2:E:397:ASN:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:339:THR:CG2	1:F:218:GLN:CD	2.62	0.46
1:H:206:ARG:HG3	1:H:206:ARG:HH11	1.80	0.46
1:A:52:LYS:CA	1:A:53:THR:N	2.69	0.46
1:A:74:PRO:CA	1:A:215:ALA:HB3	2.43	0.46
2:B:248:GLN:HA	2:B:249:SER:HA	1.82	0.46
1:D:192:PHE:CE1	1:D:206:ARG:HG2	2.51	0.46
1:F:192:PHE:CE1	1:F:206:ARG:HG2	2.51	0.46
1:A:84:VAL:O	1:A:100:ASN:HB2	2.16	0.45
1:A:192:PHE:CE1	1:A:206:ARG:HG2	2.51	0.45
2:E:237:PRO:HG2	2:E:238:ASP:H	1.81	0.45
1:F:60:VAL:HG22	1:F:102:GLN:HG3	1.97	0.45
1:F:93:TYR:O	2:G:290:HIS:CE1	2.69	0.45
2:G:206:HIS:CD2	2:I:173:GLU:C	2.89	0.45
1:F:84:VAL:O	1:F:100:ASN:HB2	2.16	0.45
2:B:274:LEU:HD22	2:B:311:GLU:CB	2.46	0.45
2:G:312:LEU:HD13	2:G:315:ARG:HB2	1.98	0.45
2:G:378:LYS:NZ	1:H:238:SER:O	2.50	0.45
1:H:91:GLY:C	2:I:240:PRO:HB2	2.37	0.45
1:D:7:ILE:HD11	1:D:33:LEU:HD12	1.90	0.45
1:A:126:THR:HG1	1:H:126:THR:HG1	1.60	0.45
1:D:253:HIS:O	2:E:368:PRO:HG3	2.16	0.45
2:E:90:HIS:CD2	2:I:208:ARG:NH2	2.85	0.45
1:H:127:ALA:HB2	1:H:171:THR:OG1	2.15	0.45
1:A:90:GLY:C	2:B:240:PRO:CA	2.83	0.45
2:B:237:PRO:CB	2:B:306:VAL:HG12	2.47	0.45
1:D:84:VAL:O	1:D:100:ASN:HB2	2.16	0.45
2:E:206:HIS:NE2	2:G:173:GLU:CB	2.80	0.45
1:F:206:ARG:HG3	1:F:206:ARG:HH11	1.80	0.45
2:I:312:LEU:HD13	2:I:315:ARG:HB2	1.98	0.45
2:E:334:LYS:HD3	2:E:396:ASN:O	2.14	0.45
1:F:112:GLU:CB	2:G:229:GLU:HG2	2.46	0.45
1:H:88:MET:O	2:I:240:PRO:HG2	2.13	0.45
1:H:192:PHE:CE1	1:H:206:ARG:HG2	2.51	0.45
1:D:206:ARG:HG3	1:D:206:ARG:HH11	1.80	0.45
1:F:249:ALA:HB2	2:G:370:TYR:CD2	2.51	0.45
1:F:273:VAL:O	1:F:273:VAL:CG1	2.65	0.45
1:A:34:LEU:HD13	1:A:132:LYS:CE	2.09	0.45
1:A:149:ASN:H	1:A:149:ASN:HD22	1.63	0.45
1:H:84:VAL:O	1:H:100:ASN:HB2	2.16	0.45
1:H:91:GLY:O	2:I:240:PRO:HB2	2.17	0.45
1:A:170:TRP:CE3	1:A:172:PRO:CD	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:ARG:HG2	2:B:358:LEU:HD13	1.98	0.44
1:D:34:LEU:HD13	1:D:132:LYS:CD	2.43	0.44
2:G:378:LYS:HE3	1:H:237:PRO:HB2	1.99	0.44
1:A:172:PRO:CG	1:A:268:ALA:HB3	2.35	0.44
1:D:51:TYR:HE1	1:D:108:VAL:HG22	1.81	0.44
1:F:116:THR:HG23	2:G:327:ASN:CG	2.37	0.44
2:G:199:VAL:HG11	2:G:374:TRP:CZ2	2.52	0.44
2:G:238:ASP:HB3	2:G:292:ALA:HB1	1.98	0.44
2:I:295:ASN:HB2	2:I:296:HIS:H	1.55	0.44
2:E:174:THR:HG21	2:I:206:HIS:CB	2.45	0.44
2:G:378:LYS:CE	1:H:237:PRO:HB2	2.47	0.44
1:H:90:GLY:O	2:I:241:ASP:CA	2.65	0.44
1:A:41:THR:HG21	1:H:41:THR:HG21	1.99	0.44
1:F:93:TYR:CE1	2:G:238:ASP:CB	3.00	0.44
1:H:88:MET:CE	2:I:239:THR:CA	2.95	0.44
2:E:237:PRO:O	2:E:238:ASP:OD1	2.36	0.44
1:H:84:VAL:HG12	1:H:86:PRO:HD3	2.00	0.44
1:A:88:MET:C	2:B:240:PRO:CG	2.85	0.44
1:D:84:VAL:HG12	1:D:86:PRO:HD3	2.00	0.44
2:E:208:ARG:CG	2:G:89:GLY:C	2.85	0.44
1:F:84:VAL:HG12	1:F:86:PRO:HD3	2.00	0.44
1:A:84:VAL:HG12	1:A:86:PRO:HD3	2.00	0.44
1:D:171:THR:O	1:D:171:THR:HG23	2.18	0.44
1:D:256:PRO:HA	2:E:365:GLY:O	2.18	0.44
1:H:252:GLN:HE21	2:I:362:ARG:NH1	2.16	0.44
1:H:385:ASP:HB3	2:I:405:GLN:H	1.63	0.44
1:A:172:PRO:O	1:A:173:PHE:HB2	2.17	0.44
2:B:238:ASP:CB	2:B:292:ALA:HB1	2.45	0.44
2:E:235:MET:O	2:E:236:PRO:O	2.36	0.44
2:G:334:LYS:HA	2:G:396:ASN:HB2	1.99	0.44
1:H:11:VAL:HG21	1:H:35:SER:CA	2.48	0.44
1:A:271:CYS:O	1:A:273:VAL:N	2.51	0.43
1:D:95:PHE:CD2	2:E:271:ASN:ND2	2.84	0.43
1:F:90:GLY:CA	2:G:240:PRO:HG2	2.48	0.43
2:G:213:LYS:HB3	2:G:332:VAL:HG23	2.00	0.43
1:H:62:CYS:CB	2:I:264:LYS:HE2	2.28	0.43
1:H:116:THR:HG23	2:I:327:ASN:CG	2.34	0.43
2:I:274:LEU:HD23	2:I:311:GLU:OE2	2.17	0.43
2:E:202:ARG:O	2:E:358:LEU:HB2	2.18	0.43
2:G:352:TYR:CZ	1:H:198:GLY:HA3	2.53	0.43
2:G:274:LEU:CD2	2:G:296:HIS:HE1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:TRP:CH2	1:A:172:PRO:CA	3.01	0.43
2:I:274:LEU:HD12	2:I:294:THR:CG2	2.48	0.43
2:B:237:PRO:O	2:B:238:ASP:CG	2.57	0.43
1:D:245:LYS:CE	2:I:378:LYS:CD	2.96	0.43
1:F:170:TRP:CH2	1:F:172:PRO:HD3	2.39	0.43
2:G:202:ARG:HG2	2:G:358:LEU:HD13	2.01	0.43
1:A:88:MET:CE	2:B:238:ASP:N	2.81	0.43
1:F:363:ALA:HB3	1:F:378:ALA:HB3	2.01	0.43
2:G:274:LEU:HD21	2:G:296:HIS:NE2	2.34	0.43
1:H:9:ASN:O	1:H:272:ALA:HA	2.19	0.43
1:A:244:LEU:HA	1:A:247:ARG:HD3	2.01	0.43
1:D:170:TRP:O	1:D:171:THR:HB	2.19	0.43
1:H:273:VAL:O	1:H:273:VAL:CG1	2.65	0.43
1:A:218:GLN:H	1:A:236:ALA:HB3	1.84	0.43
1:D:363:ALA:HB3	1:D:378:ALA:HB3	2.01	0.43
1:H:363:ALA:HB3	1:H:378:ALA:HB3	2.01	0.43
1:A:90:GLY:O	2:B:240:PRO:CA	2.65	0.42
1:F:244:LEU:HA	1:F:247:ARG:HD3	2.01	0.42
1:A:363:ALA:HB3	1:A:378:ALA:HB3	2.01	0.42
2:G:211:HIS:HB3	1:H:225:ALA:CB	2.49	0.42
2:G:378:LYS:HD2	1:H:242:TYR:HD1	1.64	0.42
1:H:333:MET:HB2	1:H:366:ARG:HB2	2.01	0.42
1:A:173:PHE:HE1	1:A:251:LEU:CD1	2.31	0.42
2:E:202:ARG:O	2:E:374:TRP:CH2	2.73	0.42
1:H:385:ASP:N	1:H:386:HIS:HB2	2.30	0.42
2:B:237:PRO:C	2:B:238:ASP:CG	2.77	0.42
2:B:237:PRO:HB3	2:B:306:VAL:HG12	2.00	0.42
1:D:244:LEU:HA	1:D:247:ARG:HD3	2.01	0.42
2:G:334:LYS:HG2	2:G:396:ASN:CB	2.49	0.42
1:H:90:GLY:H	2:I:240:PRO:HG2	1.85	0.42
1:H:95:PHE:CB	2:I:264:LYS:HB2	2.31	0.42
1:A:86:PRO:HA	1:A:227:GLY:HA2	2.02	0.42
1:A:173:PHE:CE1	1:A:251:LEU:HD12	2.54	0.42
1:D:51:TYR:HB2	1:D:108:VAL:HG12	1.47	0.42
1:F:93:TYR:HE1	2:G:238:ASP:CB	2.33	0.42
1:F:170:TRP:CE3	1:F:171:THR:HA	2.55	0.42
1:A:34:LEU:CB	1:A:132:LYS:HD3	2.49	0.42
1:A:51:TYR:HB2	1:A:108:VAL:HG13	2.01	0.42
1:A:333:MET:HB2	1:A:366:ARG:HB2	2.01	0.42
1:F:33:LEU:O	1:F:34:LEU:C	2.57	0.42
2:I:77:ARG:HE	2:I:300:GLN:HE21	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:PHE:CD1	1:A:177:ILE:HG21	2.54	0.42
1:A:387:ILE:CG2	2:B:342:TYR:CD2	3.00	0.42
2:B:204:LYS:HG3	2:B:374:TRP:CZ3	2.54	0.42
1:D:86:PRO:HA	1:D:227:GLY:HA2	2.02	0.42
1:F:170:TRP:CE3	1:F:171:THR:CA	3.03	0.42
2:G:203:GLU:OE2	2:G:334:LYS:HA	2.19	0.42
1:A:147:TYR:H	1:A:152:HIS:CD2	2.37	0.42
1:D:88:MET:HE1	2:E:239:THR:CA	2.50	0.42
2:E:77:ARG:HE	2:E:300:GLN:HE21	1.68	0.42
1:H:86:PRO:HA	1:H:227:GLY:HA2	2.02	0.42
1:H:244:LEU:HA	1:H:247:ARG:HD3	2.01	0.42
1:D:7:ILE:HD12	1:D:33:LEU:HD12	2.01	0.42
2:E:248:GLN:HA	2:E:249:SER:HA	1.82	0.42
2:E:334:LYS:CE	2:E:396:ASN:O	2.68	0.42
2:G:102:ARG:HB2	2:G:111:LYS:HB3	2.02	0.42
2:G:207:SER:CB	2:I:85:ASP:HB3	2.48	0.42
2:B:77:ARG:HE	2:B:300:GLN:HE21	1.68	0.41
2:E:90:HIS:N	2:I:208:ARG:HH12	2.18	0.41
1:F:170:TRP:CH2	1:F:172:PRO:HA	2.49	0.41
2:G:203:GLU:OE2	2:G:396:ASN:ND2	2.52	0.41
2:G:248:GLN:HA	2:G:249:SER:HA	1.82	0.41
1:A:11:VAL:HA	1:A:33:LEU:O	2.20	0.41
1:D:256:PRO:HB3	2:E:366:GLU:C	2.33	0.41
2:E:102:ARG:HB2	2:E:111:LYS:HB3	2.02	0.41
1:D:333:MET:HB2	1:D:366:ARG:HB2	2.01	0.41
1:A:51:TYR:OH	1:A:235:GLN:HG2	2.20	0.41
2:E:274:LEU:HD21	2:E:311:GLU:OE2	2.21	0.41
1:F:51:TYR:CD1	1:F:108:VAL:HG13	2.55	0.41
1:F:170:TRP:CH2	1:F:172:PRO:CG	3.02	0.41
1:F:257:PHE:CG	1:F:272:ALA:O	2.74	0.41
2:G:334:LYS:HG2	2:G:396:ASN:HB2	2.01	0.41
1:H:59:TYR:HB3	1:H:103:LEU:HB3	2.03	0.41
1:D:34:LEU:HD13	1:D:132:LYS:HD3	2.03	0.41
1:D:218:GLN:CB	1:D:236:ALA:HB2	2.50	0.41
1:F:86:PRO:HA	1:F:227:GLY:HA2	2.02	0.41
2:G:103:ASN:H	2:G:103:ASN:HD22	1.69	0.41
2:G:213:LYS:HB3	2:G:332:VAL:CG2	2.50	0.41
2:G:274:LEU:HD22	2:G:311:GLU:CB	2.50	0.41
1:H:11:VAL:HG21	1:H:35:SER:HA	2.02	0.41
2:B:102:ARG:HB2	2:B:111:LYS:HB3	2.02	0.41
1:D:59:TYR:HB3	1:D:103:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:CYS:HB3	1:D:271:CYS:HG	1.81	0.41
2:B:103:ASN:H	2:B:103:ASN:HD22	1.69	0.41
2:B:294:THR:O	2:B:295:ASN:CA	2.69	0.41
1:D:256:PRO:CB	2:E:366:GLU:C	2.88	0.41
1:F:11:VAL:HG21	1:F:36:VAL:N	2.36	0.41
2:G:336:ARG:HD2	1:H:235:GLN:N	2.36	0.41
1:H:89:TRP:N	2:I:240:PRO:HG2	2.31	0.41
1:A:59:TYR:HB3	1:A:103:LEU:HB3	2.03	0.41
1:D:95:PHE:CZ	2:E:271:ASN:CG	2.88	0.41
2:E:103:ASN:H	2:E:103:ASN:HD22	1.68	0.41
2:G:77:ARG:HE	2:G:300:GLN:HE21	1.68	0.41
1:A:38:LEU:HD13	1:A:172:PRO:HD3	2.02	0.41
1:A:95:PHE:CA	2:B:290:HIS:HB3	2.51	0.41
1:A:112:GLU:HB2	2:B:102:ARG:HH21	1.86	0.41
1:A:256:PRO:HB3	2:B:366:GLU:CA	2.51	0.41
2:B:236:PRO:CB	2:B:237:PRO:CD	2.99	0.41
2:E:336:ARG:CG	1:F:234:SER:HB2	2.42	0.41
1:F:31:MET:HB3	1:F:133:LEU:HD21	2.03	0.41
1:F:59:TYR:HB3	1:F:103:LEU:HB3	2.03	0.41
1:F:147:TYR:H	1:F:152:HIS:CD2	2.37	0.41
1:F:256:PRO:HG3	2:G:368:PRO:HD3	2.02	0.41
1:A:95:PHE:HA	2:B:290:HIS:CB	2.51	0.41
1:D:259:CYS:HB3	1:D:271:CYS:SG	2.61	0.41
1:H:88:MET:SD	2:I:240:PRO:HD3	2.60	0.41
1:H:89:TRP:N	2:I:240:PRO:HD2	2.36	0.41
2:I:235:MET:HA	2:I:236:PRO:HD3	1.85	0.41
1:A:11:VAL:CG2	1:A:35:SER:CA	2.73	0.40
1:F:129:ALA:HB2	1:F:166:MET:CE	2.37	0.40
1:F:249:ALA:HB2	2:G:370:TYR:CZ	2.56	0.40
1:F:333:MET:HB2	1:F:366:ARG:HB2	2.01	0.40
1:F:95:PHE:HZ	2:G:267:CYS:H	1.69	0.40
2:B:274:LEU:CD2	2:B:296:HIS:HE1	2.33	0.40
1:D:254:THR:C	2:E:368:PRO:CG	2.88	0.40
2:G:211:HIS:CB	1:H:225:ALA:HB1	2.51	0.40
1:H:172:PRO:HG3	1:H:271:CYS:SG	2.60	0.40
1:A:133:LEU:HG	1:A:134:ARG:N	2.37	0.40
2:B:237:PRO:CG	2:B:306:VAL:HG12	2.34	0.40
1:H:112:GLU:HB2	2:I:102:ARG:NH2	2.36	0.40
2:I:102:ARG:HB2	2:I:111:LYS:HB3	2.02	0.40
2:B:236:PRO:CB	2:B:237:PRO:HD2	2.51	0.40
1:F:257:PHE:N	2:G:365:GLY:N	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:252:GLN:NE2	2:I:362:ARG:NH2	2.34	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	380/439 (87%)	356 (94%)	16 (4%)	8 (2%)	7	36
1	D	381/439 (87%)	358 (94%)	15 (4%)	8 (2%)	7	36
1	F	383/439 (87%)	365 (95%)	14 (4%)	4 (1%)	15	55
1	H	387/439 (88%)	364 (94%)	14 (4%)	9 (2%)	6	34
2	B	327/423 (77%)	303 (93%)	19 (6%)	5 (2%)	10	46
2	E	329/423 (78%)	301 (92%)	22 (7%)	6 (2%)	8	40
2	G	329/423 (78%)	303 (92%)	19 (6%)	7 (2%)	7	36
2	I	331/423 (78%)	300 (91%)	26 (8%)	5 (2%)	10	46
All	All	2847/3448 (83%)	2650 (93%)	145 (5%)	52 (2%)	12	40

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	173	PHE
1	A	272	ALA
1	A	386	HIS
1	A	390	TYR
2	B	181	ASP
2	B	237	PRO
1	D	34	LEU
1	D	172	PRO

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Mol	Chain	Res	Type
1	D	383	PRO
1	D	390	TYR
2	E	181	ASP
2	E	236	PRO
2	E	237	PRO
1	F	172	PRO
1	F	218	GLN
1	F	390	TYR
2	G	181	ASP
2	G	237	PRO
1	H	34	LEU
1	H	174	ASP
1	H	218	GLN
1	H	272	ALA
1	H	390	TYR
2	I	181	ASP
2	I	237	PRO
2	I	295	ASN
1	A	172	PRO
2	B	185	ILE
1	D	132	LYS
1	D	272	ALA
2	E	185	ILE
2	G	185	ILE
1	H	172	PRO
1	H	386	HIS
2	I	185	ILE
1	A	126	THR
2	B	136	ASN
1	D	126	THR
2	E	136	ASN
1	F	126	THR
2	G	136	ASN
2	G	236	PRO
2	G	333	PRO
1	H	126	THR
2	I	136	ASN
2	B	296	HIS
2	E	296	HIS
2	G	296	HIS
1	D	171	THR
1	H	173	PHE

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Mol	Chain	Res	Type
1	A	174	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	327/366 (89%)	314 (96%)	13 (4%)	31	55
1	D	327/366 (89%)	313 (96%)	14 (4%)	29	53
1	F	327/366 (89%)	312 (95%)	15 (5%)	27	52
1	H	327/366 (89%)	316 (97%)	11 (3%)	37	60
2	B	295/372 (79%)	282 (96%)	13 (4%)	28	53
2	E	295/372 (79%)	281 (95%)	14 (5%)	26	51
2	G	295/372 (79%)	281 (95%)	14 (5%)	26	51
2	I	295/372 (79%)	280 (95%)	15 (5%)	24	48
All	All	2488/2952 (84%)	2379 (96%)	109 (4%)	32	53

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	69	LYS
1	A	136	LEU
1	A	149	ASN
1	A	212	ASP
1	A	219	LEU
1	A	247	ARG
1	A	267	ARG
1	A	327	LYS
1	A	346	VAL
1	A	352	LEU
1	A	364	GLU
1	A	386	HIS
2	B	88	GLU

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Mol	Chain	Res	Type
2	B	92	CYS
2	B	103	ASN
2	B	144	ARG
2	B	183	ARG
2	B	247	GLN
2	B	255	THR
2	B	256	VAL
2	B	272	GLU
2	B	276	THR
2	B	299	TRP
2	B	371	GLN
2	B	406	LEU
1	D	69	LYS
1	D	132	LYS
1	D	136	LEU
1	D	149	ASN
1	D	170	TRP
1	D	212	ASP
1	D	219	LEU
1	D	247	ARG
1	D	267	ARG
1	D	327	LYS
1	D	346	VAL
1	D	352	LEU
1	D	364	GLU
1	D	384	LYS
2	E	88	GLU
2	E	92	CYS
2	E	103	ASN
2	E	144	ARG
2	E	183	ARG
2	E	247	GLN
2	E	255	THR
2	E	256	VAL
2	E	272	GLU
2	E	276	THR
2	E	299	TRP
2	E	312	LEU
2	E	371	GLN
2	E	406	LEU
1	F	69	LYS
1	F	136	LEU

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Mol	Chain	Res	Type
1	F	149	ASN
1	F	171	THR
1	F	212	ASP
1	F	219	LEU
1	F	247	ARG
1	F	267	ARG
1	F	275	ASN
1	F	327	LYS
1	F	346	VAL
1	F	352	LEU
1	F	364	GLU
1	F	384	LYS
1	F	385	ASP
2	G	88	GLU
2	G	92	CYS
2	G	103	ASN
2	G	144	ARG
2	G	183	ARG
2	G	247	GLN
2	G	255	THR
2	G	256	VAL
2	G	272	GLU
2	G	276	THR
2	G	299	TRP
2	G	312	LEU
2	G	371	GLN
2	G	406	LEU
1	H	69	LYS
1	H	136	LEU
1	H	149	ASN
1	H	212	ASP
1	H	219	LEU
1	H	247	ARG
1	H	267	ARG
1	H	327	LYS
1	H	346	VAL
1	H	352	LEU
1	H	364	GLU
2	I	88	GLU
2	I	92	CYS
2	I	103	ASN
2	I	144	ARG

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Mol	Chain	Res	Type
2	I	183	ARG
2	I	238	ASP
2	I	247	GLN
2	I	255	THR
2	I	256	VAL
2	I	272	GLU
2	I	276	THR
2	I	295	ASN
2	I	299	TRP
2	I	371	GLN
2	I	406	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	HIS
1	A	230	HIS
1	A	235	GLN
1	A	252	GLN
1	A	373	GLN
2	B	103	ASN
2	B	346	GLN
2	B	405	GLN
1	D	149	ASN
1	D	152	HIS
1	D	230	HIS
1	D	235	GLN
1	D	252	GLN
1	D	373	GLN
2	E	90	HIS
2	E	103	ASN
2	E	210	GLN
2	E	271	ASN
2	E	296	HIS
2	E	346	GLN
1	F	149	ASN
1	F	152	HIS
1	F	218	GLN
1	F	230	HIS
1	F	373	GLN
2	G	82	HIS
2	G	90	HIS

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Mol	Chain	Res	Type
2	G	103	ASN
2	G	210	GLN
2	G	296	HIS
2	G	327	ASN
2	G	346	GLN
2	G	396	ASN
1	H	149	ASN
1	H	152	HIS
1	H	230	HIS
1	H	252	GLN
1	H	373	GLN
2	I	82	HIS
2	I	90	HIS
2	I	103	ASN
2	I	296	HIS
2	I	346	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	7
1	D	4
1	F	4
1	H	4
2	B	2
2	G	1
2	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	321:ALA	C	322:ALA	N	20.90
1	A	323:SER	C	324:LYS	N	19.06
1	A	283:PRO	C	284:GLU	N	13.12
1	A	284:GLU	C	285:ALA	N	12.29
1	D	235:GLN	C	236:ALA	N	4.87
1	D	217:THR	C	218:GLN	N	3.54
1	D	52:LYS	C	53:THR	N	3.47
1	B	333:PRO	C	334:LYS	N	3.04
1	A	235:GLN	C	236:ALA	N	2.96
1	D	108:VAL	C	109:GLU	N	2.81
1	B	294:THR	C	295:ASN	N	2.62
1	F	52:LYS	C	53:THR	N	2.53
1	G	294:THR	C	295:ASN	N	2.32
1	H	235:GLN	C	236:ALA	N	2.15
1	F	108:VAL	C	109:GLU	N	2.14
1	F	235:GLN	C	236:ALA	N	2.13
1	E	294:THR	C	295:ASN	N	2.01
1	F	217:THR	C	218:GLN	N	1.91
1	A	52:LYS	C	53:THR	N	1.69
1	H	52:LYS	C	53:THR	N	1.69
1	A	108:VAL	C	109:GLU	N	1.67
1	H	108:VAL	C	109:GLU	N	1.67
1	H	217:THR	C	218:GLN	N	0.96

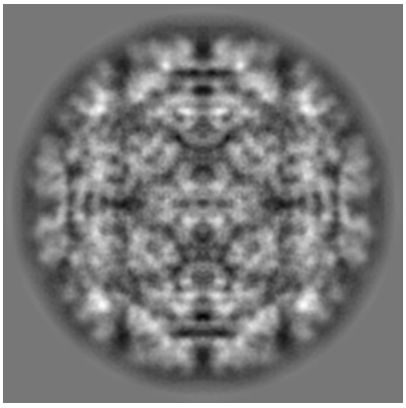
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-1015. These allow visual inspection of the internal detail of the map and identification of artifacts.

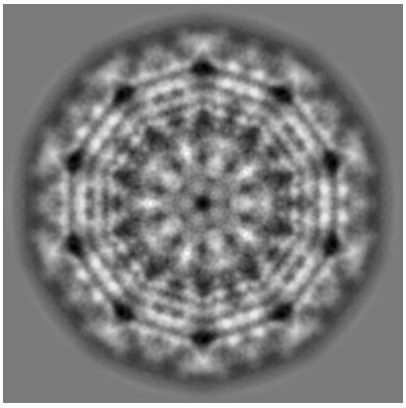
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

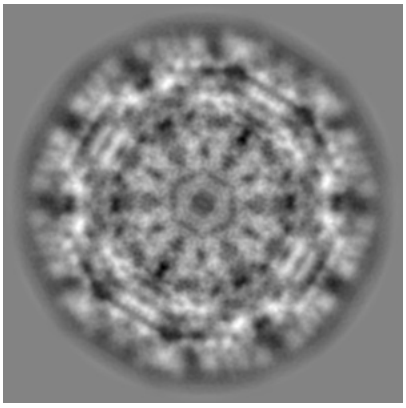
6.1.1 Primary map



X



Y

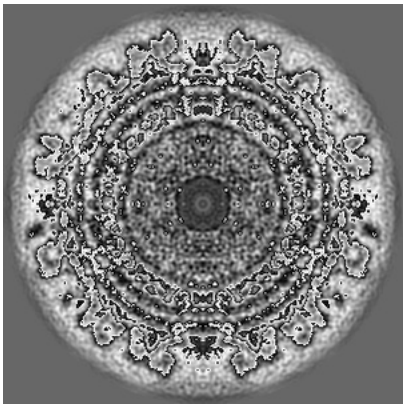


Z

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

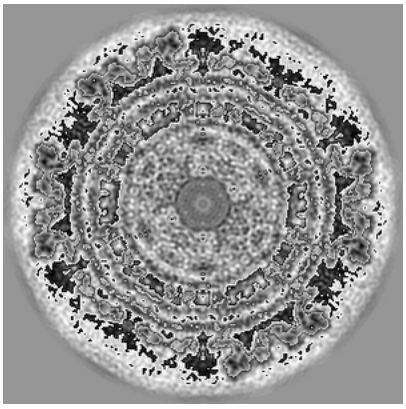
6.2 Central slices (i)

6.2.1 Primary map



X Index: 150

Y Index: 150

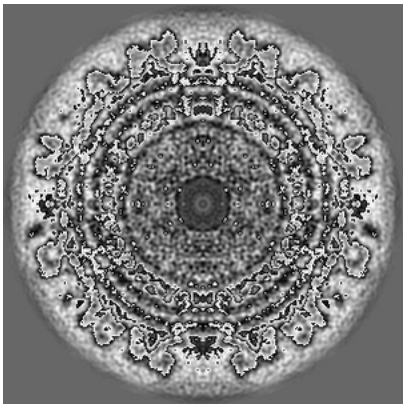


Z Index: 150

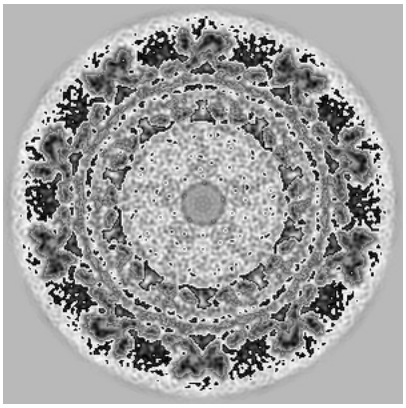
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

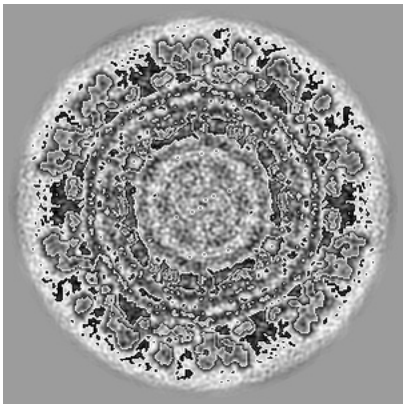
6.3.1 Primary map



X Index: 150



Y Index: 137

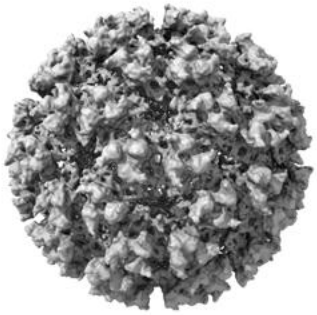


Z Index: 112

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

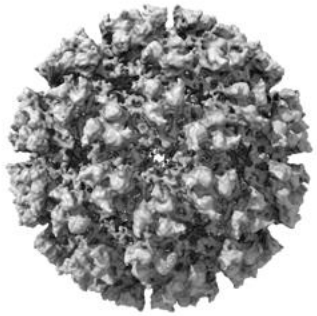
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 9460.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

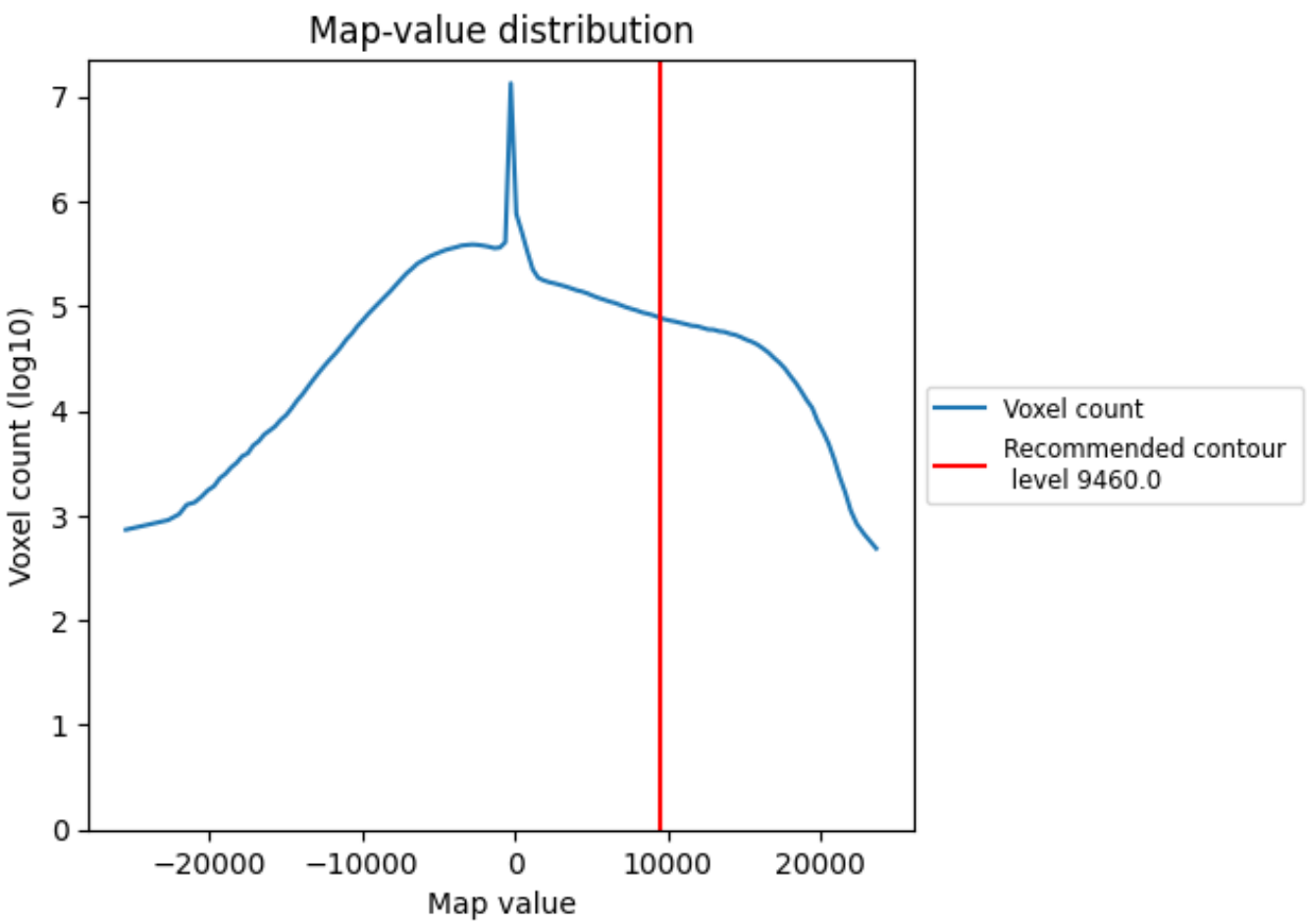
6.5 Mask visualisation (i)

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

7 Map analysis (i)

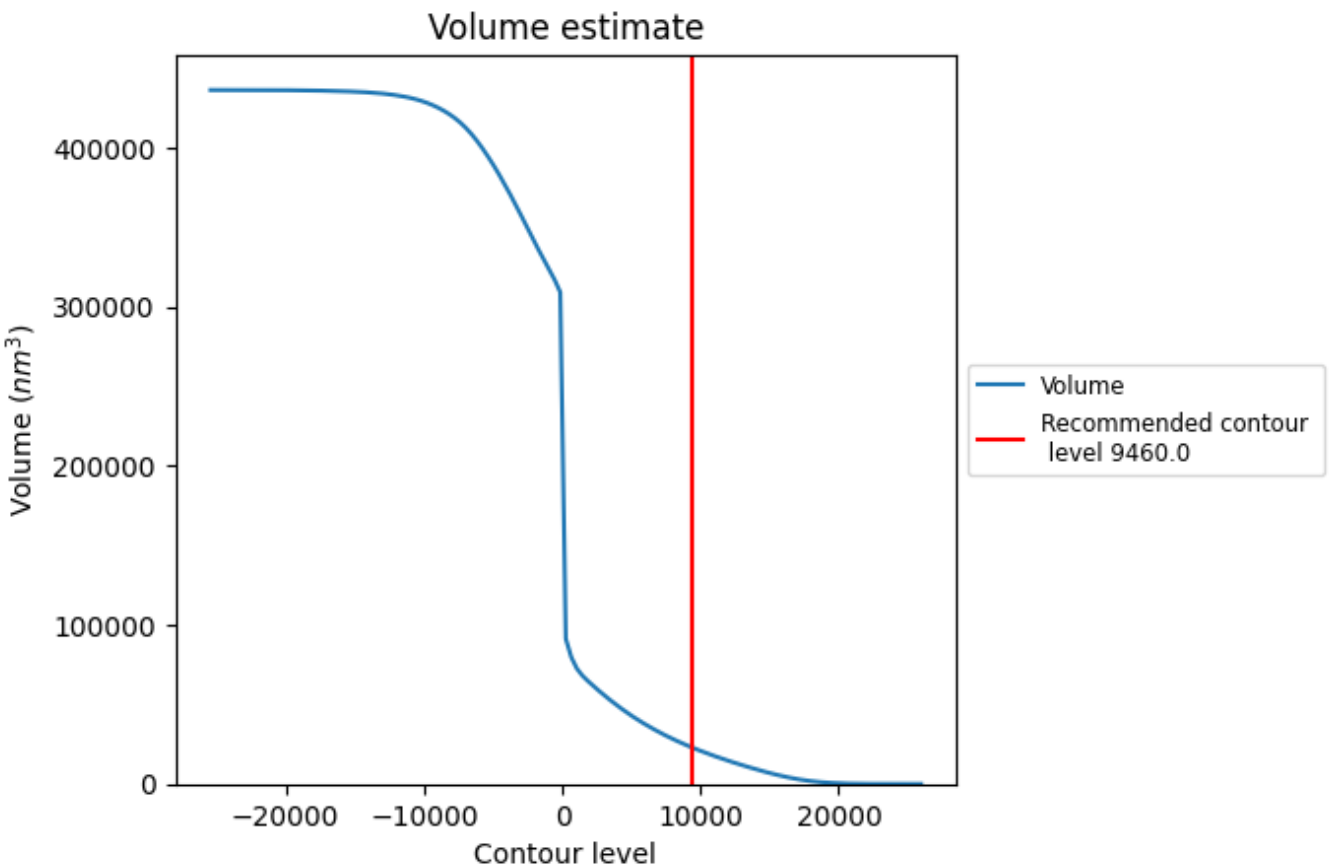
This section contains the results of statistical analysis of the map.

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.

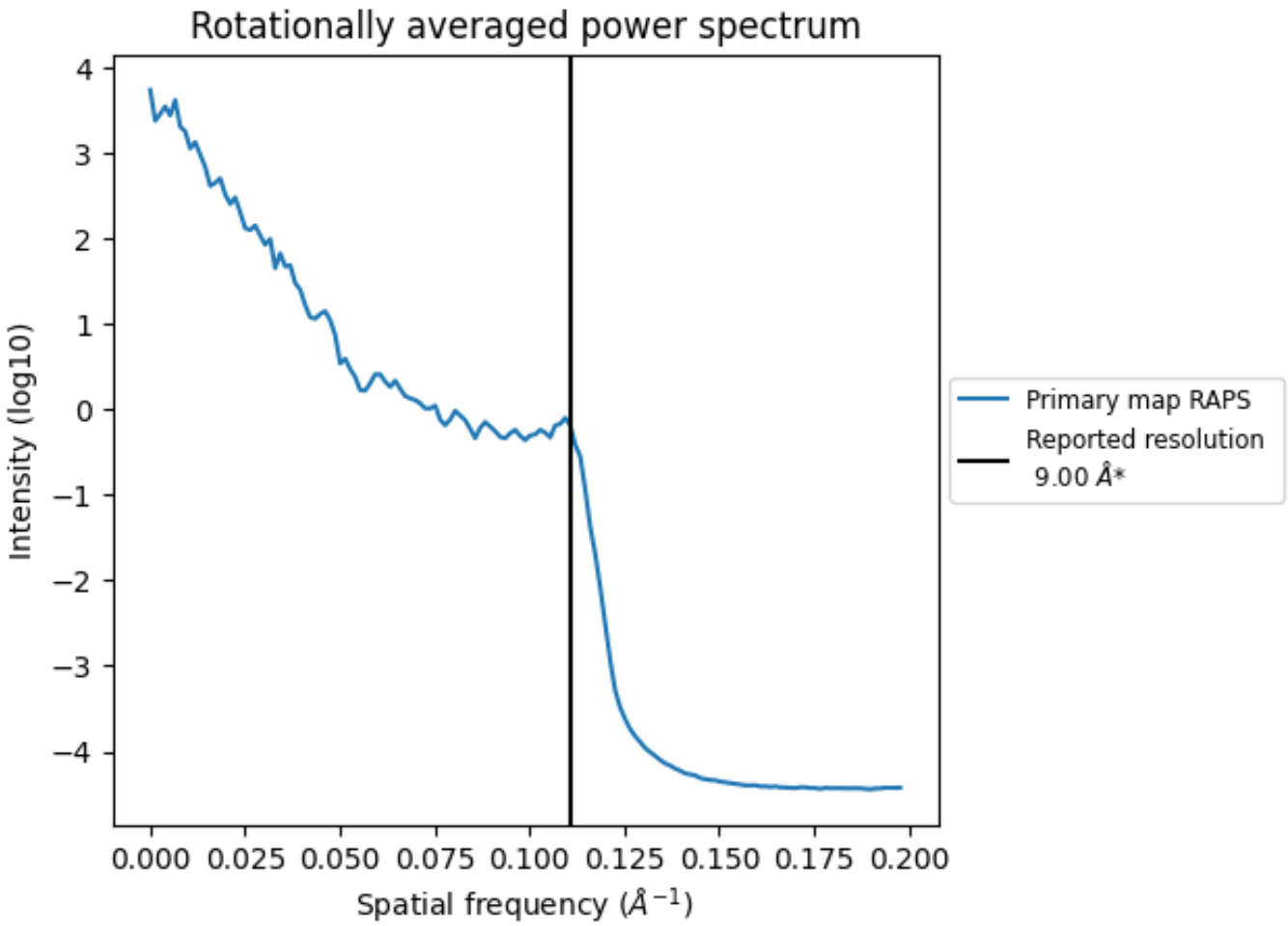
7.2 Volume estimate (i)



The volume at the recommended contour level is 22687 nm^3; this corresponds to an approximate mass of 20494 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 (i)



*Reported resolution corresponds to spatial frequency of 0.111 Å^{-1}

8 Fourier-Shell correlation (i)

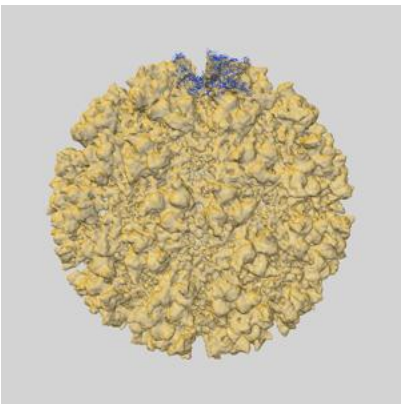
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

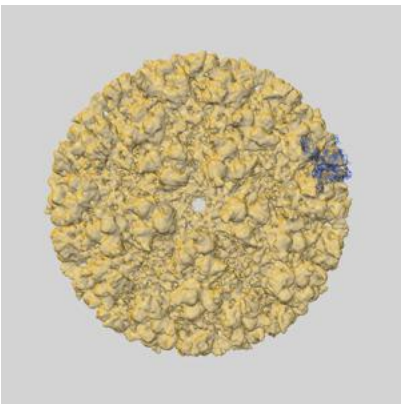
This section contains information regarding the fit between EMDB map EMD-1015 and PDB model 2XFC. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

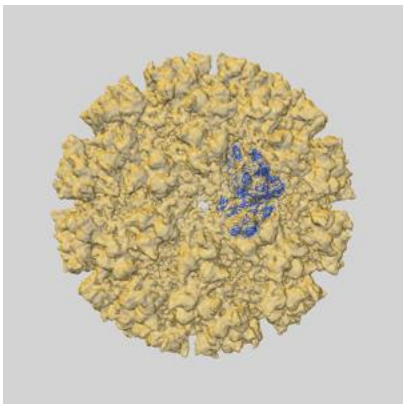
9.1.1 Map-model overlay (i)



X

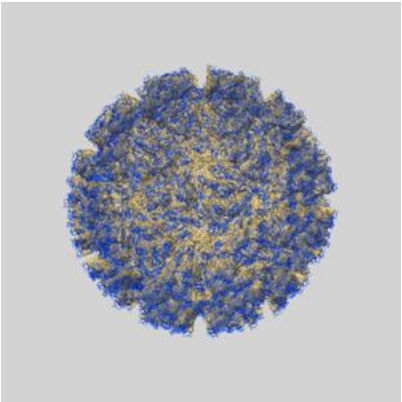


Y

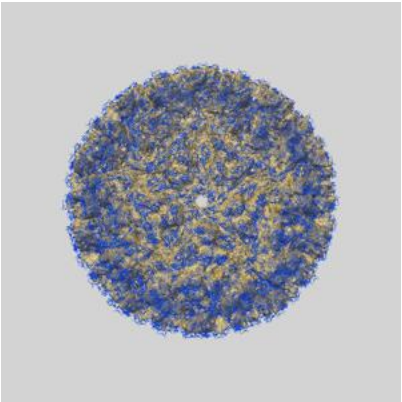


Z

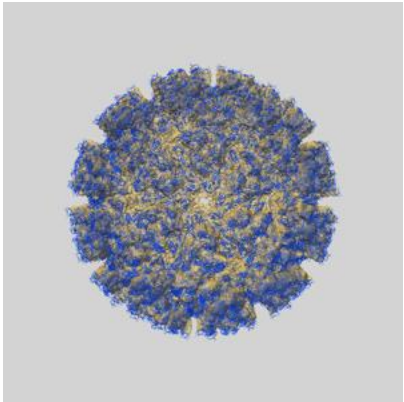
9.1.2 Map-model assembly overlay (i)



X



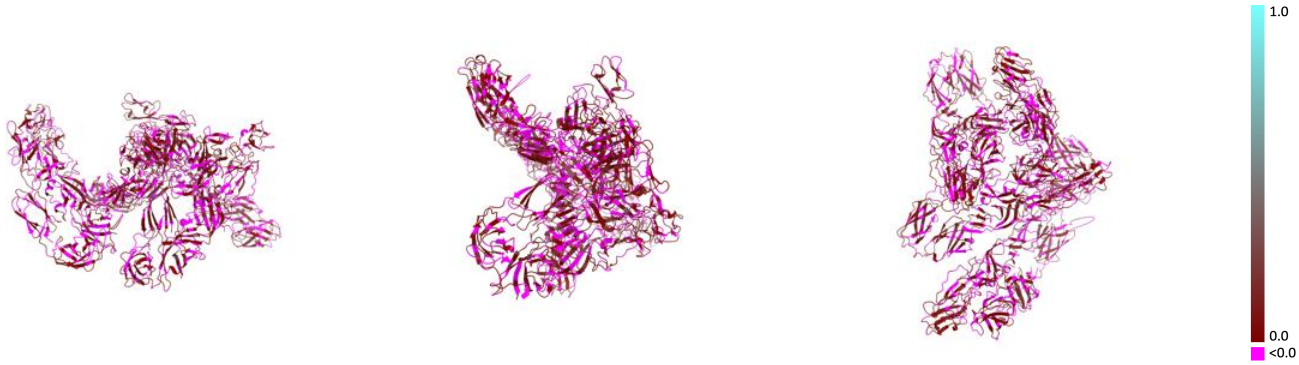
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 9460.0 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.

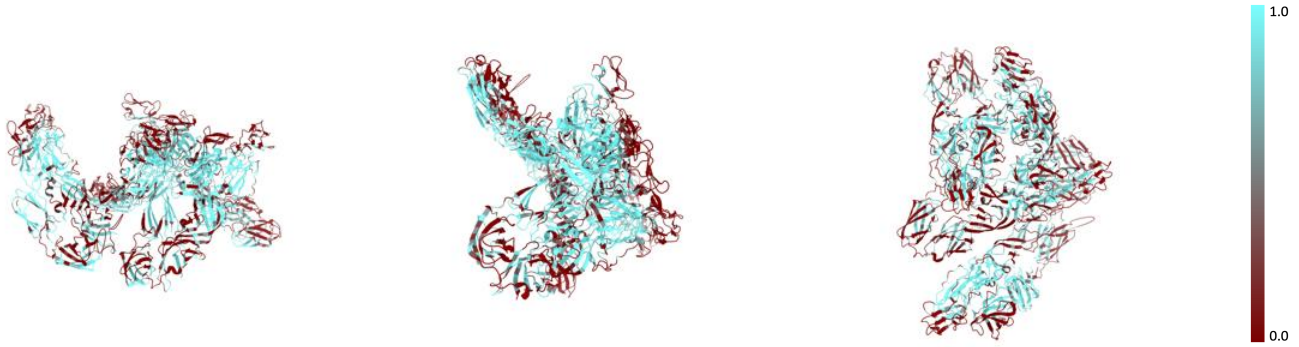
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

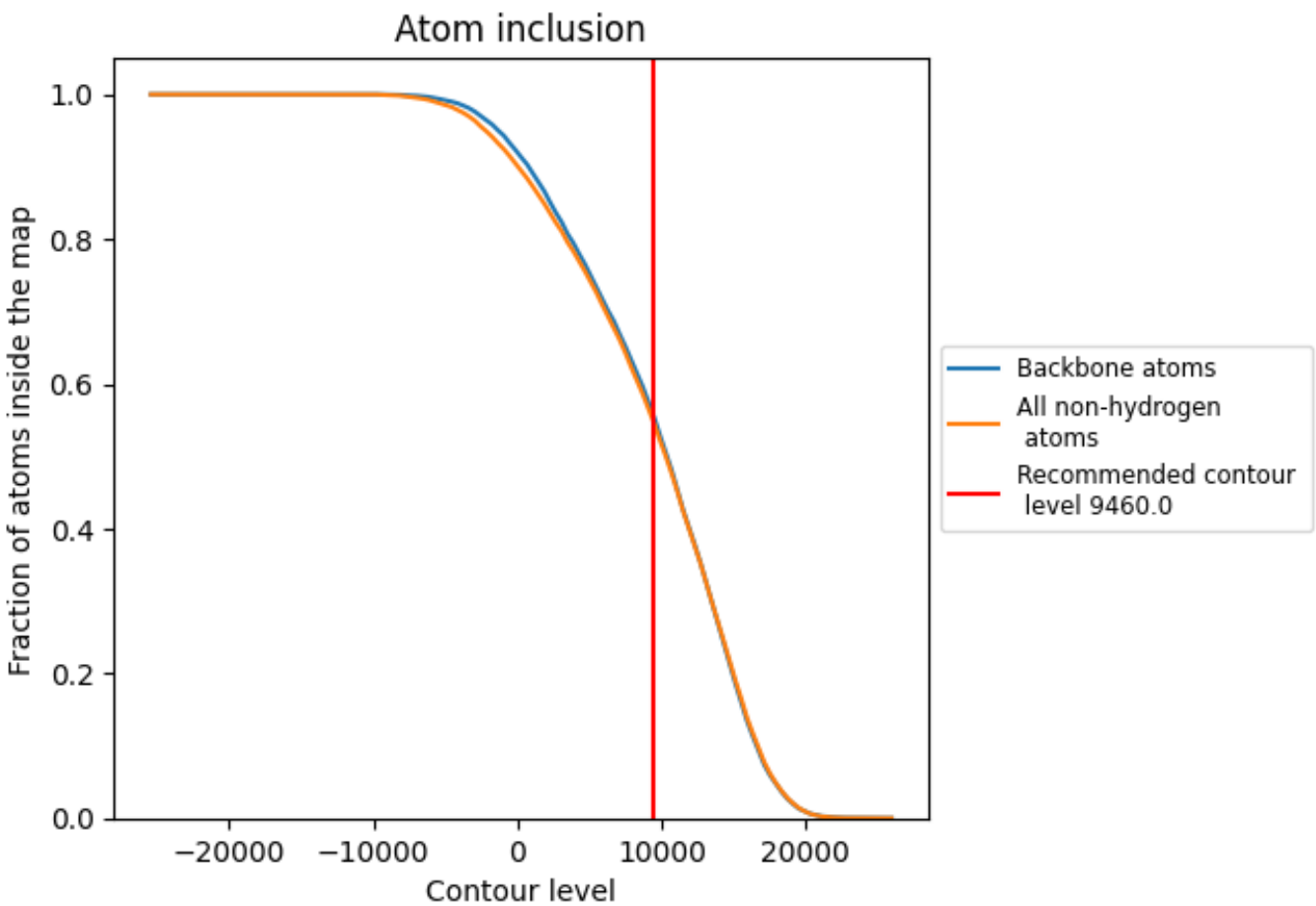
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (9460.0).

9.4 Atom inclusion (i)



At the recommended contour level, 56% of all backbone atoms, 55% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (9460.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5468	0.0400
A	0.5526	0.0290
B	0.5983	0.0460
D	0.5239	0.0400
E	0.5680	0.0440
F	0.5324	0.0260
G	0.6169	0.0530
H	0.4515	0.0360
I	0.5483	0.0510