Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 06:44 pm GMT

PDB ID	:	4CI0
EMDB ID	:	EMD-2513
Title	:	Electron cryo-microscopy of F420-reducing NiFe hydrogenase Frh
Authors	:	Allegretti, M.; Mills, D.J.; McMullan, G.; Kuehlbrandt, W.; Vonck, J.
Deposited on	:	2013-12-05
Resolution	:	3.36 Å(reported)
Based on initial model	:	3ZFS

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:

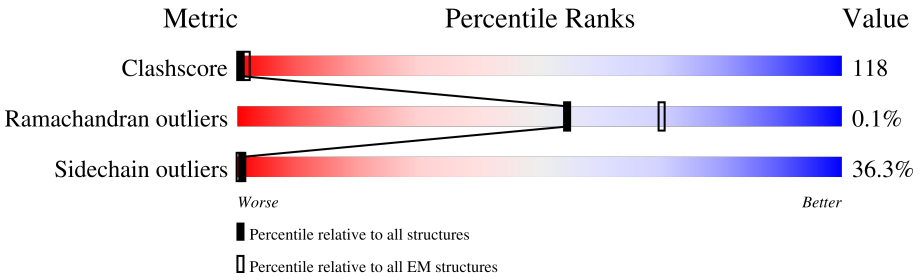
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.36 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	386	13% 17% 53% 28%
2	B	275	11% 14% 44% 24% 17%
3	C	281	19% 16% 52% 31%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	SF4	B	1274	-	-	X	-
7	SF4	B	1275	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	SF4	B	1276	-	-	X	-
7	SF4	C	1282	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 6956 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 F420-REDUCING HYDROGENASE, SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	385	2985	1875	532	561	17	0	0

- Molecule 2 is a protein called F420-REDUCING HYDROGENASE, SUBUNIT GAMMA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	228	1737	1085	290	338	24	0	0

- Molecule 3 is a protein called F420-REDUCING HYDROGENASE, SUBUNIT BETA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	280	2145	1376	347	407	15	0	0

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
			Total	Fe	
4	A	1	1	1	0

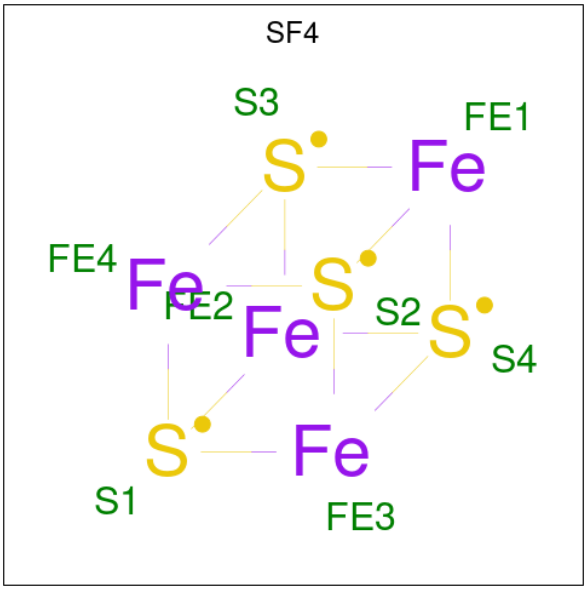
- Molecule 5 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ni	
5	A	1	1	1	0

- Molecule 6 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
			Total	Fe	
6	A	1	1	1	0

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

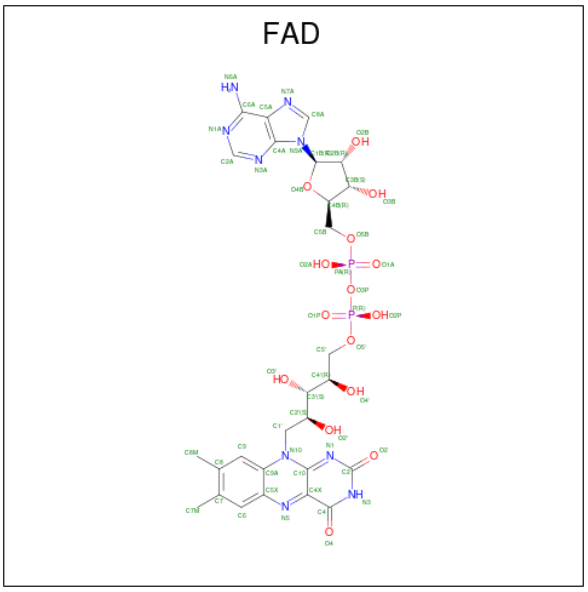


Mol	Chain	Residues	Atoms	AltConf
7	B	1	Total Fe S 24 12 12	0
7	B	1	Total Fe S 24 12 12	0
7	B	1	Total Fe S 24 12 12	0
7	C	1	Total Fe S 8 4 4	0

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
8	B	1	Total Zn 1 1	0

- Molecule 9 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

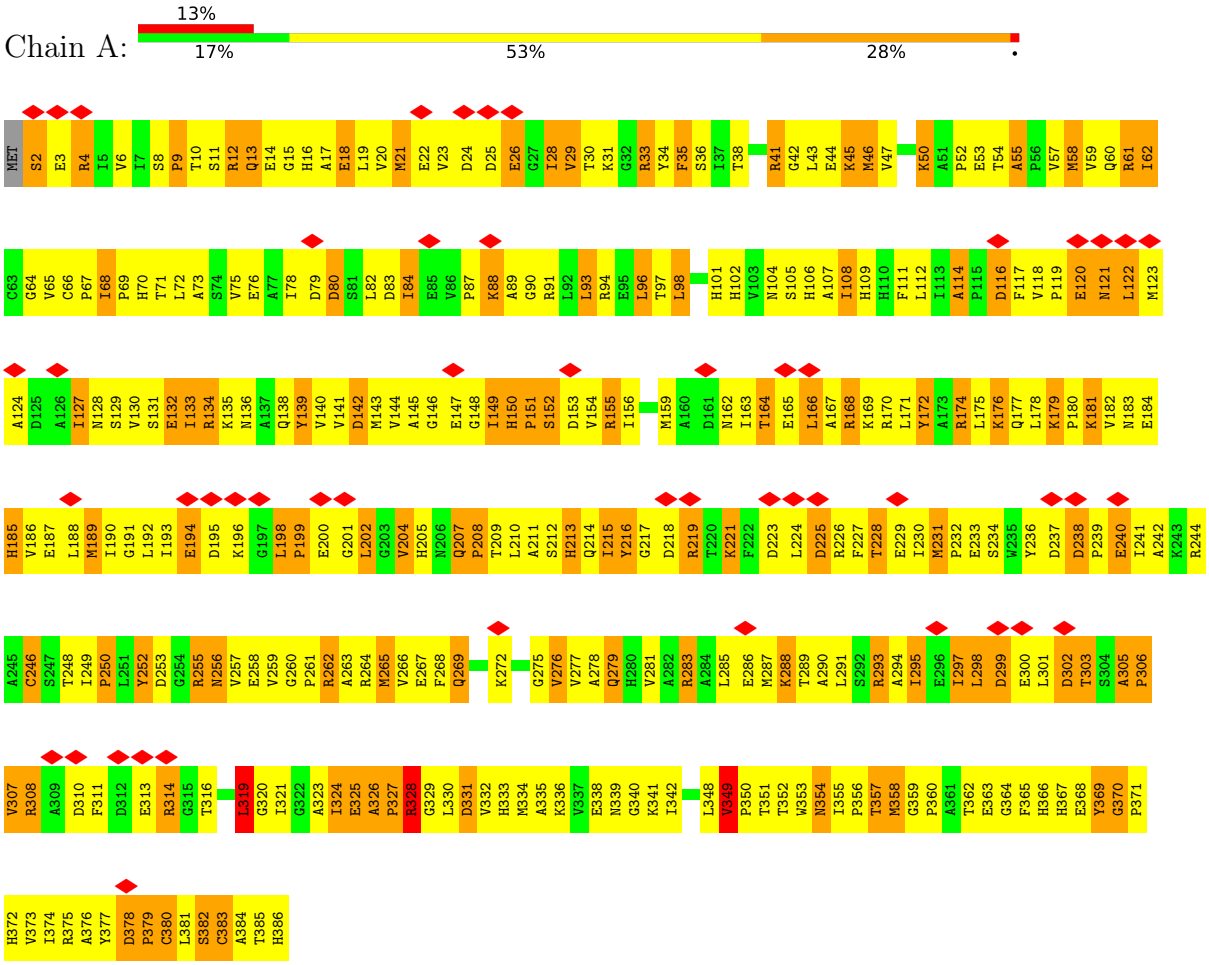


Mol	Chain	Residues	Atoms					AltConf
9	C	1	Total	C	N	O	P	0
			53	27	9	15	2	

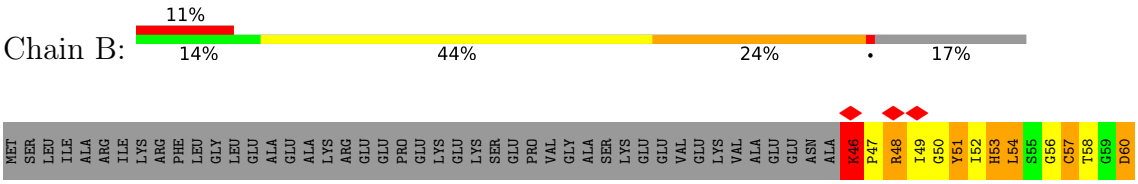
3 Residue-property plots (i)

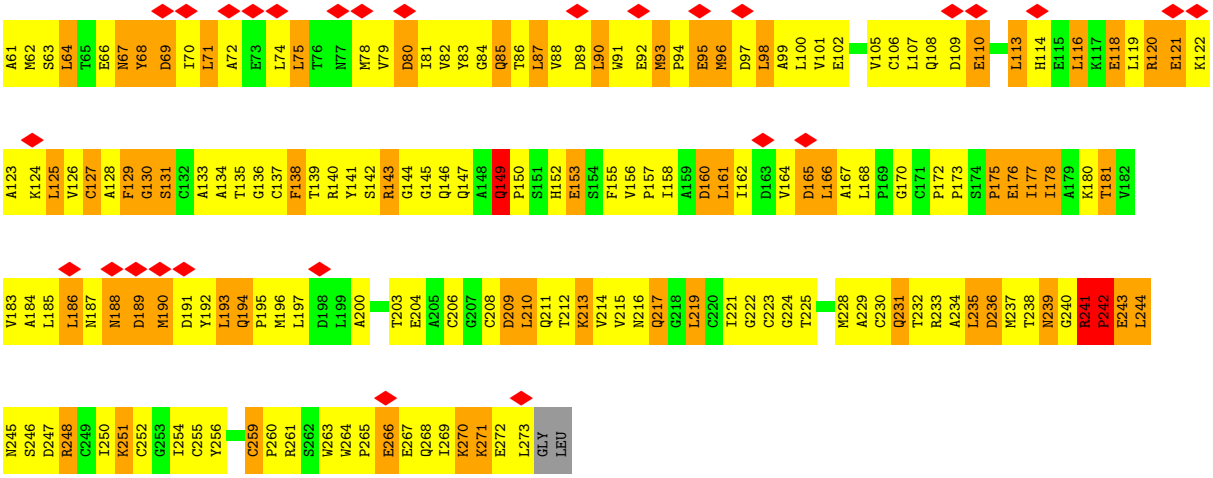
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: F420-REDUCING HYDROGENASE, SUBUNIT ALPHA



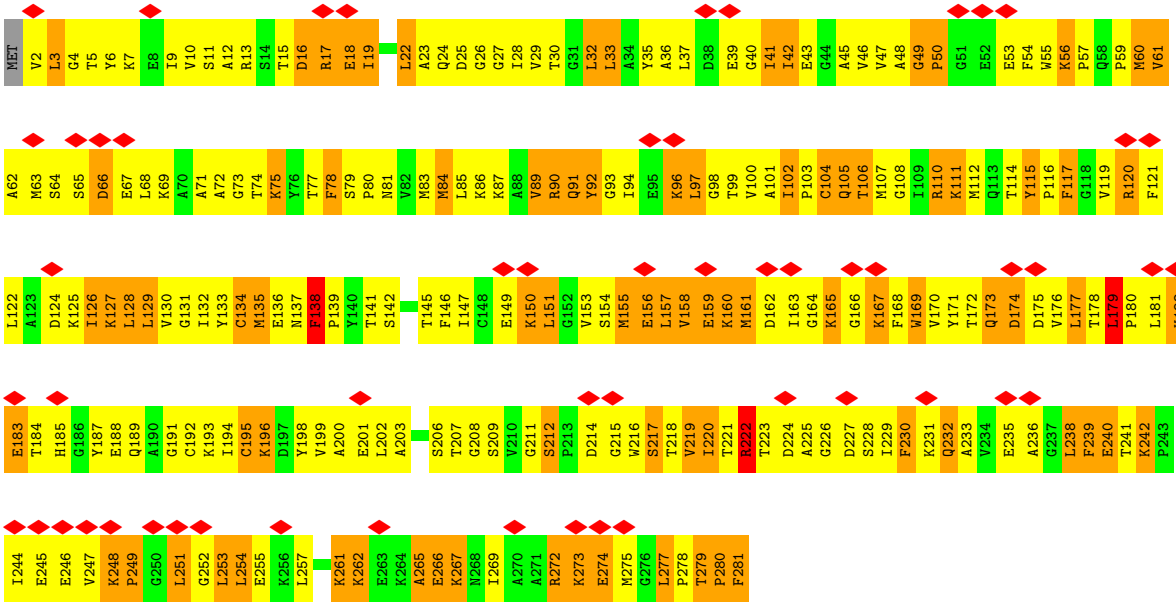
• Molecule 2: F420-REDUCING HYDROGENASE, SUBUNIT GAMMA





• Molecule 3: F420-REDUCING HYDROGENASE, SUBUNIT BETA

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, T	Depositor
Number of particles used	26000	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH IMAGE	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	22	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	106000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.628	Depositor
Minimum map value	-0.198	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	295.68002, 295.68002, 295.68002	wwPDB
Map dimensions	224, 224, 224	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, FE, ZN, FAD, NI, FE2

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	0.69	9/3048 (0.3%)	0.82	19/4133 (0.5%)
2	B	0.67	2/1768 (0.1%)	0.83	6/2400 (0.2%)
3	C	0.70	3/2184 (0.1%)	0.82	8/2946 (0.3%)
All	All	0.69	14/7000 (0.2%)	0.82	33/9479 (0.3%)

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	2
2	B	0	1
3	C	0	3
All	All	0	6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	249	PRO	N-CD	5.54	1.55	1.47
1	A	9	PRO	N-CD	5.44	1.55	1.47
1	A	360	PRO	N-CD	5.42	1.55	1.47
3	C	280	PRO	N-CD	5.27	1.55	1.47
1	A	379	PRO	N-CD	5.26	1.55	1.47
2	B	242	PRO	N-CD	5.21	1.55	1.47
3	C	278	PRO	N-CD	5.18	1.55	1.47
1	A	239	PRO	N-CD	5.13	1.55	1.47
1	A	232	PRO	N-CD	5.10	1.54	1.47
1	A	306	PRO	N-CD	5.09	1.54	1.47
2	B	175	PRO	N-CD	5.07	1.54	1.47
1	A	208	PRO	N-CD	5.02	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	PRO	N-CD	5.01	1.54	1.47
1	A	151	PRO	N-CD	5.00	1.54	1.47

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	327	PRO	CA-N-CD	-8.71	99.31	111.50
1	A	55	ALA	C-N-CD	6.01	141.01	128.40
3	C	115	TYR	C-N-CD	5.98	140.96	128.40
2	B	194	GLN	C-N-CD	5.98	140.96	128.40
3	C	102	ILE	C-N-CD	5.95	140.90	128.40
1	A	355	ILE	C-N-CD	5.95	140.89	128.40
1	A	370	GLY	C-N-CD	5.92	140.82	128.40
1	A	179	LYS	C-N-CD	5.88	140.75	128.40
1	A	349	VAL	C-N-CD	5.86	140.70	128.40
1	A	114	ALA	C-N-CD	5.84	140.68	128.40
1	A	68	ILE	C-N-CD	5.84	140.67	128.40
3	C	279	THR	C-N-CD	5.83	140.65	128.40
3	C	138	PHE	C-N-CD	5.83	140.63	128.40
1	A	198	LEU	C-N-CD	5.80	140.59	128.40
3	C	212	SER	C-N-CD	5.79	140.56	128.40
1	A	305	ALA	C-N-CD	5.79	140.55	128.40
1	A	238	ASP	C-N-CD	5.74	140.45	128.40
1	A	207	GLN	C-N-CD	5.72	140.42	128.40
3	C	179	LEU	C-N-CD	5.72	140.42	128.40
2	B	149	GLN	C-N-CD	5.72	140.40	128.40
2	B	46	LYS	C-N-CD	5.71	140.39	128.40
1	A	150	HIS	C-N-CD	5.70	140.38	128.40
2	B	259	CYS	C-N-CD	5.68	140.34	128.40
1	A	378	ASP	C-N-CD	5.67	140.30	128.40
2	B	241	ARG	C-N-CD	5.64	140.24	128.40
1	A	319	LEU	CA-CB-CG	5.58	128.15	115.30
1	A	326	ALA	C-N-CD	-5.54	108.41	120.60
2	B	130	GLY	N-CA-C	-5.38	99.66	113.10
3	C	49	GLY	C-N-CD	5.38	139.69	128.40
1	A	359	GLY	C-N-CD	5.36	139.66	128.40
3	C	50	PRO	CA-N-CD	-5.29	104.09	111.50
1	A	253	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	331	ASP	CB-CG-OD2	5.21	122.99	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	ARG	Sidechain
1	A	328	ARG	Sidechain
2	B	248	ARG	Sidechain
3	C	222	ARG	Sidechain
3	C	265	ALA	Peptide
3	C	272	ARG	Sidechain

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	2985	0	2970	712	0
2	B	1737	0	1699	468	0
3	C	2145	0	2192	577	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	B	24	0	0	7	0
7	C	8	0	0	6	0
8	B	1	0	0	0	0
9	C	53	0	31	13	0
All	All	6956	0	6892	1637	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 118.

All (1637) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:164:GLY:HA3	3:C:169:TRP:CZ3	1.46	1.48
2:B:101:VAL:HG21	2:B:158:ILE:CD1	1.54	1.35
1:A:18:GLU:HG2	1:A:35:PHE:CZ	1.61	1.35
2:B:195:PRO:HG3	3:C:115:TYR:CE2	1.62	1.34
2:B:219:LEU:CD1	3:C:272:ARG:HH21	1.40	1.33
3:C:78:PHE:HE2	3:C:189:GLN:NE2	1.23	1.33
2:B:219:LEU:CD1	3:C:272:ARG:NH2	1.92	1.32
3:C:36:ALA:CB	3:C:42:ILE:HD11	1.58	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:139:PRO:HD2	3:C:142:SER:CB	1.60	1.30
3:C:28:ILE:HG13	3:C:239:PHE:CE2	1.66	1.29
2:B:127:CYS:HB2	2:B:166:LEU:CD1	1.63	1.29
1:A:73:ALA:HB2	1:A:324:ILE:CD1	1.62	1.28
1:A:84:ILE:HD12	1:A:311:PHE:CB	1.63	1.26
2:B:267:GLU:O	2:B:270:LYS:HG3	1.34	1.25
3:C:203:ALA:O	3:C:222:ARG:HG3	1.16	1.25
3:C:114:THR:HG23	3:C:115:TYR:CD1	1.73	1.24
2:B:219:LEU:HD13	3:C:272:ARG:NH2	1.48	1.23
1:A:28:ILE:HG23	1:A:364:GLY:O	1.39	1.20
2:B:237:MET:HE2	3:C:80:PRO:CG	1.72	1.20
2:B:101:VAL:CG2	2:B:158:ILE:HD13	1.70	1.20
2:B:225:THR:HG22	7:B:1276:SF4:S1	1.80	1.19
3:C:242:LYS:CE	3:C:247:VAL:HG11	1.71	1.19
1:A:84:ILE:CG2	1:A:311:PHE:HB3	1.73	1.18
3:C:26:GLY:HA3	3:C:217:SER:HB3	1.22	1.17
1:A:199:PRO:CD	1:A:369:TYR:CE2	2.28	1.16
2:B:170:GLY:HA2	2:B:254:ILE:HD11	1.17	1.15
3:C:164:GLY:HA3	3:C:169:TRP:CE3	1.81	1.15
1:A:199:PRO:HD3	1:A:369:TYR:CE2	1.81	1.15
2:B:232:THR:HG21	2:B:248:ARG:O	1.47	1.15
1:A:71:THR:HG21	1:A:154:VAL:CG1	1.77	1.14
3:C:139:PRO:HD2	3:C:142:SER:HB3	1.17	1.13
1:A:68:ILE:HD13	1:A:101:HIS:HD2	1.12	1.12
2:B:128:ALA:HB2	2:B:158:ILE:HD11	1.26	1.12
3:C:78:PHE:CE2	3:C:189:GLN:NE2	2.16	1.12
1:A:118:VAL:CG1	1:A:192:LEU:HD13	1.79	1.12
3:C:168:PHE:HB3	3:C:179:LEU:CD1	1.79	1.12
3:C:103:PRO:HG2	7:C:1282:SF4:S3	1.90	1.11
3:C:228:SER:O	3:C:232:GLN:HG2	1.48	1.11
1:A:71:THR:HG21	1:A:154:VAL:HG11	1.31	1.10
1:A:147:GLU:OE2	3:C:120:ARG:HD3	1.50	1.10
3:C:9:ILE:HD13	3:C:220:ILE:HB	1.27	1.10
1:A:62:ILE:CG2	1:A:70:HIS:CD2	2.35	1.09
3:C:151:LEU:HD23	3:C:170:VAL:HG21	1.31	1.09
2:B:106:CYS:O	2:B:113:LEU:HD21	1.52	1.09
3:C:206:SER:OG	3:C:222:ARG:HD3	1.52	1.09
2:B:93:MET:HG3	2:B:122:LYS:HG3	1.32	1.08
2:B:260:PRO:HG3	3:C:108:GLY:HA2	1.29	1.08
3:C:242:LYS:HE3	3:C:247:VAL:HG11	1.16	1.08
1:A:96:LEU:HD11	1:A:144:VAL:HG11	1.20	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ILE:HD13	1:A:101:HIS:CD2	1.88	1.08
3:C:85:LEU:HD21	3:C:99:THR:HG21	1.36	1.08
3:C:167:LYS:HD3	3:C:178:THR:CB	1.84	1.08
3:C:96:LYS:CG	3:C:127:LYS:HE3	1.83	1.08
3:C:28:ILE:CG2	3:C:207:THR:HG21	1.84	1.07
3:C:153:VAL:HG22	3:C:157:LEU:HD23	1.33	1.07
3:C:36:ALA:HB3	3:C:42:ILE:HD11	1.11	1.07
1:A:84:ILE:HD12	1:A:311:PHE:CG	1.88	1.07
2:B:237:MET:CE	3:C:80:PRO:CG	2.32	1.07
1:A:84:ILE:CD1	1:A:311:PHE:HB2	1.83	1.07
3:C:78:PHE:HE1	3:C:139:PRO:HA	1.18	1.07
3:C:28:ILE:HG22	3:C:207:THR:HG21	1.34	1.06
2:B:127:CYS:HB2	2:B:166:LEU:HD11	1.35	1.06
1:A:149:ILE:HD11	2:B:172:PRO:HG3	1.38	1.05
1:A:84:ILE:HD12	1:A:311:PHE:HB2	1.33	1.05
1:A:231:MET:HE3	1:A:248:THR:HG22	1.34	1.05
2:B:170:GLY:CA	2:B:254:ILE:HD11	1.87	1.05
3:C:133:TYR:OH	3:C:220:ILE:CG2	2.05	1.05
3:C:275:MET:HE2	3:C:277:LEU:HD21	1.05	1.05
1:A:327:PRO:HD2	1:A:328:ARG:H	1.20	1.04
1:A:71:THR:CG2	1:A:154:VAL:HG11	1.86	1.04
2:B:125:LEU:HD21	2:B:165:ASP:CB	1.86	1.04
1:A:73:ALA:HB2	1:A:324:ILE:HD11	1.10	1.03
2:B:74:LEU:O	2:B:74:LEU:HD23	1.58	1.03
1:A:96:LEU:CD1	1:A:144:VAL:HG11	1.87	1.03
2:B:225:THR:CG2	2:B:260:PRO:HD3	1.88	1.03
3:C:24:GLN:NE2	3:C:74:THR:HB	1.73	1.03
1:A:18:GLU:HG2	1:A:35:PHE:CE1	1.93	1.03
1:A:207:GLN:HG3	1:A:256:ASN:O	1.56	1.03
3:C:28:ILE:HD13	3:C:219:VAL:HG11	1.39	1.03
3:C:96:LYS:HG2	3:C:127:LYS:HE3	1.40	1.03
3:C:203:ALA:O	3:C:222:ARG:CG	2.06	1.03
3:C:195:CYS:SG	3:C:261:LYS:NZ	2.30	1.03
1:A:190:ILE:HD11	1:A:285:LEU:HD21	1.39	1.03
2:B:49:ILE:CD1	2:B:98:LEU:HD22	1.88	1.03
3:C:242:LYS:HE3	3:C:247:VAL:CG1	1.89	1.03
1:A:84:ILE:HG23	1:A:311:PHE:HB3	1.06	1.02
3:C:164:GLY:CA	3:C:169:TRP:CZ3	2.41	1.02
3:C:28:ILE:HG13	3:C:239:PHE:HE2	0.88	1.02
1:A:14:GLU:OE1	1:A:65:VAL:HG21	1.59	1.02
1:A:214:GLN:OE1	1:A:214:GLN:N	1.92	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:142:SER:OG	3:C:187:TYR:HB3	1.58	1.02
3:C:279:THR:HG22	3:C:280:PRO:O	1.60	1.02
2:B:168:LEU:HD12	2:B:168:LEU:O	1.58	1.02
2:B:237:MET:HE2	3:C:80:PRO:HG2	1.38	1.02
2:B:225:THR:HG21	2:B:260:PRO:HD3	1.07	1.01
1:A:172:TYR:HE1	1:A:176:LYS:HG3	1.23	1.01
1:A:313:GLU:OE1	1:A:313:GLU:N	1.93	1.01
1:A:231:MET:CE	1:A:248:THR:CG2	2.39	1.01
2:B:219:LEU:HD11	3:C:272:ARG:NH2	1.75	1.01
2:B:49:ILE:HD13	2:B:98:LEU:CD2	1.91	1.01
3:C:28:ILE:CG1	3:C:239:PHE:HE2	1.74	1.01
3:C:114:THR:CG2	3:C:115:TYR:HD1	1.73	1.00
3:C:139:PRO:HD2	3:C:142:SER:HB2	1.42	1.00
3:C:164:GLY:CA	3:C:169:TRP:HZ3	1.75	1.00
1:A:202:LEU:HA	1:A:365:PHE:CE2	1.97	1.00
3:C:89:VAL:HG21	3:C:125:LYS:HD3	1.41	1.00
3:C:153:VAL:CG2	3:C:157:LEU:HD23	1.91	0.99
2:B:128:ALA:CB	2:B:158:ILE:HD11	1.91	0.99
3:C:9:ILE:CD1	3:C:220:ILE:HB	1.91	0.99
2:B:125:LEU:HD21	2:B:165:ASP:HB2	1.40	0.98
2:B:49:ILE:HD13	2:B:98:LEU:HD22	1.01	0.98
3:C:37:LEU:HD23	3:C:42:ILE:HD13	1.42	0.98
2:B:219:LEU:HD11	3:C:272:ARG:HH21	1.27	0.98
1:A:210:LEU:CD2	1:A:330:LEU:HD22	1.93	0.98
3:C:36:ALA:CB	3:C:42:ILE:CD1	2.41	0.98
3:C:16:ASP:HB2	3:C:19:ILE:HG12	1.44	0.98
3:C:24:GLN:HE21	3:C:74:THR:HB	1.24	0.98
3:C:111:LYS:O	3:C:114:THR:HG22	1.62	0.98
3:C:96:LYS:CB	3:C:127:LYS:HE3	1.94	0.97
1:A:97:THR:OG1	1:A:144:VAL:HG21	1.64	0.97
3:C:7:LYS:HD3	3:C:227:ASP:OD2	1.64	0.97
3:C:28:ILE:CD1	3:C:219:VAL:HG11	1.94	0.97
1:A:70:HIS:HE1	1:A:349:VAL:CG1	1.76	0.97
1:A:201:GLY:O	1:A:365:PHE:HZ	1.46	0.97
3:C:133:TYR:CD2	3:C:208:GLY:HA3	1.98	0.97
1:A:84:ILE:HG23	1:A:311:PHE:CB	1.94	0.97
3:C:96:LYS:HB3	3:C:127:LYS:CE	1.94	0.97
1:A:238:ASP:HB2	1:A:241:ILE:HG22	1.42	0.97
2:B:74:LEU:HD23	2:B:74:LEU:C	1.85	0.97
2:B:144:GLY:H	2:B:153:GLU:HB2	1.27	0.97
1:A:118:VAL:HG12	1:A:192:LEU:HD13	1.44	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:25:ASP:OD2	3:C:209:SER:HA	1.64	0.96
3:C:30:THR:OG1	3:C:72:ALA:HB2	1.65	0.96
3:C:36:ALA:HB3	3:C:42:ILE:CD1	1.95	0.96
2:B:237:MET:HE2	3:C:80:PRO:CB	1.96	0.96
3:C:96:LYS:HB3	3:C:127:LYS:HE3	1.46	0.96
1:A:210:LEU:HB3	1:A:259:VAL:HG12	1.47	0.96
1:A:323:ALA:HB2	1:A:332:VAL:HG12	1.44	0.96
2:B:195:PRO:CG	3:C:115:TYR:HE2	1.78	0.96
1:A:41:ARG:HG3	1:A:41:ARG:HH11	1.25	0.96
2:B:125:LEU:CD2	2:B:165:ASP:HB2	1.95	0.95
3:C:167:LYS:HD3	3:C:178:THR:OG1	1.65	0.95
1:A:18:GLU:CG	1:A:35:PHE:CZ	2.47	0.95
1:A:231:MET:HE3	1:A:248:THR:CG2	1.94	0.95
3:C:169:TRP:CD1	3:C:178:THR:HG22	2.01	0.95
3:C:275:MET:HE2	3:C:277:LEU:CD2	1.97	0.95
1:A:246:CYS:SG	1:A:385:THR:CG2	2.55	0.95
3:C:102:ILE:HG23	3:C:103:PRO:HD2	1.49	0.95
2:B:98:LEU:HD13	2:B:185:LEU:HD23	1.49	0.94
2:B:195:PRO:HG3	3:C:115:TYR:HE2	1.00	0.94
1:A:319:LEU:CB	1:A:336:LYS:HG2	1.96	0.94
3:C:151:LEU:CD2	3:C:170:VAL:HG21	1.97	0.94
3:C:139:PRO:CD	3:C:142:SER:HB3	1.98	0.93
3:C:168:PHE:HB3	3:C:179:LEU:HD11	1.50	0.93
1:A:107:ALA:HB2	1:A:133:ILE:HD11	1.48	0.93
1:A:286:GLU:O	1:A:289:THR:HG22	1.68	0.93
1:A:159:MET:HB2	1:A:307:VAL:HG11	1.49	0.92
3:C:114:THR:HG23	3:C:115:TYR:HD1	0.80	0.92
2:B:219:LEU:HD13	3:C:272:ARG:HH22	1.22	0.92
1:A:8:SER:OG	1:A:18:GLU:HB2	1.69	0.92
1:A:199:PRO:HD3	1:A:369:TYR:CZ	2.04	0.92
2:B:121:GLU:N	2:B:121:GLU:OE1	2.03	0.92
1:A:238:ASP:HB2	1:A:241:ILE:CG2	1.99	0.92
3:C:153:VAL:HG22	3:C:157:LEU:CD2	1.99	0.92
1:A:143:MET:CE	1:A:171:LEU:HG	2.01	0.91
1:A:46:MET:CE	2:B:142:SER:CA	2.49	0.91
1:A:73:ALA:CB	1:A:324:ILE:CD1	2.48	0.91
1:A:147:GLU:O	1:A:151:PRO:HA	1.70	0.91
2:B:120:ARG:NH1	2:B:126:VAL:HG12	1.83	0.91
2:B:143:ARG:HG2	2:B:143:ARG:HH11	1.35	0.91
2:B:139:THR:CG2	2:B:155:PHE:HB2	2.01	0.91
1:A:62:ILE:CG1	1:A:386:HIS:HB3	2.01	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:MET:CE	2:B:142:SER:HA	2.01	0.90
1:A:120:GLU:N	1:A:120:GLU:OE1	2.03	0.90
3:C:167:LYS:HD3	3:C:178:THR:HB	1.52	0.90
1:A:26:GLU:N	1:A:26:GLU:OE1	2.04	0.90
1:A:244:ARG:HH11	1:A:244:ARG:HG2	1.34	0.90
2:B:90:LEU:HD22	2:B:90:LEU:H	1.32	0.90
1:A:84:ILE:CD1	1:A:311:PHE:CB	2.44	0.90
1:A:71:THR:CG2	1:A:154:VAL:CG1	2.47	0.90
3:C:24:GLN:HE21	3:C:74:THR:CB	1.84	0.90
1:A:264:ARG:HD3	1:A:325:GLU:HG2	1.54	0.90
3:C:253:LEU:HD13	3:C:254:LEU:N	1.87	0.90
2:B:237:MET:HG3	3:C:83:MET:HE3	1.53	0.90
2:B:237:MET:CE	3:C:80:PRO:HG2	1.95	0.90
1:A:172:TYR:HE1	1:A:176:LYS:CG	1.85	0.89
1:A:62:ILE:HG23	1:A:70:HIS:CD2	2.08	0.89
1:A:210:LEU:HD21	1:A:330:LEU:HD22	1.54	0.89
3:C:275:MET:CE	3:C:277:LEU:HD21	1.99	0.89
1:A:349:VAL:HG21	1:A:383:CYS:O	1.73	0.88
3:C:28:ILE:HD13	3:C:219:VAL:CG1	2.03	0.88
3:C:78:PHE:CE1	3:C:139:PRO:HA	2.08	0.88
3:C:154:SER:H	3:C:157:LEU:CD2	1.86	0.88
2:B:85:GLN:HA	2:B:85:GLN:NE2	1.86	0.88
2:B:267:GLU:O	2:B:270:LYS:CG	2.21	0.88
1:A:10:THR:HB	1:A:13:GLN:NE2	1.88	0.88
3:C:23:ALA:HB1	3:C:27:GLY:HA2	1.53	0.88
1:A:70:HIS:HE1	1:A:349:VAL:HG13	1.36	0.88
1:A:175:LEU:HD12	1:A:298:LEU:HD23	1.53	0.88
1:A:43:LEU:CD2	2:B:138:PHE:CE2	2.57	0.88
1:A:71:THR:O	1:A:75:VAL:HG23	1.74	0.88
1:A:201:GLY:O	1:A:365:PHE:CZ	2.26	0.88
2:B:135:THR:HG23	2:B:203:THR:O	1.74	0.88
1:A:189:MET:O	1:A:193:ILE:HD12	1.73	0.87
1:A:323:ALA:CB	1:A:332:VAL:HG12	2.03	0.87
2:B:144:GLY:N	2:B:153:GLU:HB2	1.87	0.87
1:A:19:LEU:HD13	1:A:374:ILE:HD11	1.54	0.87
1:A:36:SER:HB2	1:A:381:LEU:HD12	1.56	0.87
1:A:159:MET:HB2	1:A:307:VAL:CG1	2.04	0.87
1:A:3:GLU:O	1:A:23:VAL:HG22	1.73	0.87
2:B:109:ASP:O	2:B:113:LEU:HD23	1.75	0.87
3:C:132:ILE:CG2	9:C:1283:FAD:H1'2	2.03	0.87
1:A:308:ARG:HG3	1:A:308:ARG:HH11	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:PHE:CZ	1:A:348:LEU:HD11	2.10	0.87
3:C:78:PHE:HE2	3:C:189:GLN:CD	1.79	0.87
3:C:151:LEU:HD23	3:C:170:VAL:CG2	2.05	0.87
2:B:160:ASP:OD1	2:B:161:LEU:HD23	1.75	0.87
1:A:185:HIS:O	1:A:188:LEU:HG	1.75	0.86
2:B:235:LEU:HD13	7:B:1275:SF4:S2	2.14	0.86
3:C:26:GLY:HA3	3:C:217:SER:CB	2.05	0.86
1:A:132:GLU:HG3	1:A:181:LYS:HZ1	1.41	0.86
1:A:102:HIS:HE1	1:A:325:GLU:O	1.58	0.86
1:A:319:LEU:HB3	1:A:336:LYS:CG	2.05	0.86
1:A:123:MET:O	1:A:127:ILE:HG22	1.76	0.86
1:A:46:MET:HE2	2:B:142:SER:HA	1.57	0.86
2:B:232:THR:CG2	2:B:248:ARG:O	2.24	0.86
1:A:265:MET:CE	1:A:269:GLN:OE1	2.23	0.85
2:B:58:THR:HG22	2:B:58:THR:O	1.75	0.85
3:C:129:LEU:HD12	3:C:130:VAL:N	1.92	0.85
1:A:109:HIS:CD2	1:A:378:ASP:CG	2.49	0.85
2:B:101:VAL:HG23	2:B:101:VAL:O	1.74	0.85
3:C:55:TRP:HZ2	3:C:159:GLU:O	1.58	0.85
3:C:78:PHE:HE2	3:C:189:GLN:HE22	1.20	0.85
1:A:260:GLY:H	1:A:263:ALA:HB3	1.40	0.85
2:B:265:PRO:HG2	2:B:268:GLN:OE1	1.77	0.85
3:C:80:PRO:O	3:C:83:MET:HG2	1.77	0.85
2:B:260:PRO:CG	3:C:108:GLY:HA2	2.06	0.85
1:A:52:PRO:CD	1:A:340:GLY:O	2.25	0.84
1:A:119:PRO:HB2	1:A:121:ASN:ND2	1.91	0.84
3:C:91:GLN:N	3:C:91:GLN:HE21	1.76	0.84
3:C:226:GLY:O	3:C:229:ILE:HG22	1.75	0.84
1:A:52:PRO:HD3	1:A:340:GLY:O	1.76	0.84
3:C:158:VAL:O	3:C:158:VAL:CG2	2.24	0.84
1:A:96:LEU:HB2	1:A:297:ILE:HD11	1.59	0.84
2:B:48:ARG:HB2	2:B:48:ARG:HH11	1.42	0.84
2:B:237:MET:HG3	3:C:83:MET:CE	2.06	0.84
1:A:10:THR:HB	1:A:13:GLN:HE21	1.43	0.84
1:A:34:TYR:CE2	1:A:358:MET:CE	2.60	0.84
1:A:70:HIS:CE1	1:A:349:VAL:CG1	2.61	0.84
2:B:49:ILE:HG23	2:B:98:LEU:HD21	1.60	0.84
1:A:65:VAL:C	1:A:67:PRO:CD	2.46	0.84
1:A:88:LYS:HB2	1:A:88:LYS:NZ	1.91	0.84
1:A:326:ALA:HB1	1:A:327:PRO:HD3	1.60	0.84
3:C:96:LYS:CG	3:C:127:LYS:CE	2.56	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ILE:HD13	1:A:62:ILE:O	1.79	0.83
2:B:186:LEU:HD22	2:B:186:LEU:O	1.79	0.83
3:C:24:GLN:OE1	3:C:160:LYS:HE3	1.78	0.83
3:C:32:LEU:HD12	3:C:32:LEU:O	1.79	0.83
1:A:43:LEU:CD1	1:A:62:ILE:HB	2.07	0.83
2:B:266:GLU:O	2:B:269:ILE:HG22	1.76	0.83
3:C:26:GLY:CA	3:C:217:SER:HB3	2.06	0.83
3:C:43:GLU:HB3	3:C:94:ILE:HG23	1.59	0.83
1:A:43:LEU:CD2	2:B:138:PHE:HE2	1.91	0.83
1:A:96:LEU:HB2	1:A:297:ILE:CD1	2.08	0.83
1:A:43:LEU:HD11	1:A:62:ILE:HA	1.61	0.83
2:B:120:ARG:CZ	2:B:126:VAL:HG12	2.08	0.83
3:C:254:LEU:HD12	3:C:254:LEU:O	1.77	0.83
3:C:251:LEU:HD13	3:C:252:GLY:N	1.93	0.83
1:A:231:MET:CE	1:A:248:THR:HG22	2.06	0.82
2:B:139:THR:HG21	2:B:155:PHE:CB	2.09	0.82
2:B:225:THR:CG2	7:B:1276:SF4:S1	2.65	0.82
1:A:175:LEU:CD1	1:A:298:LEU:HD23	2.08	0.82
2:B:116:LEU:HD12	2:B:162:ILE:HD13	1.61	0.82
1:A:36:SER:CB	1:A:381:LEU:HD12	2.09	0.82
1:A:190:ILE:HD11	1:A:285:LEU:CD2	2.09	0.82
2:B:93:MET:HE3	2:B:118:GLU:HG2	1.61	0.82
2:B:106:CYS:O	2:B:113:LEU:CD2	2.28	0.82
1:A:265:MET:CE	1:A:269:GLN:HG3	2.08	0.82
2:B:48:ARG:HH11	2:B:48:ARG:CB	1.93	0.82
2:B:127:CYS:CB	2:B:166:LEU:CD1	2.53	0.82
1:A:249:ILE:CG2	1:A:356:PRO:HG3	2.10	0.82
3:C:78:PHE:CE2	3:C:189:GLN:CD	2.52	0.81
1:A:327:PRO:HD2	1:A:328:ARG:N	1.93	0.81
1:A:380:CYS:SG	1:A:383:CYS:HB2	2.19	0.81
2:B:119:LEU:HD13	2:B:119:LEU:O	1.80	0.81
2:B:127:CYS:HB2	2:B:166:LEU:HD13	1.60	0.81
3:C:28:ILE:CG2	3:C:207:THR:CG2	2.58	0.81
1:A:175:LEU:CD1	1:A:298:LEU:CD2	2.59	0.81
2:B:58:THR:HA	2:B:102:GLU:OE1	1.80	0.81
1:A:328:ARG:HH12	1:A:380:CYS:HB3	1.45	0.81
3:C:132:ILE:HG22	9:C:1283:FAD:H1'2	1.61	0.81
1:A:57:VAL:CG2	2:B:248:ARG:NH1	2.43	0.81
1:A:62:ILE:HG21	1:A:70:HIS:CD2	2.16	0.81
1:A:208:PRO:O	1:A:257:VAL:HG23	1.80	0.81
3:C:17:ARG:HB3	3:C:17:ARG:CZ	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:GLU:HB3	3:C:41:ILE:HD11	1.60	0.81
1:A:62:ILE:CG2	1:A:70:HIS:HD2	1.93	0.81
3:C:175:ASP:OD1	3:C:176:VAL:N	2.14	0.81
3:C:277:LEU:HD23	3:C:277:LEU:H	1.45	0.81
1:A:118:VAL:CG1	1:A:192:LEU:CD1	2.56	0.80
1:A:118:VAL:HG12	1:A:192:LEU:CD1	2.10	0.80
1:A:147:GLU:OE2	3:C:120:ARG:CD	2.29	0.80
2:B:168:LEU:HB2	3:C:117:PHE:HE1	1.45	0.80
3:C:122:LEU:HD12	3:C:122:LEU:O	1.81	0.80
3:C:179:LEU:HD12	3:C:179:LEU:H	1.45	0.80
1:A:213:HIS:HB3	1:A:216:TYR:O	1.81	0.80
1:A:43:LEU:CD1	1:A:62:ILE:CB	2.60	0.80
2:B:93:MET:CG	2:B:122:LYS:HG3	2.10	0.80
1:A:109:HIS:NE2	1:A:378:ASP:HB2	1.96	0.80
1:A:293:ARG:CD	1:A:297:ILE:CG2	2.59	0.80
1:A:319:LEU:CA	1:A:336:LYS:HG2	2.11	0.80
2:B:244:LEU:O	2:B:244:LEU:HD13	1.81	0.80
3:C:15:THR:N	3:C:238:LEU:O	2.14	0.80
1:A:246:CYS:SG	1:A:385:THR:HG21	2.21	0.80
1:A:319:LEU:CB	1:A:336:LYS:CG	2.59	0.80
3:C:168:PHE:HB3	3:C:179:LEU:HD12	1.64	0.80
2:B:177:ILE:HB	3:C:116:PRO:HG2	1.64	0.80
1:A:164:THR:OG1	3:C:92:TYR:HA	1.81	0.80
2:B:260:PRO:HG3	3:C:108:GLY:CA	2.10	0.80
1:A:199:PRO:CD	1:A:369:TYR:CZ	2.64	0.79
3:C:119:VAL:HG12	3:C:122:LEU:HB3	1.62	0.79
1:A:143:MET:HE3	1:A:171:LEU:HG	1.63	0.79
2:B:225:THR:HG21	2:B:260:PRO:CD	2.03	0.79
3:C:142:SER:O	3:C:145:THR:HG22	1.82	0.79
2:B:108:GLN:OE1	2:B:108:GLN:N	2.15	0.79
3:C:171:TYR:HD1	3:C:176:VAL:HG12	1.47	0.79
1:A:102:HIS:CE1	1:A:325:GLU:O	2.35	0.79
3:C:253:LEU:O	3:C:253:LEU:HD22	1.83	0.79
1:A:231:MET:SD	2:B:147:GLN:NE2	2.56	0.79
1:A:140:VAL:HG22	1:A:171:LEU:HD22	1.63	0.79
2:B:71:LEU:HD22	2:B:71:LEU:O	1.82	0.79
1:A:199:PRO:HD2	1:A:369:TYR:CE2	2.17	0.79
2:B:74:LEU:C	2:B:74:LEU:CD2	2.51	0.79
2:B:224:GLY:N	7:B:1276:SF4:S3	2.55	0.79
1:A:213:HIS:CB	1:A:216:TYR:O	2.31	0.79
1:A:262:ARG:HD2	1:A:262:ARG:O	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LEU:HD23	1:A:330:LEU:HD22	1.63	0.79
1:A:9:PRO:HG2	2:B:85:GLN:CG	2.14	0.78
3:C:248:LYS:HG3	3:C:249:PRO:HA	1.65	0.78
1:A:257:VAL:HG11	1:A:353:TRP:CE3	2.19	0.78
1:A:291:LEU:HD23	1:A:291:LEU:O	1.83	0.78
3:C:182:LYS:HA	3:C:185:HIS:CE1	2.19	0.78
1:A:96:LEU:O	1:A:96:LEU:HD22	1.81	0.78
1:A:43:LEU:HD13	1:A:62:ILE:HB	1.65	0.78
1:A:60:GLN:HE21	1:A:61:ARG:NH1	1.80	0.78
2:B:192:TYR:O	2:B:195:PRO:HD2	1.84	0.78
3:C:206:SER:HG	3:C:222:ARG:HD3	1.46	0.78
3:C:221:THR:HG21	3:C:227:ASP:CB	2.14	0.78
1:A:319:LEU:HB3	1:A:336:LYS:HG2	1.63	0.78
2:B:49:ILE:HG23	2:B:98:LEU:CD2	2.14	0.78
2:B:57:CYS:N	7:B:1274:SF4:S3	2.57	0.78
2:B:98:LEU:CD1	2:B:185:LEU:HD23	2.15	0.77
2:B:210:LEU:HD12	2:B:211:GLN:N	1.98	0.77
1:A:60:GLN:HE21	1:A:61:ARG:HH12	1.33	0.77
1:A:66:CYS:N	1:A:67:PRO:CD	2.47	0.77
1:A:88:LYS:NZ	1:A:88:LYS:CB	2.46	0.77
1:A:265:MET:HE3	1:A:269:GLN:HG3	1.64	0.77
1:A:132:GLU:HG3	1:A:181:LYS:NZ	1.98	0.77
1:A:261:PRO:HB3	1:A:286:GLU:HG3	1.66	0.77
2:B:261:ARG:O	3:C:280:PRO:HB3	1.84	0.77
1:A:208:PRO:HD3	1:A:255:ARG:NH1	1.99	0.77
1:A:257:VAL:CG1	1:A:353:TRP:HE3	1.97	0.77
3:C:89:VAL:CG2	3:C:125:LYS:HD3	2.12	0.77
1:A:175:LEU:HD12	1:A:298:LEU:CD2	2.13	0.77
3:C:221:THR:HG21	3:C:227:ASP:HB2	1.65	0.77
3:C:216:TRP:CH2	3:C:240:GLU:CG	2.68	0.77
2:B:101:VAL:CG2	2:B:101:VAL:O	2.32	0.77
1:A:128:ASN:OD1	2:B:72:ALA:CB	2.33	0.77
3:C:96:LYS:CB	3:C:127:LYS:CE	2.60	0.77
3:C:151:LEU:CD2	3:C:170:VAL:CG2	2.61	0.77
1:A:97:THR:OG1	1:A:144:VAL:CG2	2.32	0.77
2:B:166:LEU:HD12	2:B:166:LEU:H	1.49	0.77
3:C:90:ARG:HB3	3:C:91:GLN:NE2	2.00	0.77
3:C:206:SER:OG	3:C:222:ARG:CD	2.33	0.77
3:C:272:ARG:NH1	3:C:277:LEU:HD12	1.99	0.77
1:A:9:PRO:CG	2:B:85:GLN:HG2	2.15	0.77
1:A:119:PRO:HB2	1:A:121:ASN:HD21	1.45	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:MET:CE	1:A:248:THR:HG21	2.15	0.77
2:B:116:LEU:CD1	2:B:162:ILE:HD13	2.15	0.77
3:C:164:GLY:CA	3:C:169:TRP:CE3	2.63	0.77
1:A:114:ALA:O	1:A:118:VAL:HG22	1.85	0.76
1:A:65:VAL:C	1:A:67:PRO:HD2	2.04	0.76
3:C:167:LYS:CD	3:C:178:THR:HB	2.14	0.76
1:A:62:ILE:HG12	1:A:386:HIS:HB3	1.67	0.76
3:C:139:PRO:CD	3:C:142:SER:CB	2.54	0.76
1:A:46:MET:HE2	2:B:142:SER:CA	2.13	0.76
2:B:85:GLN:HA	2:B:85:GLN:HE21	1.49	0.76
3:C:164:GLY:HA3	3:C:169:TRP:HZ3	0.95	0.76
1:A:227:PHE:CE2	1:A:348:LEU:HD11	2.21	0.76
3:C:55:TRP:NE1	3:C:158:VAL:HG22	1.99	0.76
3:C:169:TRP:CD1	3:C:178:THR:CG2	2.69	0.76
1:A:43:LEU:HD21	2:B:138:PHE:CZ	2.20	0.76
1:A:80:ASP:OD1	1:A:320:GLY:HA3	1.86	0.76
2:B:191:ASP:OD1	2:B:192:TYR:N	2.18	0.76
3:C:35:TYR:CZ	3:C:39:GLU:CG	2.69	0.76
3:C:216:TRP:HH2	3:C:240:GLU:CG	1.98	0.76
1:A:172:TYR:CE1	1:A:176:LYS:CG	2.69	0.76
1:A:249:ILE:HG22	1:A:356:PRO:HG3	1.66	0.76
1:A:262:ARG:HD2	1:A:262:ARG:C	2.05	0.76
2:B:237:MET:HE3	2:B:240:GLY:O	1.86	0.76
1:A:73:ALA:CB	1:A:324:ILE:HD11	2.04	0.76
1:A:188:LEU:HD12	1:A:189:MET:N	2.01	0.75
1:A:230:ILE:HD12	1:A:234:SER:OG	1.86	0.75
3:C:16:ASP:HB2	3:C:19:ILE:CG1	2.16	0.75
1:A:149:ILE:HD11	2:B:172:PRO:CG	2.15	0.75
1:A:238:ASP:CB	1:A:241:ILE:HG22	2.17	0.75
1:A:127:ILE:HD12	2:B:72:ALA:HA	1.67	0.75
1:A:321:ILE:N	1:A:321:ILE:HD12	2.02	0.75
1:A:167:ALA:HB2	3:C:93:GLY:H	1.50	0.75
3:C:102:ILE:HG22	3:C:104:CYS:H	1.50	0.75
1:A:210:LEU:HB3	1:A:259:VAL:CG1	2.17	0.74
1:A:143:MET:HE1	1:A:171:LEU:HG	1.69	0.74
2:B:237:MET:CE	3:C:80:PRO:HG3	2.16	0.74
3:C:78:PHE:HE1	3:C:139:PRO:CA	1.97	0.74
3:C:87:LYS:HB2	3:C:87:LYS:HZ3	1.53	0.74
1:A:118:VAL:HG13	1:A:192:LEU:HD13	1.65	0.74
1:A:34:TYR:CE2	1:A:358:MET:HE2	2.21	0.74
1:A:221:LYS:NZ	1:A:221:LYS:HB3	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:GLY:HA2	1:A:307:VAL:HG12	1.69	0.74
1:A:275:GLY:H	1:A:278:ALA:HB3	1.53	0.74
1:A:295:ILE:HD12	1:A:295:ILE:O	1.88	0.74
1:A:210:LEU:CD2	1:A:330:LEU:CD2	2.65	0.74
3:C:28:ILE:HG21	3:C:207:THR:CG2	2.18	0.74
3:C:133:TYR:OH	3:C:220:ILE:HG23	1.87	0.74
3:C:168:PHE:O	3:C:178:THR:HA	1.88	0.74
3:C:28:ILE:CG1	3:C:239:PHE:CE2	2.56	0.74
2:B:90:LEU:HD22	2:B:90:LEU:N	2.03	0.73
2:B:144:GLY:HA3	2:B:153:GLU:CB	2.16	0.73
3:C:55:TRP:NE1	3:C:158:VAL:CG2	2.51	0.73
1:A:286:GLU:O	1:A:289:THR:CG2	2.37	0.73
2:B:58:THR:HA	2:B:102:GLU:CD	2.08	0.73
2:B:98:LEU:HD23	2:B:98:LEU:O	1.88	0.73
2:B:143:ARG:HG2	2:B:143:ARG:NH1	1.99	0.73
3:C:62:ALA:HB1	3:C:67:GLU:HB3	1.69	0.73
3:C:132:ILE:CG2	9:C:1283:FAD:C1'	2.66	0.73
1:A:90:GLY:HA2	1:A:307:VAL:CG1	2.19	0.73
1:A:210:LEU:HD21	1:A:330:LEU:CD2	2.17	0.73
2:B:125:LEU:HD21	2:B:165:ASP:HB3	1.66	0.73
2:B:238:THR:OG1	2:B:243:GLU:OE1	2.06	0.73
3:C:55:TRP:CZ2	3:C:159:GLU:O	2.41	0.73
3:C:87:LYS:HB2	3:C:87:LYS:NZ	2.02	0.73
1:A:72:LEU:HD12	1:A:98:LEU:HG	1.71	0.73
3:C:12:ALA:HB2	3:C:241:THR:HG22	1.70	0.73
3:C:23:ALA:CB	3:C:27:GLY:HA2	2.18	0.73
1:A:9:PRO:HG2	2:B:85:GLN:HG2	1.70	0.73
3:C:19:ILE:N	3:C:19:ILE:HD13	2.02	0.73
2:B:101:VAL:CG2	2:B:158:ILE:CD1	2.45	0.72
3:C:36:ALA:HB1	3:C:42:ILE:CD1	2.19	0.72
2:B:101:VAL:HG21	2:B:158:ILE:HD13	0.78	0.72
3:C:167:LYS:CA	3:C:181:LEU:CD2	2.67	0.72
1:A:121:ASN:H	1:A:121:ASN:HD22	1.36	0.72
1:A:223:ASP:HB2	1:A:226:ARG:HB2	1.71	0.72
3:C:23:ALA:HB1	3:C:27:GLY:CA	2.20	0.72
2:B:139:THR:HG22	2:B:155:PHE:HB2	1.71	0.72
3:C:42:ILE:CG2	3:C:98:GLY:N	2.53	0.72
1:A:3:GLU:HG2	1:A:23:VAL:HG23	1.70	0.72
2:B:144:GLY:CA	2:B:153:GLU:HB2	2.18	0.72
1:A:177:GLN:O	1:A:180:PRO:HD2	1.90	0.72
1:A:249:ILE:HG23	1:A:356:PRO:HD3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:SER:O	2:B:91:TRP:CD1	2.42	0.72
1:A:143:MET:HE3	1:A:171:LEU:CG	2.19	0.72
1:A:166:LEU:HD13	3:C:43:GLU:OE2	1.89	0.72
3:C:154:SER:H	3:C:157:LEU:HD22	1.54	0.72
2:B:120:ARG:CZ	2:B:126:VAL:CG1	2.67	0.72
2:B:170:GLY:HA2	2:B:254:ILE:CD1	2.09	0.72
1:A:265:MET:HE1	1:A:269:GLN:OE1	1.89	0.71
1:A:186:VAL:HG21	1:A:288:LYS:HE3	1.70	0.71
1:A:349:VAL:HG11	1:A:383:CYS:SG	2.29	0.71
2:B:166:LEU:HD12	2:B:166:LEU:N	2.04	0.71
3:C:30:THR:HG1	3:C:72:ALA:HB2	1.55	0.71
3:C:228:SER:O	3:C:232:GLN:CG	2.32	0.71
1:A:14:GLU:OE1	1:A:65:VAL:CG2	2.37	0.71
1:A:146:GLY:CA	1:A:153:ASP:OD2	2.38	0.71
3:C:280:PRO:HG2	3:C:281:PHE:CD1	2.25	0.71
1:A:152:SER:O	1:A:155:ARG:NH1	2.22	0.71
1:A:264:ARG:CD	1:A:325:GLU:HG2	2.21	0.71
1:A:34:TYR:CD2	1:A:358:MET:HE2	2.25	0.71
1:A:65:VAL:C	1:A:67:PRO:HD3	2.09	0.71
3:C:96:LYS:HG2	3:C:127:LYS:CE	2.20	0.71
3:C:194:ILE:HB	3:C:269:ILE:HD11	1.73	0.71
1:A:96:LEU:HB2	1:A:297:ILE:CG1	2.21	0.71
2:B:261:ARG:NH2	3:C:191:GLY:O	2.23	0.71
3:C:154:SER:N	3:C:157:LEU:HD22	2.06	0.71
1:A:104:ASN:OD1	1:A:134:ARG:NH1	2.23	0.71
3:C:154:SER:HB3	3:C:157:LEU:HD22	1.73	0.71
3:C:41:ILE:HD13	3:C:41:ILE:N	2.03	0.70
1:A:117:PHE:HE2	1:A:193:ILE:HG12	1.56	0.70
3:C:11:SER:HA	3:C:218:THR:HA	1.71	0.70
3:C:165:LYS:N	3:C:165:LYS:HD2	2.04	0.70
3:C:236:ALA:CB	3:C:238:LEU:HD22	2.22	0.70
1:A:18:GLU:O	1:A:35:PHE:CE1	2.44	0.70
1:A:293:ARG:HD3	1:A:297:ILE:HG23	1.73	0.70
3:C:25:ASP:OD2	3:C:209:SER:CA	2.39	0.70
3:C:150:LYS:HE2	3:C:183:GLU:OE2	1.92	0.70
2:B:239:ASN:O	2:B:239:ASN:ND2	2.25	0.70
2:B:194:GLN:HA	2:B:194:GLN:NE2	2.05	0.70
3:C:46:VAL:HG22	3:C:99:THR:HB	1.74	0.70
3:C:167:LYS:HG2	3:C:178:THR:HB	1.74	0.70
3:C:176:VAL:C	3:C:177:LEU:HD12	2.12	0.70
3:C:167:LYS:CA	3:C:181:LEU:HD21	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:THR:HG22	2:B:87:LEU:CD1	2.22	0.70
2:B:139:THR:CG2	2:B:155:PHE:CB	2.68	0.70
1:A:43:LEU:CD1	1:A:62:ILE:HG12	2.21	0.70
2:B:49:ILE:HG13	2:B:79:VAL:HG11	1.73	0.70
3:C:35:TYR:CE2	3:C:39:GLU:HG3	2.27	0.70
2:B:101:VAL:HG22	2:B:128:ALA:HA	1.73	0.69
3:C:36:ALA:CA	3:C:42:ILE:HD11	2.21	0.69
3:C:111:LYS:O	3:C:115:TYR:N	2.23	0.69
3:C:216:TRP:HH2	3:C:240:GLU:HG3	1.55	0.69
1:A:4:ARG:HA	1:A:21:MET:O	1.92	0.69
1:A:84:ILE:HD13	1:A:311:PHE:HB2	1.70	0.69
3:C:36:ALA:C	3:C:42:ILE:HD11	2.13	0.69
3:C:47:VAL:HG21	3:C:71:ALA:CB	2.22	0.69
3:C:30:THR:OG1	3:C:72:ALA:CB	2.40	0.69
3:C:158:VAL:O	3:C:158:VAL:HG23	1.92	0.69
1:A:88:LYS:HB2	1:A:88:LYS:HZ2	1.57	0.69
1:A:116:ASP:OD1	1:A:116:ASP:N	2.26	0.69
1:A:8:SER:HG	1:A:18:GLU:HB2	1.56	0.69
1:A:43:LEU:HD21	2:B:138:PHE:HZ	1.58	0.69
1:A:308:ARG:HG3	1:A:308:ARG:NH1	2.02	0.69
2:B:128:ALA:O	2:B:167:ALA:HA	1.93	0.69
3:C:102:ILE:CG2	3:C:103:PRO:HD2	2.21	0.69
3:C:134:CYS:SG	7:C:1282:SF4:FE4	1.83	0.69
3:C:168:PHE:CB	3:C:179:LEU:CD1	2.67	0.69
3:C:177:LEU:HD12	3:C:177:LEU:N	2.05	0.69
3:C:218:THR:HG23	3:C:218:THR:O	1.93	0.69
3:C:251:LEU:HD13	3:C:252:GLY:H	1.57	0.69
1:A:44:GLU:H	2:B:146:GLN:NE2	1.90	0.69
1:A:68:ILE:CD1	1:A:101:HIS:HD2	1.98	0.69
1:A:79:ASP:OD1	1:A:80:ASP:N	2.26	0.69
1:A:246:CYS:SG	1:A:385:THR:HG22	2.31	0.69
1:A:319:LEU:HB3	1:A:336:LYS:CD	2.22	0.69
2:B:129:PHE:CD2	2:B:178:ILE:HD11	2.27	0.69
1:A:65:VAL:O	1:A:101:HIS:CE1	2.46	0.69
1:A:214:GLN:O	1:A:215:ILE:HD12	1.93	0.69
1:A:221:LYS:HB3	1:A:221:LYS:HZ3	1.58	0.69
1:A:117:PHE:CE2	1:A:193:ILE:HG12	2.28	0.69
1:A:326:ALA:HB3	1:A:350:PRO:HG2	1.74	0.69
1:A:165:GLU:OE1	1:A:168:ARG:NH1	2.25	0.68
1:A:295:ILE:HD12	1:A:295:ILE:C	2.14	0.68
2:B:98:LEU:CD1	2:B:185:LEU:CD2	2.71	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:ASP:O	2:B:213:LYS:HB2	1.92	0.68
3:C:244:ILE:HG13	3:C:251:LEU:HB3	1.74	0.68
1:A:289:THR:HG23	1:A:290:ALA:N	2.09	0.68
1:A:327:PRO:CD	1:A:328:ARG:H	2.03	0.68
3:C:157:LEU:N	3:C:157:LEU:HD13	2.09	0.68
2:B:192:TYR:HD1	2:B:193:LEU:HD22	1.58	0.68
3:C:9:ILE:HD11	3:C:220:ILE:HD13	1.75	0.68
1:A:202:LEU:HA	1:A:365:PHE:CZ	2.28	0.68
1:A:255:ARG:NH1	1:A:255:ARG:HG2	2.08	0.68
3:C:39:GLU:CB	3:C:41:ILE:HD11	2.24	0.68
3:C:133:TYR:CE2	3:C:208:GLY:HA3	2.27	0.68
2:B:210:LEU:O	2:B:214:VAL:HG12	1.93	0.68
3:C:45:ALA:HA	3:C:98:GLY:O	1.94	0.68
3:C:220:ILE:HG12	3:C:222:ARG:NH1	2.09	0.68
1:A:46:MET:HE2	2:B:142:SER:N	2.09	0.68
1:A:172:TYR:CE1	1:A:176:LYS:HG3	2.16	0.68
3:C:221:THR:HG21	3:C:227:ASP:CA	2.24	0.68
1:A:43:LEU:CD1	1:A:62:ILE:CG1	2.71	0.68
1:A:66:CYS:O	1:A:69:PRO:HG2	1.94	0.68
2:B:193:LEU:N	2:B:193:LEU:HD23	2.07	0.68
3:C:266:GLU:HG3	3:C:267:LYS:N	2.07	0.68
1:A:297:ILE:HD12	1:A:297:ILE:C	2.15	0.68
1:A:349:VAL:HG12	1:A:350:PRO:HD3	1.75	0.68
2:B:232:THR:HG22	2:B:248:ARG:HG2	1.74	0.68
2:B:260:PRO:CG	3:C:108:GLY:CA	2.71	0.68
3:C:111:LYS:HA	3:C:114:THR:HG22	1.75	0.68
3:C:4:GLY:HA3	3:C:201:GLU:HG3	1.75	0.67
3:C:7:LYS:NZ	3:C:224:ASP:CG	2.47	0.67
3:C:9:ILE:HD11	3:C:220:ILE:CD1	2.24	0.67
1:A:70:HIS:CE1	1:A:349:VAL:HG13	2.23	0.67
1:A:96:LEU:C	1:A:96:LEU:HD13	2.15	0.67
2:B:52:ILE:N	2:B:100:LEU:O	2.26	0.67
2:B:125:LEU:CD2	2:B:165:ASP:CB	2.63	0.67
1:A:107:ALA:CB	1:A:133:ILE:HD11	2.22	0.67
1:A:328:ARG:NH1	1:A:380:CYS:HB3	2.10	0.67
2:B:192:TYR:HD1	2:B:193:LEU:CD2	2.08	0.67
2:B:235:LEU:CD1	7:B:1275:SF4:S2	2.82	0.67
1:A:119:PRO:HG2	1:A:122:LEU:HB2	1.76	0.67
1:A:82:LEU:O	1:A:83:ASP:HB2	1.94	0.67
3:C:6:TYR:HB3	3:C:220:ILE:HD11	1.76	0.67
3:C:253:LEU:HD13	3:C:253:LEU:C	2.15	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:62:ALA:HB2	3:C:67:GLU:HG2	1.76	0.67
3:C:233:ALA:O	3:C:236:ALA:HB3	1.94	0.67
3:C:254:LEU:HD12	3:C:254:LEU:C	2.15	0.67
1:A:246:CYS:HG	1:A:385:THR:CG2	2.05	0.67
2:B:186:LEU:HD13	2:B:186:LEU:C	2.15	0.67
3:C:47:VAL:CG2	3:C:71:ALA:CB	2.73	0.67
1:A:155:ARG:HD3	2:B:248:ARG:HH22	1.60	0.67
3:C:64:SER:OG	3:C:67:GLU:HB2	1.95	0.67
2:B:83:TYR:H	2:B:90:LEU:HD21	1.59	0.66
2:B:125:LEU:HD23	2:B:126:VAL:N	2.10	0.66
2:B:221:ILE:HG21	7:C:1282:SF4:S4	2.35	0.66
3:C:90:ARG:HB3	3:C:91:GLN:HE22	1.60	0.66
1:A:28:ILE:CG2	1:A:364:GLY:O	2.32	0.66
1:A:121:ASN:HD22	1:A:121:ASN:N	1.94	0.66
1:A:133:ILE:HD12	1:A:133:ILE:C	2.14	0.66
1:A:319:LEU:HA	1:A:336:LYS:HG2	1.78	0.66
2:B:51:TYR:HA	2:B:100:LEU:O	1.95	0.66
3:C:45:ALA:CB	3:C:98:GLY:O	2.43	0.66
3:C:133:TYR:CD1	3:C:199:VAL:HA	2.30	0.66
1:A:127:ILE:CD1	2:B:72:ALA:HA	2.26	0.66
1:A:291:LEU:HD23	1:A:291:LEU:C	2.16	0.66
1:A:145:ALA:C	1:A:153:ASP:HB2	2.15	0.66
1:A:349:VAL:CG2	1:A:383:CYS:O	2.43	0.66
2:B:131:SER:OG	2:B:252:CYS:O	2.14	0.66
1:A:275:GLY:N	1:A:278:ALA:HB3	2.10	0.66
2:B:237:MET:HB2	3:C:83:MET:HE1	1.78	0.66
2:B:264:TRP:CH2	3:C:107:MET:O	2.48	0.66
1:A:166:LEU:CD1	3:C:43:GLU:OE2	2.44	0.66
2:B:83:TYR:HA	2:B:90:LEU:CD2	2.26	0.66
2:B:244:LEU:C	2:B:244:LEU:HD22	2.15	0.66
3:C:147:ILE:HD12	3:C:155:MET:SD	2.36	0.66
1:A:276:VAL:HG21	1:A:373:VAL:HA	1.78	0.66
2:B:119:LEU:HD13	2:B:119:LEU:C	2.15	0.66
3:C:167:LYS:C	3:C:181:LEU:HD21	2.16	0.66
1:A:41:ARG:HG3	1:A:41:ARG:NH1	2.04	0.65
1:A:43:LEU:HD11	1:A:62:ILE:CA	2.27	0.65
1:A:131:SER:HB3	2:B:68:TYR:HB3	1.79	0.65
3:C:3:LEU:HD13	3:C:3:LEU:N	2.11	0.65
3:C:36:ALA:O	3:C:40:GLY:N	2.28	0.65
3:C:133:TYR:OH	3:C:220:ILE:HG21	1.96	0.65
3:C:133:TYR:CE1	3:C:199:VAL:HG23	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:MET:CE	2:B:142:SER:CB	2.74	0.65
1:A:240:GLU:O	1:A:244:ARG:HG3	1.96	0.65
2:B:83:TYR:O	2:B:83:TYR:CD2	2.48	0.65
3:C:167:LYS:N	3:C:181:LEU:CD2	2.60	0.65
1:A:9:PRO:HG2	2:B:85:GLN:HG3	1.78	0.65
1:A:73:ALA:CA	1:A:324:ILE:HD12	2.26	0.65
1:A:127:ILE:HD13	1:A:127:ILE:C	2.15	0.65
1:A:255:ARG:HG2	1:A:255:ARG:HH11	1.61	0.65
1:A:265:MET:HE2	1:A:269:GLN:CG	2.27	0.65
2:B:264:TRP:CZ2	2:B:268:GLN:NE2	2.65	0.65
1:A:183:ASN:O	1:A:186:VAL:HG22	1.96	0.65
1:A:199:PRO:HD3	1:A:369:TYR:HE2	1.52	0.65
1:A:249:ILE:CG2	1:A:356:PRO:CG	2.74	0.65
2:B:52:ILE:O	2:B:101:VAL:HA	1.96	0.65
3:C:23:ALA:CB	3:C:27:GLY:CA	2.75	0.65
1:A:178:LEU:HD12	1:A:178:LEU:O	1.96	0.65
1:A:201:GLY:C	1:A:365:PHE:CZ	2.69	0.65
3:C:85:LEU:CD2	3:C:99:THR:HG21	2.22	0.65
3:C:42:ILE:HG22	3:C:98:GLY:N	2.12	0.65
1:A:265:MET:CE	1:A:269:GLN:CG	2.75	0.65
2:B:271:LYS:HG3	2:B:272:GLU:N	2.12	0.65
3:C:77:THR:HG22	3:C:78:PHE:N	2.12	0.65
3:C:92:TYR:O	3:C:94:ILE:HG13	1.97	0.65
1:A:202:LEU:HD22	1:A:373:VAL:HG22	1.78	0.65
3:C:171:TYR:CD1	3:C:176:VAL:HG12	2.31	0.65
1:A:14:GLU:OE2	1:A:65:VAL:HG23	1.96	0.65
1:A:43:LEU:CD2	2:B:138:PHE:CZ	2.80	0.65
1:A:155:ARG:HD3	2:B:248:ARG:NH2	2.12	0.65
2:B:89:ASP:N	2:B:89:ASP:OD1	2.27	0.65
2:B:241:ARG:HG3	2:B:241:ARG:HH11	1.61	0.65
1:A:96:LEU:HB2	1:A:297:ILE:HG12	1.77	0.64
1:A:162:ASN:HB2	1:A:307:VAL:CG2	2.27	0.64
1:A:191:GLY:HA2	1:A:194:GLU:OE1	1.96	0.64
3:C:4:GLY:O	3:C:6:TYR:HD1	1.78	0.64
3:C:17:ARG:HB3	3:C:17:ARG:NH1	2.13	0.64
1:A:369:TYR:O	1:A:372:HIS:HB2	1.96	0.64
2:B:144:GLY:HA3	2:B:153:GLU:HB2	1.77	0.64
3:C:28:ILE:HG13	3:C:239:PHE:CD2	2.30	0.64
3:C:167:LYS:CG	3:C:178:THR:HB	2.27	0.64
1:A:98:LEU:HD12	1:A:216:TYR:HD1	1.62	0.64
1:A:162:ASN:HB2	1:A:307:VAL:HG22	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLN:CD	1:A:256:ASN:ND2	2.50	0.64
1:A:227:PHE:CZ	1:A:348:LEU:CD1	2.80	0.64
3:C:154:SER:HB3	3:C:157:LEU:CD2	2.28	0.64
1:A:293:ARG:HD2	1:A:297:ILE:CG2	2.27	0.64
1:A:354:ASN:HD22	1:A:354:ASN:N	1.95	0.64
2:B:127:CYS:CB	2:B:166:LEU:HD13	2.23	0.64
3:C:158:VAL:O	3:C:158:VAL:HG22	1.97	0.64
1:A:265:MET:HE2	1:A:269:GLN:HG3	1.79	0.64
3:C:179:LEU:HD12	3:C:179:LEU:N	2.13	0.64
1:A:293:ARG:O	1:A:297:ILE:HG23	1.97	0.64
1:A:70:HIS:CE1	1:A:349:VAL:HG11	2.31	0.64
1:A:262:ARG:HH11	1:A:262:ARG:CG	2.10	0.64
1:A:366:HIS:O	1:A:369:TYR:HB2	1.97	0.64
3:C:111:LYS:O	3:C:114:THR:CG2	2.42	0.64
1:A:46:MET:HE3	2:B:142:SER:HA	1.79	0.64
1:A:190:ILE:CD1	1:A:285:LEU:HD21	2.22	0.64
3:C:36:ALA:C	3:C:42:ILE:CD1	2.66	0.64
3:C:167:LYS:N	3:C:181:LEU:HD21	2.11	0.64
1:A:19:LEU:HD22	1:A:374:ILE:HD12	1.79	0.64
1:A:41:ARG:HH11	1:A:41:ARG:CG	2.08	0.64
2:B:168:LEU:HD12	2:B:168:LEU:C	2.18	0.64
1:A:231:MET:HE1	1:A:248:THR:CG2	2.25	0.64
2:B:49:ILE:CD1	2:B:98:LEU:CD2	2.63	0.64
1:A:168:ARG:HG2	1:A:168:ARG:HH11	1.63	0.63
2:B:93:MET:HG3	2:B:122:LYS:CG	2.19	0.63
1:A:62:ILE:HG23	1:A:70:HIS:HD2	1.58	0.63
3:C:221:THR:CG2	3:C:227:ASP:HB2	2.28	0.63
2:B:241:ARG:HH11	2:B:241:ARG:CG	2.12	0.63
1:A:214:GLN:C	1:A:215:ILE:HD12	2.19	0.63
1:A:329:GLY:O	1:A:350:PRO:HG3	1.99	0.63
1:A:34:TYR:CE2	1:A:358:MET:HE1	2.34	0.63
1:A:43:LEU:HD11	1:A:62:ILE:CB	2.29	0.63
1:A:57:VAL:HG21	2:B:248:ARG:NH1	2.12	0.63
2:B:266:GLU:OE1	2:B:266:GLU:HA	1.98	0.63
3:C:53:GLU:HA	3:C:53:GLU:OE1	1.97	0.63
1:A:244:ARG:HH11	1:A:244:ARG:CG	2.10	0.63
1:A:65:VAL:O	1:A:67:PRO:HD2	1.98	0.62
2:B:58:THR:O	2:B:58:THR:CG2	2.45	0.62
2:B:203:THR:HG22	2:B:204:GLU:N	2.14	0.62
3:C:236:ALA:HB1	3:C:238:LEU:HD22	1.81	0.62
3:C:246:GLU:OE2	3:C:247:VAL:HG12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:MET:HE3	2:B:142:SER:CB	2.29	0.62
2:B:89:ASP:O	2:B:91:TRP:HZ3	1.80	0.62
3:C:111:LYS:C	3:C:114:THR:HG22	2.18	0.62
3:C:129:LEU:HD12	3:C:129:LEU:C	2.20	0.62
2:B:139:THR:HG21	2:B:155:PHE:HB3	1.81	0.62
2:B:235:LEU:HD12	2:B:244:LEU:HB2	1.80	0.62
3:C:42:ILE:HG21	3:C:98:GLY:HA3	1.80	0.62
3:C:55:TRP:NE1	3:C:158:VAL:O	2.26	0.62
3:C:17:ARG:HG3	3:C:17:ARG:HH11	1.64	0.62
3:C:167:LYS:HA	3:C:181:LEU:CD2	2.28	0.62
1:A:89:ALA:HB2	1:A:305:ALA:HB3	1.81	0.62
1:A:219:ARG:HB3	1:A:219:ARG:CZ	2.29	0.62
1:A:258:GLU:HG3	1:A:377:TYR:CE2	2.33	0.62
1:A:326:ALA:HB1	1:A:327:PRO:CD	2.27	0.62
3:C:135:MET:HG2	3:C:198:TYR:HE1	1.65	0.62
1:A:46:MET:CE	2:B:142:SER:N	2.61	0.62
1:A:257:VAL:HG11	1:A:353:TRP:HE3	1.55	0.62
1:A:330:LEU:HG	1:A:331:ASP:N	2.14	0.62
1:A:349:VAL:HG12	1:A:350:PRO:CD	2.30	0.62
3:C:180:PRO:O	3:C:183:GLU:HB3	1.99	0.62
1:A:8:SER:O	2:B:91:TRP:HD1	1.83	0.62
1:A:18:GLU:CG	1:A:35:PHE:HZ	2.08	0.62
1:A:127:ILE:HD11	2:B:71:LEU:HD13	1.81	0.62
1:A:149:ILE:HD13	1:A:149:ILE:H	1.64	0.62
2:B:90:LEU:O	2:B:90:LEU:HD23	1.99	0.62
2:B:232:THR:O	2:B:233:ARG:HB2	1.99	0.62
3:C:212:SER:OG	3:C:218:THR:HB	1.99	0.62
1:A:184:GLU:OE2	1:A:188:LEU:HD23	1.99	0.61
2:B:53:HIS:HB2	2:B:102:GLU:CB	2.29	0.61
2:B:93:MET:HB2	2:B:96:MET:CE	2.30	0.61
2:B:248:ARG:O	2:B:248:ARG:HG2	2.00	0.61
1:A:262:ARG:HH11	1:A:262:ARG:HG3	1.65	0.61
2:B:206:CYS:HB3	2:B:208:CYS:H	1.63	0.61
3:C:7:LYS:HZ1	3:C:224:ASP:CG	2.03	0.61
1:A:128:ASN:OD1	2:B:72:ALA:HB3	2.00	0.61
1:A:276:VAL:HG22	1:A:376:ALA:CB	2.31	0.61
2:B:180:LYS:O	2:B:183:VAL:HG12	2.00	0.61
2:B:268:GLN:HG2	2:B:269:ILE:N	2.15	0.61
1:A:14:GLU:CD	1:A:65:VAL:HG21	2.21	0.61
1:A:65:VAL:O	1:A:101:HIS:HE1	1.83	0.61
1:A:84:ILE:HG21	1:A:311:PHE:HB3	1.78	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:LEU:HD12	2:B:210:LEU:C	2.18	0.61
3:C:168:PHE:CB	3:C:179:LEU:HD11	2.29	0.61
1:A:43:LEU:HD11	1:A:62:ILE:HG12	1.82	0.61
1:A:293:ARG:HD3	1:A:297:ILE:CG2	2.29	0.61
3:C:42:ILE:HG21	3:C:98:GLY:N	2.16	0.61
3:C:147:ILE:HD13	3:C:158:VAL:HG11	1.82	0.61
1:A:43:LEU:HD12	1:A:62:ILE:CG1	2.31	0.61
1:A:174:ARG:HG2	1:A:174:ARG:HH11	1.66	0.61
1:A:263:ALA:O	1:A:267:GLU:HG2	2.01	0.61
1:A:310:ASP:OD1	1:A:311:PHE:N	2.34	0.61
1:A:79:ASP:O	1:A:83:ASP:N	2.34	0.61
3:C:248:LYS:HG3	3:C:249:PRO:CA	2.31	0.61
1:A:178:LEU:HD11	1:A:182:VAL:HG23	1.82	0.61
2:B:66:GLU:HB2	2:B:175:PRO:HB3	1.82	0.61
2:B:209:ASP:O	2:B:213:LYS:N	2.21	0.61
1:A:139:TYR:CD2	1:A:174:ARG:HD2	2.35	0.61
1:A:215:ILE:HG22	1:A:216:TYR:N	2.13	0.61
2:B:98:LEU:HD13	2:B:185:LEU:CD2	2.25	0.61
3:C:132:ILE:HG22	9:C:1283:FAD:C1'	2.30	0.61
1:A:62:ILE:HD13	1:A:62:ILE:C	2.20	0.60
1:A:71:THR:HG21	1:A:154:VAL:HG13	1.80	0.60
2:B:186:LEU:HD13	2:B:187:ASN:N	2.17	0.60
2:B:237:MET:HB2	3:C:83:MET:CE	2.31	0.60
1:A:29:VAL:HG13	1:A:363:GLU:HA	1.82	0.60
1:A:143:MET:CE	1:A:171:LEU:CG	2.76	0.60
3:C:17:ARG:HH11	3:C:17:ARG:CG	2.14	0.60
1:A:33:ARG:CG	1:A:33:ARG:HH11	2.14	0.60
1:A:41:ARG:NH2	1:A:62:ILE:O	2.33	0.60
1:A:255:ARG:HH11	1:A:255:ARG:CG	2.14	0.60
3:C:28:ILE:HG21	3:C:207:THR:HG23	1.83	0.60
1:A:233:GLU:HA	1:A:242:ALA:HB1	1.82	0.60
1:A:256:ASN:HD22	1:A:256:ASN:N	1.99	0.60
3:C:106:THR:HG23	3:C:202:LEU:HB2	1.82	0.60
1:A:14:GLU:CG	2:B:58:THR:HG21	2.32	0.60
1:A:19:LEU:HD13	1:A:374:ILE:CD1	2.30	0.60
2:B:237:MET:HE3	3:C:80:PRO:HG2	1.83	0.60
3:C:221:THR:HG21	3:C:227:ASP:HA	1.83	0.60
2:B:74:LEU:HA	2:B:78:MET:HB2	1.83	0.60
3:C:211:GLY:HA2	3:C:249:PRO:HG2	1.83	0.60
3:C:226:GLY:O	3:C:229:ILE:CG2	2.46	0.60
1:A:313:GLU:H	1:A:313:GLU:CD	1.96	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:TYR:HE1	2:B:91:TRP:O	1.84	0.60
3:C:128:LEU:O	3:C:128:LEU:HG	2.02	0.60
1:A:240:GLU:HG3	1:A:241:ILE:N	2.15	0.60
3:C:7:LYS:HE3	3:C:224:ASP:HB2	1.82	0.60
3:C:162:ASP:OD1	3:C:163:ILE:N	2.35	0.60
3:C:216:TRP:CH2	3:C:240:GLU:HG2	2.36	0.60
1:A:174:ARG:HH11	1:A:174:ARG:CG	2.15	0.60
1:A:219:ARG:HG3	1:A:219:ARG:HH11	1.67	0.60
1:A:291:LEU:O	1:A:294:ALA:HB3	2.02	0.60
2:B:70:ILE:HG23	2:B:78:MET:CE	2.32	0.60
2:B:136:GLY:O	2:B:139:THR:HB	2.02	0.60
3:C:146:PHE:HA	3:C:150:LYS:HG2	1.83	0.60
3:C:163:ILE:CG2	3:C:181:LEU:HD11	2.32	0.60
1:A:199:PRO:CG	1:A:369:TYR:CE2	2.84	0.59
2:B:237:MET:CG	3:C:83:MET:CE	2.78	0.59
1:A:219:ARG:HH11	1:A:219:ARG:CG	2.14	0.59
3:C:9:ILE:HD13	3:C:220:ILE:CB	2.17	0.59
3:C:92:TYR:HD1	3:C:92:TYR:H	1.45	0.59
1:A:201:GLY:O	1:A:204:VAL:HG22	2.02	0.59
2:B:46:LYS:HG3	2:B:47:PRO:N	2.17	0.59
2:B:192:TYR:CD1	2:B:193:LEU:CD2	2.85	0.59
1:A:71:THR:HG22	1:A:154:VAL:HG11	1.78	0.59
1:A:46:MET:HE3	2:B:142:SER:CA	2.32	0.59
1:A:262:ARG:HG3	1:A:262:ARG:NH1	2.17	0.59
1:A:327:PRO:CD	1:A:328:ARG:N	2.62	0.59
3:C:55:TRP:HE1	3:C:158:VAL:HG22	1.67	0.59
1:A:55:ALA:O	1:A:59:VAL:HG23	2.03	0.59
3:C:273:LYS:HE3	3:C:279:THR:HB	1.84	0.59
2:B:70:ILE:HG22	2:B:74:LEU:HB2	1.84	0.59
2:B:71:LEU:HD22	2:B:71:LEU:C	2.22	0.59
2:B:125:LEU:HD23	2:B:165:ASP:HB2	1.80	0.59
3:C:32:LEU:HD12	3:C:32:LEU:C	2.23	0.59
3:C:66:ASP:OD1	3:C:66:ASP:N	2.24	0.59
3:C:169:TRP:NE1	3:C:178:THR:HG21	2.17	0.59
3:C:281:PHE:HD1	3:C:281:PHE:N	2.00	0.59
1:A:118:VAL:HG23	1:A:123:MET:HG3	1.84	0.59
3:C:101:ALA:HB3	3:C:129:LEU:HD11	1.85	0.59
3:C:111:LYS:CA	3:C:114:THR:HG22	2.32	0.59
1:A:201:GLY:C	1:A:365:PHE:HZ	2.06	0.58
1:A:145:ALA:O	1:A:153:ASP:HB2	2.02	0.58
2:B:106:CYS:HB2	2:B:155:PHE:CE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:220:ILE:HG12	3:C:222:ARG:HH11	1.66	0.58
1:A:119:PRO:CB	1:A:121:ASN:HD21	2.13	0.58
1:A:147:GLU:OE2	3:C:120:ARG:HG3	2.03	0.58
2:B:128:ALA:HB1	2:B:133:ALA:HB1	1.86	0.58
1:A:14:GLU:OE2	1:A:65:VAL:CG2	2.51	0.58
1:A:43:LEU:HD12	1:A:62:ILE:HG12	1.85	0.58
1:A:73:ALA:HB2	1:A:324:ILE:HD12	1.78	0.58
2:B:88:VAL:HG12	2:B:89:ASP:N	2.19	0.58
3:C:41:ILE:HD13	3:C:41:ILE:H	1.67	0.58
3:C:42:ILE:HG21	3:C:98:GLY:CA	2.34	0.58
3:C:147:ILE:HD12	3:C:155:MET:CE	2.33	0.58
3:C:158:VAL:HG21	3:C:161:MET:CE	2.33	0.58
1:A:43:LEU:HD22	2:B:138:PHE:HE2	1.66	0.58
2:B:195:PRO:CG	3:C:115:TYR:CE2	2.56	0.58
3:C:253:LEU:HD22	3:C:253:LEU:C	2.24	0.58
1:A:262:ARG:O	1:A:266:VAL:HG23	2.04	0.58
3:C:35:TYR:CZ	3:C:39:GLU:HG2	2.37	0.58
1:A:70:HIS:NE2	1:A:383:CYS:SG	2.76	0.58
3:C:35:TYR:CE2	3:C:39:GLU:CG	2.87	0.58
1:A:4:ARG:HB2	1:A:21:MET:O	2.04	0.58
1:A:96:LEU:HD13	1:A:97:THR:N	2.19	0.58
2:B:168:LEU:O	2:B:168:LEU:CD1	2.43	0.58
3:C:92:TYR:CD1	3:C:92:TYR:N	2.72	0.58
1:A:12:ARG:HB3	1:A:375:ARG:HD2	1.84	0.58
1:A:329:GLY:O	1:A:350:PRO:CG	2.51	0.58
2:B:83:TYR:N	2:B:90:LEU:HD21	2.19	0.58
2:B:237:MET:HE2	3:C:80:PRO:HB3	1.81	0.58
3:C:102:ILE:H	3:C:105:GLN:HG3	1.68	0.58
1:A:210:LEU:HD23	1:A:330:LEU:CD2	2.32	0.58
1:A:319:LEU:HB3	1:A:336:LYS:HD3	1.85	0.58
3:C:106:THR:CG2	3:C:202:LEU:HB2	2.33	0.58
1:A:36:SER:HB3	1:A:381:LEU:HD12	1.85	0.57
1:A:139:TYR:CE2	1:A:174:ARG:NE	2.72	0.57
1:A:189:MET:O	1:A:193:ILE:CD1	2.50	0.57
1:A:231:MET:HE1	1:A:248:THR:HG21	1.86	0.57
2:B:230:CYS:SG	2:B:233:ARG:N	2.77	0.57
1:A:14:GLU:HG3	2:B:58:THR:HG21	1.86	0.57
1:A:62:ILE:HG12	1:A:386:HIS:CB	2.34	0.57
2:B:53:HIS:HB2	2:B:102:GLU:HB3	1.85	0.57
1:A:33:ARG:NH1	1:A:33:ARG:HG2	2.19	0.57
1:A:109:HIS:CD2	1:A:378:ASP:HB2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:LEU:O	1:A:192:LEU:HG	2.03	0.57
1:A:199:PRO:HD2	1:A:369:TYR:CZ	2.38	0.57
3:C:18:GLU:N	3:C:18:GLU:OE1	2.37	0.57
3:C:53:GLU:HB3	3:C:56:LYS:HB2	1.87	0.57
1:A:207:GLN:CD	1:A:256:ASN:HD21	2.07	0.57
3:C:244:ILE:HG23	3:C:245:GLU:N	2.19	0.57
1:A:84:ILE:HG21	1:A:311:PHE:HD2	1.68	0.57
1:A:229:GLU:OE2	1:A:248:THR:OG1	2.22	0.57
3:C:29:VAL:HG21	3:C:132:ILE:CD1	2.34	0.57
3:C:36:ALA:HB1	3:C:42:ILE:CG1	2.35	0.57
1:A:96:LEU:HD11	1:A:144:VAL:CG1	2.13	0.57
3:C:114:THR:CG2	3:C:115:TYR:CD1	2.63	0.57
1:A:43:LEU:HD22	2:B:138:PHE:CE2	2.38	0.57
1:A:109:HIS:CG	1:A:378:ASP:OD2	2.58	0.57
1:A:208:PRO:CD	1:A:255:ARG:NH1	2.68	0.57
2:B:239:ASN:N	2:B:239:ASN:HD22	2.00	0.57
3:C:135:MET:HG2	3:C:198:TYR:CE1	2.40	0.57
1:A:62:ILE:HG13	1:A:386:HIS:HB3	1.85	0.57
1:A:293:ARG:CD	1:A:297:ILE:HG22	2.35	0.57
2:B:91:TRP:HE3	2:B:91:TRP:N	2.03	0.57
1:A:212:SER:O	1:A:268:PHE:CZ	2.58	0.57
1:A:231:MET:HE1	1:A:248:THR:HB	1.87	0.57
3:C:35:TYR:CZ	3:C:39:GLU:HG3	2.39	0.57
3:C:121:PHE:O	3:C:125:LYS:HD2	2.04	0.57
3:C:163:ILE:HG21	3:C:181:LEU:HD11	1.85	0.57
3:C:236:ALA:HB3	3:C:238:LEU:HD22	1.86	0.56
1:A:57:VAL:CG2	2:B:248:ARG:HH11	2.16	0.56
1:A:68:ILE:CD1	1:A:101:HIS:CD2	2.78	0.56
1:A:156:ILE:HG22	1:A:311:PHE:CE2	2.40	0.56
2:B:91:TRP:N	2:B:91:TRP:CE3	2.73	0.56
3:C:36:ALA:CB	3:C:42:ILE:CG1	2.83	0.56
3:C:103:PRO:CG	7:C:1282:SF4:S3	2.81	0.56
3:C:132:ILE:HG21	9:C:1283:FAD:H1'1	1.87	0.56
1:A:35:PHE:CD1	1:A:35:PHE:N	2.73	0.56
1:A:76:GLU:O	1:A:79:ASP:OD1	2.23	0.56
1:A:265:MET:CE	1:A:269:GLN:CD	2.73	0.56
2:B:51:TYR:HB2	2:B:100:LEU:HB2	1.85	0.56
3:C:133:TYR:OH	3:C:220:ILE:HG22	2.03	0.56
3:C:227:ASP:OD1	3:C:231:LYS:HE3	2.04	0.56
3:C:281:PHE:CD1	3:C:281:PHE:N	2.73	0.56
1:A:199:PRO:HD3	1:A:369:TYR:OH	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:TYR:HA	2:B:90:LEU:HD21	1.86	0.56
2:B:131:SER:HB3	2:B:137:CYS:HB2	1.87	0.56
3:C:47:VAL:HG23	3:C:47:VAL:O	2.05	0.56
3:C:28:ILE:HD11	3:C:230:PHE:CE1	2.40	0.56
3:C:90:ARG:C	3:C:91:GLN:HE21	2.08	0.56
3:C:91:GLN:HE21	3:C:91:GLN:CA	2.17	0.56
3:C:133:TYR:HE1	3:C:199:VAL:HG23	1.68	0.56
2:B:187:ASN:C	2:B:188:ASN:HD22	2.09	0.56
3:C:187:TYR:CD1	3:C:187:TYR:N	2.73	0.56
1:A:82:LEU:HB3	1:A:84:ILE:HD11	1.88	0.56
1:A:109:HIS:CD2	1:A:378:ASP:CB	2.89	0.56
1:A:215:ILE:O	1:A:325:GLU:HB2	2.06	0.56
1:A:381:LEU:N	1:A:381:LEU:HD22	2.21	0.56
3:C:239:PHE:N	3:C:239:PHE:CD1	2.73	0.56
1:A:89:ALA:HB2	1:A:302:ASP:OD2	2.04	0.56
3:C:62:ALA:CB	3:C:67:GLU:HG2	2.35	0.56
1:A:66:CYS:HB2	1:A:69:PRO:HG3	1.87	0.56
1:A:351:THR:CG2	1:A:384:ALA:HB2	2.36	0.56
2:B:264:TRP:HH2	3:C:107:MET:O	1.89	0.56
3:C:138:PHE:CD1	3:C:138:PHE:N	2.74	0.56
1:A:256:ASN:ND2	1:A:256:ASN:N	2.53	0.56
2:B:196:MET:HG3	3:C:117:PHE:HZ	1.71	0.56
3:C:36:ALA:HB1	3:C:42:ILE:HG13	1.87	0.56
3:C:37:LEU:HD23	3:C:42:ILE:CD1	2.28	0.56
3:C:46:VAL:HG12	3:C:61:VAL:HB	1.88	0.56
1:A:34:TYR:CD2	1:A:358:MET:CE	2.86	0.55
1:A:71:THR:CG2	1:A:154:VAL:HG13	2.33	0.55
2:B:192:TYR:CD1	2:B:193:LEU:HD22	2.40	0.55
2:B:214:VAL:HG23	2:B:219:LEU:CB	2.36	0.55
1:A:246:CYS:HG	1:A:385:THR:HG22	1.66	0.55
2:B:101:VAL:HG23	2:B:133:ALA:CB	2.36	0.55
2:B:86:THR:HG22	2:B:87:LEU:HD13	1.89	0.55
1:A:62:ILE:CD1	1:A:383:CYS:HA	2.36	0.55
1:A:143:MET:HE3	1:A:171:LEU:CD2	2.37	0.55
2:B:66:GLU:O	2:B:68:TYR:CD1	2.59	0.55
2:B:101:VAL:HG23	2:B:133:ALA:HB2	1.87	0.55
2:B:127:CYS:SG	2:B:166:LEU:HD13	2.47	0.55
1:A:68:ILE:HB	1:A:101:HIS:CD2	2.41	0.55
2:B:137:CYS:SG	2:B:138:PHE:N	2.80	0.55
1:A:138:GLN:O	1:A:141:VAL:HG12	2.07	0.55
1:A:249:ILE:HG23	1:A:356:PRO:CD	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:VAL:CG1	1:A:156:ILE:HA	2.37	0.55
1:A:300:GLU:HG3	1:A:300:GLU:O	2.06	0.55
3:C:216:TRP:CH2	3:C:240:GLU:HG3	2.36	0.55
1:A:12:ARG:NH2	1:A:116:ASP:OD1	2.39	0.55
1:A:18:GLU:CD	1:A:35:PHE:HZ	2.11	0.55
1:A:209:THR:HB	1:A:263:ALA:HB1	1.88	0.55
3:C:265:ALA:O	3:C:269:ILE:HG12	2.07	0.55
1:A:236:TYR:HB3	1:A:241:ILE:HG23	1.89	0.54
2:B:93:MET:HE3	2:B:118:GLU:CG	2.36	0.54
2:B:269:ILE:HG23	2:B:270:LYS:N	2.22	0.54
3:C:84:MET:CE	3:C:87:LYS:HD2	2.37	0.54
2:B:135:THR:HG22	2:B:135:THR:O	2.06	0.54
2:B:186:LEU:HD22	2:B:186:LEU:C	2.27	0.54
3:C:81:ASN:ND2	3:C:100:VAL:O	2.40	0.54
3:C:153:VAL:HG23	3:C:157:LEU:HD23	1.82	0.54
1:A:366:HIS:CD2	1:A:368:GLU:HG2	2.42	0.54
2:B:67:ASN:O	2:B:71:LEU:HB2	2.07	0.54
3:C:57:PRO:HB3	3:C:75:LYS:HG3	1.89	0.54
2:B:237:MET:CG	3:C:83:MET:HE3	2.33	0.54
3:C:96:LYS:HA	3:C:125:LYS:O	2.08	0.54
3:C:247:VAL:HG23	3:C:247:VAL:O	2.07	0.54
3:C:7:LYS:HE3	3:C:224:ASP:CB	2.37	0.54
3:C:45:ALA:CA	3:C:98:GLY:O	2.55	0.54
3:C:166:GLY:C	3:C:181:LEU:HD23	2.28	0.54
1:A:329:GLY:CA	1:A:350:PRO:HB3	2.38	0.54
3:C:9:ILE:HG22	3:C:244:ILE:HB	1.89	0.54
3:C:10:VAL:HG11	3:C:241:THR:HB	1.89	0.54
1:A:66:CYS:N	1:A:67:PRO:HD3	2.19	0.54
1:A:84:ILE:HG21	1:A:311:PHE:CD2	2.43	0.54
1:A:87:PRO:HG3	1:A:306:PRO:O	2.07	0.54
1:A:132:GLU:CG	1:A:181:LYS:HZ1	2.18	0.54
1:A:108:ILE:HG12	1:A:134:ARG:NH2	2.23	0.54
1:A:367:HIS:O	1:A:371:PRO:HD3	2.07	0.54
2:B:241:ARG:HH21	3:C:189:GLN:HE21	1.56	0.54
3:C:2:VAL:HG23	3:C:3:LEU:O	2.07	0.54
3:C:165:LYS:HD2	3:C:165:LYS:H	1.71	0.54
1:A:105:SER:O	1:A:108:ILE:HG22	2.07	0.54
2:B:173:PRO:HB2	2:B:178:ILE:HD12	1.90	0.54
3:C:42:ILE:HD12	3:C:42:ILE:H	1.73	0.54
3:C:101:ALA:O	3:C:131:GLY:HA2	2.07	0.54
1:A:381:LEU:O	1:A:384:ALA:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:ARG:HD3	2:B:126:VAL:HG11	1.90	0.54
3:C:45:ALA:HB1	3:C:98:GLY:O	2.08	0.54
2:B:192:TYR:HB3	2:B:193:LEU:HD23	1.90	0.53
2:B:244:LEU:HD22	2:B:245:ASN:N	2.24	0.53
3:C:4:GLY:O	3:C:222:ARG:NH2	2.40	0.53
1:A:106:HIS:HB2	1:A:287:MET:HE2	1.88	0.53
1:A:219:ARG:NH1	1:A:321:ILE:O	2.42	0.53
1:A:257:VAL:CG1	1:A:353:TRP:CE3	2.81	0.53
2:B:51:TYR:OH	2:B:61:ALA:HB2	2.08	0.53
2:B:63:SER:OG	2:B:172:PRO:CG	2.56	0.53
1:A:172:TYR:CE1	1:A:176:LYS:HG2	2.44	0.53
1:A:231:MET:CE	1:A:248:THR:CB	2.86	0.53
2:B:69:ASP:OD1	2:B:69:ASP:N	2.37	0.53
3:C:110:ARG:HG3	3:C:202:LEU:HB3	1.90	0.53
1:A:219:ARG:CZ	1:A:219:ARG:CB	2.86	0.53
2:B:221:ILE:HD12	2:B:222:GLY:N	2.24	0.53
1:A:73:ALA:HA	1:A:324:ILE:HD12	1.89	0.53
1:A:139:TYR:O	1:A:143:MET:HB2	2.09	0.53
2:B:70:ILE:HG23	2:B:78:MET:HE1	1.90	0.53
3:C:102:ILE:CG2	3:C:103:PRO:CD	2.85	0.53
3:C:103:PRO:HD2	3:C:134:CYS:HB3	1.91	0.53
1:A:76:GLU:OE1	1:A:324:ILE:CG2	2.57	0.53
1:A:249:ILE:HG21	1:A:356:PRO:HB3	1.90	0.53
1:A:293:ARG:NE	1:A:297:ILE:HG22	2.24	0.53
1:A:26:GLU:HB2	1:A:28:ILE:HD13	1.90	0.53
2:B:64:LEU:O	2:B:67:ASN:OD1	2.27	0.53
2:B:93:MET:HB2	2:B:96:MET:HE1	1.91	0.53
2:B:213:LYS:HB3	2:B:256:TYR:CE1	2.44	0.53
3:C:7:LYS:CD	3:C:227:ASP:OD2	2.48	0.53
3:C:142:SER:OG	3:C:187:TYR:CB	2.45	0.53
1:A:9:PRO:HB3	1:A:16:HIS:HB3	1.91	0.53
1:A:14:GLU:CD	1:A:65:VAL:CG2	2.77	0.53
1:A:52:PRO:HD2	1:A:340:GLY:O	2.06	0.53
1:A:54:THR:OG1	2:B:247:ASP:O	2.25	0.53
1:A:146:GLY:N	1:A:153:ASP:OD2	2.42	0.53
2:B:57:CYS:O	2:B:58:THR:HB	2.09	0.53
2:B:134:ALA:HB2	2:B:167:ALA:HB1	1.90	0.53
3:C:55:TRP:CD1	3:C:158:VAL:HG22	2.43	0.53
3:C:119:VAL:CG1	3:C:122:LEU:HB3	2.37	0.53
2:B:83:TYR:HA	2:B:90:LEU:HD23	1.91	0.53
1:A:147:GLU:OE2	3:C:120:ARG:CG	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:28:ILE:HD11	3:C:230:PHE:CZ	2.43	0.53
3:C:242:LYS:HE2	3:C:247:VAL:HG11	1.83	0.53
3:C:169:TRP:NE1	3:C:178:THR:CG2	2.72	0.52
1:A:127:ILE:HD12	2:B:72:ALA:CA	2.37	0.52
1:A:172:TYR:CZ	1:A:295:ILE:HD13	2.44	0.52
2:B:101:VAL:O	2:B:133:ALA:HB2	2.08	0.52
1:A:72:LEU:CD1	1:A:98:LEU:HG	2.38	0.52
2:B:54:LEU:HD21	2:B:116:LEU:HD22	1.91	0.52
1:A:59:VAL:O	1:A:62:ILE:HG22	2.10	0.52
1:A:88:LYS:HB2	1:A:88:LYS:HZ3	1.70	0.52
1:A:231:MET:CE	1:A:248:THR:HB	2.39	0.52
2:B:214:VAL:HG23	2:B:219:LEU:HB2	1.91	0.52
3:C:29:VAL:O	3:C:33:LEU:HB2	2.10	0.52
1:A:174:ARG:CG	1:A:174:ARG:NH1	2.73	0.52
2:B:93:MET:CE	2:B:118:GLU:HB3	2.40	0.52
3:C:55:TRP:HZ2	3:C:159:GLU:C	2.13	0.52
3:C:103:PRO:HD3	3:C:132:ILE:O	2.09	0.52
1:A:24:ASP:OD1	1:A:30:THR:HG22	2.10	0.52
1:A:143:MET:CE	1:A:171:LEU:CD2	2.86	0.52
1:A:264:ARG:NH1	1:A:286:GLU:CD	2.62	0.52
2:B:265:PRO:O	2:B:268:GLN:OE1	2.27	0.52
2:B:270:LYS:C	2:B:270:LYS:HD3	2.30	0.52
3:C:181:LEU:CD2	3:C:181:LEU:N	2.73	0.52
1:A:329:GLY:C	1:A:350:PRO:HB3	2.30	0.52
1:A:381:LEU:N	1:A:381:LEU:CD2	2.73	0.52
2:B:70:ILE:N	2:B:70:ILE:HD13	2.24	0.52
2:B:193:LEU:N	2:B:193:LEU:CD2	2.73	0.52
3:C:53:GLU:HB3	3:C:56:LYS:CB	2.40	0.52
3:C:192:CYS:HG	7:C:1282:SF4:FE3	1.27	0.52
3:C:227:ASP:CG	3:C:231:LYS:HE3	2.30	0.52
2:B:113:LEU:CD2	2:B:113:LEU:N	2.73	0.52
2:B:235:LEU:HD12	2:B:244:LEU:CB	2.39	0.52
3:C:220:ILE:CD1	3:C:222:ARG:NH1	2.73	0.52
1:A:12:ARG:HG2	1:A:112:LEU:O	2.10	0.52
2:B:270:LYS:CD	2:B:271:LYS:N	2.73	0.52
3:C:7:LYS:NZ	3:C:224:ASP:OD1	2.41	0.52
3:C:37:LEU:N	3:C:42:ILE:CD1	2.73	0.52
1:A:11:SER:OG	1:A:375:ARG:NH1	2.43	0.52
1:A:156:ILE:O	1:A:311:PHE:HE2	1.93	0.52
1:A:219:ARG:NH1	1:A:219:ARG:CB	2.73	0.52
2:B:83:TYR:CG	2:B:93:MET:HB3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:LEU:N	2:B:90:LEU:CD2	2.73	0.52
3:C:57:PRO:HG2	3:C:79:SER:HB2	1.91	0.52
3:C:132:ILE:HG23	9:C:1283:FAD:O4'	2.09	0.52
2:B:67:ASN:ND2	2:B:175:PRO:O	2.43	0.51
2:B:223:CYS:O	3:C:105:GLN:NE2	2.43	0.51
3:C:179:LEU:HD13	3:C:179:LEU:O	2.09	0.51
3:C:181:LEU:N	3:C:181:LEU:HD22	2.25	0.51
9:C:1283:FAD:N1	9:C:1283:FAD:H2'	2.25	0.51
1:A:25:ASP:N	1:A:26:GLU:OE1	2.43	0.51
1:A:244:ARG:HG2	1:A:244:ARG:NH1	2.12	0.51
1:A:261:PRO:O	1:A:265:MET:HG3	2.09	0.51
1:A:262:ARG:HH11	1:A:262:ARG:HB3	1.76	0.51
1:A:319:LEU:HB2	1:A:336:LYS:CG	2.41	0.51
1:A:336:LYS:NZ	1:A:336:LYS:CB	2.73	0.51
3:C:157:LEU:N	3:C:157:LEU:CD1	2.73	0.51
1:A:140:VAL:HG21	1:A:175:LEU:HD21	1.92	0.51
1:A:246:CYS:SG	1:A:385:THR:CB	2.99	0.51
2:B:241:ARG:HH21	3:C:189:GLN:NE2	2.08	0.51
3:C:17:ARG:NH1	3:C:17:ARG:CG	2.73	0.51
3:C:25:ASP:OD2	3:C:209:SER:CB	2.58	0.51
3:C:177:LEU:N	3:C:177:LEU:CD1	2.73	0.51
3:C:240:GLU:HG3	3:C:240:GLU:O	2.08	0.51
1:A:33:ARG:CG	1:A:33:ARG:NH1	2.73	0.51
2:B:186:LEU:CD1	2:B:187:ASN:ND2	2.73	0.51
3:C:3:LEU:N	3:C:3:LEU:CD1	2.73	0.51
3:C:19:ILE:O	3:C:23:ALA:CB	2.58	0.51
3:C:132:ILE:HG21	9:C:1283:FAD:C1'	2.40	0.51
1:A:138:GLN:HE21	2:B:66:GLU:CD	2.14	0.51
1:A:277:VAL:O	1:A:281:VAL:HG23	2.10	0.51
2:B:113:LEU:N	2:B:113:LEU:HD22	2.25	0.51
2:B:195:PRO:HG3	3:C:115:TYR:CZ	2.36	0.51
3:C:160:LYS:CG	3:C:171:TYR:HD2	2.23	0.51
3:C:208:GLY:O	3:C:218:THR:HG22	2.11	0.51
1:A:3:GLU:O	1:A:23:VAL:CG2	2.55	0.51
1:A:121:ASN:ND2	1:A:122:LEU:H	2.09	0.51
1:A:88:LYS:CB	1:A:88:LYS:HZ3	2.24	0.51
1:A:117:PHE:CE2	1:A:193:ILE:HG23	2.46	0.51
2:B:66:GLU:O	2:B:68:TYR:CE1	2.63	0.51
3:C:150:LYS:HE2	3:C:183:GLU:CD	2.31	0.51
1:A:16:HIS:H	1:A:38:THR:CG2	2.24	0.51
2:B:98:LEU:HD23	2:B:98:LEU:C	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:154:SER:CB	3:C:157:LEU:HD22	2.39	0.51
1:A:87:PRO:CG	1:A:306:PRO:O	2.59	0.51
1:A:90:GLY:HA2	1:A:307:VAL:HG13	1.93	0.51
1:A:184:GLU:OE1	1:A:185:HIS:N	2.43	0.51
2:B:97:ASP:HA	2:B:124:LYS:HE2	1.92	0.50
3:C:120:ARG:O	3:C:121:PHE:HB2	2.10	0.50
3:C:160:LYS:HG2	3:C:171:TYR:HD2	1.76	0.50
1:A:57:VAL:HG22	2:B:248:ARG:NH1	2.24	0.50
1:A:227:PHE:HZ	1:A:348:LEU:HD21	1.76	0.50
2:B:139:THR:HG21	2:B:155:PHE:HB2	1.72	0.50
2:B:195:PRO:HG2	2:B:196:MET:SD	2.51	0.50
2:B:242:PRO:O	2:B:242:PRO:HG2	2.11	0.50
1:A:186:VAL:HG21	1:A:288:LYS:CE	2.39	0.50
2:B:98:LEU:HD12	2:B:185:LEU:HD21	1.93	0.50
2:B:236:ASP:O	2:B:243:GLU:O	2.29	0.50
3:C:218:THR:O	3:C:218:THR:CG2	2.58	0.50
3:C:223:THR:HG22	3:C:224:ASP:N	2.26	0.50
3:C:273:LYS:HA	3:C:273:LYS:HE2	1.93	0.50
2:B:93:MET:HB2	2:B:96:MET:HE2	1.93	0.50
3:C:33:LEU:CD2	3:C:100:VAL:HG23	2.41	0.50
1:A:227:PHE:CD1	1:A:228:THR:N	2.80	0.50
2:B:156:VAL:HB	2:B:160:ASP:OD2	2.11	0.50
2:B:203:THR:HG22	2:B:204:GLU:H	1.76	0.50
3:C:167:LYS:N	3:C:181:LEU:HD23	2.26	0.50
3:C:231:LYS:O	3:C:235:GLU:HG3	2.10	0.50
9:C:1283:FAD:N1	9:C:1283:FAD:C2'	2.73	0.50
1:A:98:LEU:HD12	1:A:216:TYR:CD1	2.46	0.50
1:A:249:ILE:CG2	1:A:356:PRO:HB3	2.42	0.50
2:B:229:ALA:HB1	2:B:254:ILE:HG22	1.93	0.50
2:B:84:GLY:O	2:B:88:VAL:N	2.45	0.50
3:C:209:SER:N	9:C:1283:FAD:O2	2.45	0.50
1:A:3:GLU:HG2	1:A:23:VAL:CG2	2.39	0.50
1:A:64:GLY:C	1:A:67:PRO:HD3	2.31	0.50
2:B:49:ILE:HG13	2:B:79:VAL:CG1	2.41	0.50
2:B:241:ARG:CG	2:B:241:ARG:NH1	2.73	0.50
3:C:6:TYR:HB3	3:C:220:ILE:CD1	2.41	0.50
3:C:199:VAL:HG22	3:C:200:ALA:N	2.27	0.50
3:C:220:ILE:HD11	3:C:222:ARG:NH1	2.26	0.50
3:C:220:ILE:CG1	3:C:222:ARG:NH1	2.74	0.50
3:C:242:LYS:NZ	3:C:247:VAL:HG11	2.26	0.50
1:A:311:PHE:CD1	1:A:311:PHE:C	2.85	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:MET:HE3	1:A:379:PRO:HG3	1.94	0.50
2:B:234:ALA:HB2	2:B:248:ARG:O	2.12	0.50
3:C:7:LYS:HE3	3:C:224:ASP:CA	2.41	0.50
3:C:145:THR:HG23	3:C:146:PHE:N	2.26	0.50
1:A:18:GLU:OE2	1:A:35:PHE:HZ	1.94	0.49
1:A:24:ASP:HB2	1:A:26:GLU:OE1	2.11	0.49
1:A:231:MET:HE1	1:A:248:THR:CB	2.41	0.49
3:C:165:LYS:N	3:C:165:LYS:CD	2.73	0.49
2:B:192:TYR:CD1	2:B:192:TYR:C	2.86	0.49
3:C:202:LEU:HD22	3:C:202:LEU:N	2.27	0.49
3:C:223:THR:CG2	3:C:224:ASP:N	2.75	0.49
1:A:4:ARG:CA	1:A:21:MET:O	2.59	0.49
1:A:28:ILE:CD1	1:A:28:ILE:N	2.75	0.49
1:A:66:CYS:C	1:A:69:PRO:HD2	2.31	0.49
1:A:258:GLU:HG3	1:A:377:TYR:HE2	1.75	0.49
2:B:98:LEU:HA	2:B:125:LEU:O	2.12	0.49
3:C:196:LYS:HD2	3:C:265:ALA:HB3	1.94	0.49
1:A:155:ARG:NH1	2:B:248:ARG:NH2	2.60	0.49
2:B:83:TYR:O	2:B:83:TYR:CG	2.65	0.49
3:C:280:PRO:C	3:C:281:PHE:CD1	2.85	0.49
1:A:58:MET:HE3	2:B:141:TYR:CE2	2.46	0.49
1:A:139:TYR:HD2	1:A:174:ARG:HD2	1.75	0.49
3:C:47:VAL:CG2	3:C:71:ALA:HB1	2.42	0.49
1:A:128:ASN:OD1	2:B:72:ALA:HB2	2.12	0.49
1:A:141:VAL:HG13	1:A:142:ASP:N	2.26	0.49
1:A:338:GLU:O	1:A:339:ASN:HB2	2.12	0.49
3:C:150:LYS:N	3:C:150:LYS:CD	2.75	0.49
1:A:47:VAL:O	1:A:50:LYS:HB2	2.13	0.49
1:A:78:ILE:HD13	1:A:335:ALA:HB3	1.94	0.49
1:A:218:ASP:HB2	1:A:221:LYS:HG3	1.95	0.49
2:B:110:GLU:HA	2:B:110:GLU:OE1	2.13	0.49
2:B:129:PHE:CD1	2:B:129:PHE:C	2.85	0.49
3:C:17:ARG:NH1	3:C:17:ARG:CB	2.75	0.49
1:A:259:VAL:HG23	1:A:259:VAL:O	2.13	0.49
1:A:6:VAL:HG23	1:A:6:VAL:O	2.12	0.49
1:A:136:ASN:O	1:A:139:TYR:HB2	2.12	0.49
1:A:210:LEU:CD1	1:A:252:TYR:CE2	2.96	0.49
2:B:217:GLN:NE2	2:B:217:GLN:N	2.60	0.49
3:C:96:LYS:HB3	3:C:127:LYS:CD	2.41	0.49
1:A:172:TYR:HE2	1:A:299:ASP:HB2	1.78	0.49
1:A:212:SER:O	1:A:268:PHE:HZ	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:VAL:CG1	2:B:89:ASP:N	2.76	0.49
1:A:20:VAL:HG23	1:A:35:PHE:HE1	1.77	0.48
1:A:172:TYR:CD1	1:A:172:TYR:C	2.86	0.48
1:A:381:LEU:O	1:A:382:SER:C	2.51	0.48
2:B:206:CYS:HB3	2:B:208:CYS:SG	2.52	0.48
3:C:15:THR:OG1	3:C:238:LEU:O	2.28	0.48
3:C:55:TRP:HE1	3:C:158:VAL:CG2	2.25	0.48
3:C:133:TYR:HD1	3:C:199:VAL:HA	1.76	0.48
1:A:22:GLU:O	1:A:30:THR:HG23	2.14	0.48
1:A:22:GLU:OE1	1:A:31:LYS:HB2	2.13	0.48
1:A:41:ARG:NH1	1:A:41:ARG:CG	2.72	0.48
1:A:73:ALA:CB	1:A:324:ILE:HD12	2.34	0.48
1:A:148:GLY:HA2	1:A:149:ILE:C	2.34	0.48
1:A:260:GLY:O	1:A:264:ARG:N	2.39	0.48
2:B:53:HIS:HB2	2:B:102:GLU:HB2	1.95	0.48
2:B:168:LEU:HB2	3:C:117:PHE:CE1	2.37	0.48
2:B:210:LEU:HD23	2:B:255:CYS:HB2	1.95	0.48
2:B:90:LEU:H	2:B:90:LEU:CD2	2.14	0.48
2:B:213:LYS:HG2	2:B:256:TYR:CZ	2.48	0.48
2:B:228:MET:HG3	3:C:86:LYS:HB2	1.94	0.48
1:A:142:ASP:HA	1:A:146:GLY:O	2.13	0.48
1:A:178:LEU:CD1	1:A:182:VAL:HG23	2.43	0.48
1:A:249:ILE:HG23	1:A:356:PRO:CG	2.43	0.48
2:B:106:CYS:HB2	2:B:155:PHE:CD2	2.48	0.48
3:C:35:TYR:OH	3:C:39:GLU:CD	2.52	0.48
2:B:89:ASP:O	2:B:91:TRP:CZ3	2.64	0.48
2:B:125:LEU:CD2	2:B:126:VAL:N	2.77	0.48
3:C:164:GLY:CA	3:C:169:TRP:HE3	2.24	0.48
1:A:43:LEU:HD11	1:A:62:ILE:CG1	2.41	0.48
1:A:75:VAL:HG21	1:A:154:VAL:HG22	1.96	0.48
1:A:43:LEU:HD23	2:B:138:PHE:HE2	1.71	0.48
1:A:44:GLU:N	2:B:146:GLN:HE21	2.12	0.48
1:A:96:LEU:CB	1:A:297:ILE:HD11	2.36	0.48
1:A:143:MET:HG3	3:C:90:ARG:O	2.14	0.48
1:A:257:VAL:C	1:A:357:THR:HG21	2.34	0.48
3:C:25:ASP:HB3	3:C:26:GLY:H	1.18	0.48
3:C:86:LYS:O	3:C:90:ARG:HB2	2.14	0.48
3:C:280:PRO:C	3:C:281:PHE:HD1	2.17	0.48
1:A:75:VAL:HG13	1:A:156:ILE:HA	1.95	0.48
2:B:223:CYS:HB2	3:C:105:GLN:HA	1.96	0.48
2:B:46:LYS:HG3	2:B:47:PRO:CD	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:GLU:O	2:B:180:LYS:HG2	2.14	0.48
2:B:214:VAL:HG13	2:B:215:VAL:N	2.29	0.48
3:C:73:GLY:O	9:C:1283:FAD:H51A	2.14	0.48
3:C:151:LEU:HD21	3:C:170:VAL:HG23	1.96	0.48
3:C:224:ASP:OD1	3:C:224:ASP:O	2.32	0.48
1:A:244:ARG:CG	1:A:244:ARG:NH1	2.73	0.48
3:C:35:TYR:OH	3:C:39:GLU:OE2	2.30	0.48
1:A:57:VAL:HG21	2:B:248:ARG:HH11	1.77	0.47
1:A:275:GLY:N	1:A:278:ALA:CB	2.76	0.47
1:A:289:THR:CG2	1:A:290:ALA:N	2.75	0.47
2:B:164:VAL:HG23	2:B:164:VAL:O	2.14	0.47
3:C:214:ASP:OD1	3:C:215:GLY:N	2.47	0.47
1:A:109:HIS:CD2	1:A:378:ASP:OD2	2.67	0.47
2:B:186:LEU:HD13	2:B:187:ASN:ND2	2.28	0.47
3:C:122:LEU:HD12	3:C:122:LEU:C	2.31	0.47
1:A:28:ILE:HG23	1:A:364:GLY:C	2.26	0.47
1:A:43:LEU:HD23	2:B:138:PHE:CE2	2.45	0.47
1:A:238:ASP:CA	1:A:241:ILE:HG22	2.44	0.47
1:A:246:CYS:HG	1:A:385:THR:HG21	1.73	0.47
3:C:9:ILE:CD1	3:C:220:ILE:CD1	2.90	0.47
2:B:213:LYS:HG2	2:B:256:TYR:CE1	2.50	0.47
3:C:280:PRO:HG2	3:C:281:PHE:CE1	2.49	0.47
1:A:60:GLN:NE2	1:A:61:ARG:HH12	2.09	0.47
1:A:143:MET:HE3	1:A:171:LEU:HD21	1.96	0.47
1:A:246:CYS:SG	1:A:385:THR:HB	2.55	0.47
1:A:293:ARG:HD3	1:A:293:ARG:O	2.14	0.47
1:A:328:ARG:NH1	1:A:328:ARG:HG3	2.28	0.47
1:A:11:SER:CB	2:B:89:ASP:HB3	2.44	0.47
1:A:293:ARG:O	1:A:294:ALA:C	2.52	0.47
2:B:60:ASP:OD2	2:B:130:GLY:HA3	2.15	0.47
2:B:116:LEU:CD1	2:B:162:ILE:CD1	2.90	0.47
1:A:127:ILE:HD12	2:B:72:ALA:CB	2.44	0.47
1:A:129:SER:O	1:A:133:ILE:HG23	2.14	0.47
1:A:147:GLU:O	1:A:151:PRO:CA	2.53	0.47
1:A:221:LYS:NZ	1:A:221:LYS:CB	2.73	0.47
1:A:319:LEU:HD12	1:A:319:LEU:O	2.14	0.47
3:C:112:MET:SD	3:C:119:VAL:HG21	2.54	0.47
3:C:244:ILE:CG1	3:C:251:LEU:HB3	2.43	0.47
3:C:280:PRO:O	3:C:281:PHE:HB2	2.13	0.47
3:C:280:PRO:CG	3:C:281:PHE:CD1	2.96	0.47
1:A:106:HIS:CB	1:A:287:MET:CE	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:VAL:HG23	1:A:187:GLU:N	2.30	0.47
1:A:231:MET:HE2	2:B:147:GLN:HE21	1.79	0.47
1:A:336:LYS:NZ	1:A:336:LYS:HB3	2.29	0.47
1:A:367:HIS:O	1:A:370:GLY:N	2.45	0.47
2:B:86:THR:CG2	2:B:87:LEU:HD13	2.44	0.47
2:B:221:ILE:HD12	2:B:221:ILE:C	2.35	0.47
2:B:271:LYS:HZ3	2:B:272:GLU:HG3	1.79	0.47
3:C:60:MET:CE	3:C:67:GLU:HG2	2.45	0.47
1:A:18:GLU:O	1:A:35:PHE:CD1	2.68	0.47
1:A:145:ALA:O	1:A:151:PRO:HB2	2.15	0.47
2:B:239:ASN:HA	2:B:240:GLY:HA2	1.70	0.47
1:A:223:ASP:HB3	1:A:226:ARG:H	1.80	0.47
1:A:224:LEU:HD11	1:A:321:ILE:HG12	1.97	0.47
2:B:66:GLU:O	2:B:68:TYR:CG	2.68	0.47
3:C:173:GLN:O	3:C:174:ASP:CB	2.63	0.47
1:A:172:TYR:C	1:A:172:TYR:HD1	2.19	0.46
2:B:81:ILE:HG23	2:B:81:ILE:O	2.14	0.46
2:B:129:PHE:CE2	2:B:178:ILE:HD11	2.49	0.46
2:B:224:GLY:HA3	3:C:80:PRO:HB3	1.96	0.46
3:C:47:VAL:HG23	3:C:71:ALA:CB	2.45	0.46
1:A:10:THR:CB	1:A:13:GLN:HE21	2.20	0.46
1:A:55:ALA:HB2	1:A:342:ILE:HD11	1.97	0.46
1:A:138:GLN:HA	1:A:141:VAL:HG12	1.97	0.46
1:A:162:ASN:OD1	1:A:162:ASN:C	2.53	0.46
2:B:209:ASP:OD1	2:B:210:LEU:N	2.48	0.46
3:C:37:LEU:N	3:C:42:ILE:HD11	2.30	0.46
3:C:182:LYS:HZ3	3:C:185:HIS:HE1	1.63	0.46
1:A:15:GLY:HA3	1:A:381:LEU:HB2	1.97	0.46
1:A:41:ARG:N	1:A:386:HIS:OXT	2.48	0.46
3:C:19:ILE:HD13	3:C:19:ILE:H	1.77	0.46
3:C:227:ASP:O	3:C:231:LYS:HG3	2.15	0.46
1:A:18:GLU:CD	1:A:35:PHE:CZ	2.86	0.46
1:A:319:LEU:HD12	1:A:319:LEU:C	2.36	0.46
2:B:83:TYR:HB2	2:B:94:PRO:HD2	1.97	0.46
3:C:198:TYR:HA	3:C:261:LYS:HE3	1.98	0.46
3:C:248:LYS:HA	3:C:249:PRO:C	2.35	0.46
3:C:262:LYS:HE3	3:C:262:LYS:HB2	1.70	0.46
1:A:33:ARG:HH11	1:A:33:ARG:HG2	1.77	0.46
1:A:34:TYR:CD1	1:A:374:ILE:HD13	2.50	0.46
1:A:285:LEU:O	1:A:288:LYS:HB3	2.14	0.46
2:B:164:VAL:HG23	2:B:200:ALA:HB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:ASP:C	2:B:190:MET:SD	2.94	0.46
3:C:110:ARG:HG3	3:C:202:LEU:HD12	1.97	0.46
3:C:269:ILE:O	3:C:273:LYS:HB2	2.16	0.46
1:A:265:MET:HE3	1:A:269:GLN:CG	2.42	0.46
1:A:314:ARG:HE	1:A:314:ARG:HB2	1.60	0.46
1:A:54:THR:HG23	2:B:247:ASP:O	2.15	0.46
1:A:93:LEU:HD13	1:A:93:LEU:HA	1.84	0.46
1:A:106:HIS:HB3	1:A:287:MET:HE3	1.96	0.46
1:A:199:PRO:HG3	1:A:369:TYR:CE2	2.49	0.46
1:A:283:ARG:HH11	1:A:283:ARG:CG	2.29	0.46
3:C:13:ARG:O	3:C:239:PHE:HA	2.16	0.46
3:C:19:ILE:N	3:C:19:ILE:CD1	2.69	0.46
3:C:60:MET:CE	3:C:67:GLU:CG	2.94	0.46
3:C:164:GLY:N	3:C:169:TRP:HE3	2.13	0.46
1:A:67:PRO:HG2	1:A:68:ILE:HD12	1.97	0.46
2:B:143:ARG:HH11	2:B:143:ARG:CG	2.13	0.46
2:B:210:LEU:O	2:B:214:VAL:CG1	2.62	0.46
3:C:7:LYS:HE3	3:C:224:ASP:HA	1.98	0.46
3:C:65:SER:O	3:C:69:LYS:HD2	2.16	0.46
1:A:262:ARG:HH11	1:A:262:ARG:CB	2.29	0.46
2:B:75:LEU:O	2:B:79:VAL:O	2.34	0.46
2:B:252:CYS:SG	2:B:254:ILE:HG12	2.55	0.46
3:C:225:ALA:O	3:C:228:SER:OG	2.25	0.46
1:A:231:MET:HE3	1:A:248:THR:CB	2.46	0.46
1:A:289:THR:HG23	1:A:290:ALA:H	1.80	0.46
2:B:221:ILE:CG2	2:B:261:ARG:NH2	2.79	0.46
3:C:46:VAL:HG23	3:C:46:VAL:O	2.16	0.46
3:C:77:THR:CG2	3:C:78:PHE:N	2.79	0.46
1:A:119:PRO:CG	1:A:121:ASN:HD21	2.29	0.45
1:A:209:THR:HB	1:A:263:ALA:CB	2.46	0.45
1:A:215:ILE:CD1	1:A:215:ILE:N	2.80	0.45
3:C:105:GLN:H	3:C:105:GLN:HG2	1.58	0.45
3:C:251:LEU:HD13	3:C:251:LEU:C	2.34	0.45
1:A:62:ILE:CD1	1:A:386:HIS:HB3	2.46	0.45
1:A:121:ASN:ND2	1:A:121:ASN:N	2.60	0.45
1:A:124:ALA:O	1:A:127:ILE:HG23	2.16	0.45
1:A:140:VAL:O	1:A:144:VAL:HG13	2.16	0.45
1:A:213:HIS:O	1:A:264:ARG:HD3	2.17	0.45
2:B:183:VAL:HG13	2:B:184:ALA:N	2.32	0.45
2:B:214:VAL:HG23	2:B:219:LEU:HB3	1.98	0.45
2:B:237:MET:CB	3:C:83:MET:CE	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:260:PRO:HG2	3:C:108:GLY:CA	2.45	0.45
3:C:251:LEU:C	3:C:251:LEU:HD22	2.36	0.45
1:A:106:HIS:HB3	1:A:287:MET:CE	2.46	0.45
3:C:60:MET:HE3	3:C:67:GLU:CG	2.47	0.45
3:C:62:ALA:HB1	3:C:67:GLU:CB	2.45	0.45
9:C:1283:FAD:H1'1	9:C:1283:FAD:H9	1.79	0.45
1:A:182:VAL:O	1:A:186:VAL:HG13	2.16	0.45
1:A:302:ASP:OD1	1:A:302:ASP:N	2.49	0.45
1:A:319:LEU:C	1:A:319:LEU:CD1	2.85	0.45
2:B:53:HIS:C	2:B:53:HIS:CD2	2.88	0.45
3:C:4:GLY:C	3:C:222:ARG:NH2	2.69	0.45
1:A:144:VAL:HG23	1:A:145:ALA:N	2.30	0.45
1:A:146:GLY:HA3	1:A:153:ASP:OD2	2.13	0.45
1:A:321:ILE:N	1:A:321:ILE:CD1	2.73	0.45
1:A:362:THR:HG21	1:A:374:ILE:HG13	1.98	0.45
2:B:114:HIS:CD2	2:B:114:HIS:C	2.88	0.45
2:B:237:MET:CE	3:C:80:PRO:CB	2.80	0.45
1:A:42:GLY:HA2	2:B:146:GLN:NE2	2.32	0.45
2:B:53:HIS:CD2	2:B:56:GLY:H	2.35	0.45
3:C:29:VAL:CG1	3:C:100:VAL:HG21	2.47	0.45
3:C:163:ILE:HG12	3:C:168:PHE:CE2	2.52	0.45
2:B:63:SER:HA	2:B:66:GLU:HG2	1.98	0.45
2:B:125:LEU:CD2	2:B:125:LEU:C	2.85	0.45
2:B:145:GLY:N	2:B:150:PRO:O	2.49	0.45
2:B:248:ARG:O	2:B:248:ARG:CG	2.65	0.45
3:C:251:LEU:N	3:C:251:LEU:CD1	2.79	0.45
1:A:47:VAL:HG12	1:A:342:ILE:HD13	1.99	0.45
1:A:62:ILE:C	1:A:62:ILE:CD1	2.86	0.45
1:A:62:ILE:HD11	1:A:383:CYS:HA	1.98	0.45
2:B:51:TYR:CA	2:B:100:LEU:O	2.64	0.45
2:B:53:HIS:CD2	2:B:53:HIS:O	2.70	0.45
2:B:93:MET:HE3	2:B:118:GLU:HB3	1.99	0.45
2:B:221:ILE:CD1	2:B:223:CYS:H	2.30	0.45
2:B:237:MET:HE3	3:C:80:PRO:CG	2.36	0.45
3:C:131:GLY:HA3	3:C:200:ALA:CB	2.47	0.45
3:C:154:SER:CA	3:C:157:LEU:HD22	2.46	0.45
1:A:47:VAL:CG1	1:A:342:ILE:HD13	2.47	0.45
1:A:68:ILE:O	1:A:72:LEU:HG	2.16	0.45
2:B:190:MET:SD	2:B:190:MET:N	2.90	0.45
2:B:217:GLN:N	2:B:217:GLN:HE21	2.15	0.45
3:C:25:ASP:HB3	3:C:217:SER:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:199:VAL:CG2	3:C:200:ALA:N	2.79	0.45
3:C:277:LEU:HD23	3:C:277:LEU:N	2.24	0.45
9:C:1283:FAD:H1'2	9:C:1283:FAD:O4'	2.16	0.45
1:A:109:HIS:HB2	1:A:378:ASP:OD2	2.17	0.45
1:A:167:ALA:CB	3:C:93:GLY:H	2.26	0.45
1:A:205:HIS:CD2	1:A:377:TYR:OH	2.69	0.45
1:A:219:ARG:CG	1:A:219:ARG:NH1	2.73	0.45
2:B:105:VAL:CG2	2:B:116:LEU:HD23	2.47	0.45
1:A:210:LEU:CB	1:A:259:VAL:HG12	2.33	0.44
2:B:98:LEU:CD1	2:B:185:LEU:HD21	2.47	0.44
2:B:221:ILE:C	2:B:221:ILE:CD1	2.85	0.44
2:B:221:ILE:CG2	7:C:1282:SF4:S4	3.05	0.44
2:B:232:THR:O	2:B:233:ARG:CB	2.64	0.44
3:C:36:ALA:HB3	3:C:42:ILE:CG1	2.47	0.44
3:C:257:LEU:HD12	3:C:257:LEU:HA	1.75	0.44
2:B:107:LEU:HB2	2:B:108:GLN:OE1	2.17	0.44
2:B:129:PHE:CD1	2:B:129:PHE:O	2.70	0.44
1:A:66:CYS:O	1:A:69:PRO:CG	2.65	0.44
1:A:279:GLN:HE21	1:A:279:GLN:HB3	1.54	0.44
2:B:263:TRP:O	2:B:263:TRP:CE3	2.70	0.44
2:B:83:TYR:CA	2:B:90:LEU:HD21	2.47	0.44
3:C:6:TYR:CD1	3:C:6:TYR:N	2.86	0.44
3:C:19:ILE:O	3:C:23:ALA:HB3	2.16	0.44
3:C:222:ARG:H	3:C:222:ARG:HG2	1.55	0.44
3:C:232:GLN:HG2	3:C:232:GLN:H	1.54	0.44
1:A:225:ASP:OD1	1:A:225:ASP:N	2.36	0.44
1:A:265:MET:HE2	1:A:269:GLN:CD	2.36	0.44
2:B:185:LEU:HD12	2:B:185:LEU:HA	1.85	0.44
2:B:221:ILE:HG23	2:B:261:ARG:NH2	2.33	0.44
3:C:111:LYS:HA	3:C:114:THR:CG2	2.46	0.44
3:C:163:ILE:HG12	3:C:168:PHE:CD2	2.53	0.44
1:A:4:ARG:CB	1:A:21:MET:O	2.66	0.44
3:C:37:LEU:CD1	3:C:63:MET:O	2.66	0.44
3:C:41:ILE:H	3:C:41:ILE:CD1	2.27	0.44
3:C:119:VAL:HG11	3:C:122:LEU:HD23	1.99	0.44
3:C:236:ALA:CB	3:C:238:LEU:CD2	2.94	0.44
1:A:46:MET:HE1	2:B:142:SER:HB3	2.00	0.44
1:A:78:ILE:HD13	1:A:335:ALA:CB	2.47	0.44
2:B:269:ILE:CG2	2:B:270:LYS:N	2.81	0.44
3:C:54:PHE:CE2	3:C:156:GLU:CD	2.91	0.44
1:A:82:LEU:HD21	1:A:313:GLU:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:TYR:O	2:B:51:TYR:CD1	2.70	0.44
2:B:194:GLN:NE2	2:B:194:GLN:CA	2.73	0.44
2:B:210:LEU:C	2:B:210:LEU:CD1	2.85	0.44
3:C:19:ILE:H	3:C:19:ILE:CD1	2.30	0.44
3:C:26:GLY:CA	3:C:217:SER:CB	2.82	0.44
3:C:29:VAL:CG1	3:C:100:VAL:CG2	2.95	0.44
3:C:126:ILE:H	3:C:126:ILE:HG12	1.61	0.44
1:A:261:PRO:HG2	1:A:283:ARG:NH1	2.33	0.44
2:B:79:VAL:CG1	2:B:80:ASP:N	2.81	0.44
2:B:264:TRP:CH2	2:B:268:GLN:NE2	2.86	0.44
3:C:78:PHE:N	3:C:78:PHE:CD1	2.75	0.44
3:C:102:ILE:HG22	3:C:103:PRO:N	2.33	0.44
3:C:274:GLU:OE1	3:C:275:MET:N	2.50	0.44
1:A:34:TYR:HE2	1:A:358:MET:HE1	1.81	0.43
1:A:57:VAL:HG21	2:B:248:ARG:HG3	1.99	0.43
1:A:96:LEU:HD12	1:A:144:VAL:HG11	1.89	0.43
2:B:144:GLY:HA3	2:B:153:GLU:CA	2.47	0.43
3:C:139:PRO:CD	3:C:142:SER:HB2	2.31	0.43
3:C:239:PHE:N	3:C:239:PHE:HD1	2.14	0.43
1:A:256:ASN:ND2	1:A:256:ASN:H	2.14	0.43
3:C:138:PHE:HE2	3:C:184:THR:CG2	2.31	0.43
3:C:236:ALA:HB1	3:C:238:LEU:CD2	2.48	0.43
3:C:253:LEU:HD13	3:C:254:LEU:CA	2.47	0.43
1:A:14:GLU:CD	2:B:58:THR:HG21	2.38	0.43
1:A:45:LYS:HB2	2:B:146:GLN:HB2	2.00	0.43
1:A:82:LEU:HB3	1:A:84:ILE:CD1	2.48	0.43
1:A:84:ILE:CG2	1:A:311:PHE:CB	2.66	0.43
3:C:49:GLY:O	3:C:60:MET:SD	2.76	0.43
3:C:242:LYS:CE	3:C:247:VAL:CG1	2.61	0.43
1:A:2:SER:HB2	1:A:3:GLU:H	1.63	0.43
2:B:244:LEU:HD13	2:B:244:LEU:C	2.37	0.43
3:C:48:ALA:HA	3:C:59:PRO:HA	2.00	0.43
3:C:133:TYR:HD2	3:C:208:GLY:HA3	1.70	0.43
1:A:212:SER:C	1:A:268:PHE:CZ	2.92	0.43
1:A:73:ALA:CA	1:A:324:ILE:CD1	2.92	0.43
1:A:141:VAL:CG1	1:A:142:ASP:N	2.82	0.43
1:A:168:ARG:NH1	1:A:168:ARG:HG2	2.30	0.43
2:B:114:HIS:CD2	2:B:114:HIS:O	2.70	0.43
3:C:78:PHE:H	3:C:78:PHE:HD1	1.60	0.43
3:C:179:LEU:HD22	3:C:183:GLU:HG2	2.00	0.43
3:C:244:ILE:CG2	3:C:245:GLU:N	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:ASN:ND2	2:B:239:ASN:N	2.67	0.43
3:C:196:LYS:HD2	3:C:265:ALA:CB	2.49	0.43
1:A:36:SER:HB3	1:A:381:LEU:CD1	2.49	0.43
1:A:214:GLN:C	1:A:215:ILE:CD1	2.85	0.43
1:A:293:ARG:HD3	1:A:293:ARG:C	2.38	0.43
2:B:48:ARG:CB	2:B:48:ARG:NH1	2.73	0.43
2:B:125:LEU:HD23	2:B:126:VAL:H	1.84	0.43
3:C:96:LYS:HB3	3:C:127:LYS:HE2	1.95	0.43
1:A:139:TYR:CE2	1:A:174:ARG:CD	3.02	0.43
2:B:266:GLU:O	2:B:269:ILE:CG2	2.60	0.43
3:C:176:VAL:HG23	3:C:176:VAL:O	2.18	0.43
1:A:12:ARG:CG	1:A:112:LEU:O	2.67	0.43
1:A:162:ASN:OD1	1:A:163:ILE:N	2.52	0.43
1:A:172:TYR:HD1	1:A:172:TYR:O	2.02	0.43
2:B:128:ALA:HB1	2:B:158:ILE:HD11	1.93	0.43
2:B:180:LYS:O	2:B:183:VAL:CG1	2.65	0.43
3:C:18:GLU:O	3:C:22:LEU:HG	2.19	0.43
1:A:213:HIS:HB2	1:A:217:GLY:HA2	2.01	0.42
1:A:207:GLN:CG	1:A:256:ASN:ND2	2.82	0.42
2:B:116:LEU:HD11	2:B:162:ILE:HD13	1.97	0.42
2:B:156:VAL:CG2	2:B:160:ASP:OD2	2.68	0.42
3:C:46:VAL:HG22	3:C:99:THR:CB	2.46	0.42
3:C:189:GLN:HG3	3:C:192:CYS:SG	2.59	0.42
2:B:62:MET:O	2:B:66:GLU:HG2	2.19	0.42
3:C:42:ILE:CG2	3:C:98:GLY:H	2.28	0.42
3:C:65:SER:OG	3:C:69:LYS:NZ	2.50	0.42
1:A:8:SER:HA	1:A:9:PRO:HA	1.81	0.42
2:B:50:GLY:O	2:B:99:ALA:HA	2.19	0.42
2:B:60:ASP:CG	2:B:102:GLU:HG3	2.39	0.42
3:C:7:LYS:CE	3:C:224:ASP:HA	2.49	0.42
3:C:29:VAL:HG21	3:C:132:ILE:HD11	2.01	0.42
3:C:85:LEU:HD22	3:C:97:LEU:HD11	2.02	0.42
3:C:153:VAL:HG22	3:C:157:LEU:HB2	2.02	0.42
3:C:226:GLY:C	3:C:229:ILE:HG22	2.37	0.42
1:A:33:ARG:HA	1:A:33:ARG:HD3	1.69	0.42
1:A:57:VAL:HG11	2:B:232:THR:HG23	2.00	0.42
1:A:132:GLU:CG	1:A:181:LYS:NZ	2.76	0.42
2:B:149:GLN:HG3	2:B:152:HIS:NE2	2.34	0.42
3:C:33:LEU:HD12	3:C:33:LEU:HA	1.78	0.42
3:C:175:ASP:OD1	3:C:177:LEU:HD12	2.19	0.42
3:C:187:TYR:H	3:C:187:TYR:HD1	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:GLU:N	2:B:146:GLN:NE2	2.62	0.42
1:A:59:VAL:CG1	1:A:333:HIS:HE1	2.32	0.42
1:A:96:LEU:HD22	1:A:96:LEU:C	2.40	0.42
1:A:154:VAL:O	1:A:155:ARG:HG2	2.20	0.42
1:A:165:GLU:OE1	1:A:169:LYS:NZ	2.52	0.42
1:A:165:GLU:CD	1:A:168:ARG:NH1	2.73	0.42
1:A:293:ARG:CZ	1:A:297:ILE:HG22	2.50	0.42
2:B:89:ASP:C	2:B:91:TRP:CZ3	2.92	0.42
2:B:95:GLU:HA	2:B:122:LYS:O	2.19	0.42
2:B:176:GLU:O	2:B:180:LYS:CG	2.67	0.42
1:A:202:LEU:HD22	1:A:373:VAL:CG2	2.47	0.42
1:A:223:ASP:HB2	1:A:226:ARG:CB	2.46	0.42
1:A:250:PRO:HB3	1:A:348:LEU:HD22	2.02	0.42
1:A:338:GLU:O	1:A:339:ASN:CB	2.66	0.42
2:B:56:GLY:CA	7:B:1274:SF4:S3	3.07	0.42
2:B:79:VAL:HG12	2:B:80:ASP:N	2.34	0.42
2:B:113:LEU:CD2	2:B:113:LEU:H	2.32	0.42
2:B:241:ARG:HA	2:B:241:ARG:HD3	1.72	0.42
2:B:120:ARG:NE	2:B:126:VAL:HG11	2.34	0.42
2:B:187:ASN:C	2:B:188:ASN:ND2	2.73	0.42
2:B:232:THR:CG2	2:B:248:ARG:HG2	2.44	0.42
3:C:39:GLU:HB3	3:C:41:ILE:CD1	2.41	0.42
1:A:111:PHE:CD2	1:A:112:LEU:HD23	2.55	0.42
2:B:87:LEU:C	2:B:88:VAL:HG23	2.40	0.42
2:B:124:LYS:HE2	2:B:124:LYS:HB3	1.73	0.42
2:B:244:LEU:C	2:B:244:LEU:CD2	2.85	0.42
2:B:261:ARG:O	3:C:280:PRO:CB	2.63	0.42
2:B:74:LEU:HD22	2:B:75:LEU:HD12	2.02	0.42
3:C:91:GLN:NE2	3:C:91:GLN:CA	2.82	0.42
1:A:185:HIS:HA	1:A:188:LEU:CD2	2.50	0.41
1:A:366:HIS:HD2	1:A:368:GLU:H	1.68	0.41
1:A:154:VAL:C	1:A:155:ARG:HG2	2.41	0.41
1:A:249:ILE:CG2	1:A:356:PRO:CB	2.98	0.41
2:B:119:LEU:C	2:B:119:LEU:CD1	2.86	0.41
2:B:170:GLY:N	2:B:254:ILE:HD11	2.31	0.41
3:C:280:PRO:HB2	3:C:281:PHE:HD1	1.85	0.41
1:A:54:THR:HG23	1:A:58:MET:HE1	2.01	0.41
1:A:84:ILE:HD12	1:A:311:PHE:CD2	2.49	0.41
1:A:167:ALA:HB2	3:C:93:GLY:N	2.28	0.41
2:B:93:MET:HE1	2:B:118:GLU:HB3	2.01	0.41
2:B:99:ALA:HB2	2:B:123:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:HIS:O	2:B:114:HIS:HD2	2.04	0.41
2:B:237:MET:CE	3:C:80:PRO:HB3	2.48	0.41
3:C:4:GLY:C	3:C:222:ARG:HH22	2.23	0.41
3:C:60:MET:HE2	3:C:67:GLU:HG2	2.02	0.41
3:C:245:GLU:HG2	3:C:246:GLU:N	2.35	0.41
1:A:14:GLU:O	1:A:381:LEU:HD23	2.20	0.41
1:A:89:ALA:CB	1:A:305:ALA:HB3	2.49	0.41
2:B:70:ILE:O	2:B:74:LEU:HB2	2.19	0.41
2:B:175:PRO:HG3	3:C:121:PHE:CE1	2.56	0.41
3:C:229:ILE:HG23	3:C:230:PHE:N	2.34	0.41
1:A:59:VAL:HG11	1:A:333:HIS:CE1	2.55	0.41
1:A:162:ASN:HB2	1:A:307:VAL:HG21	2.02	0.41
2:B:82:VAL:HG21	2:B:94:PRO:HG2	2.02	0.41
2:B:157:PRO:HG2	2:B:203:THR:HG23	2.01	0.41
2:B:208:CYS:O	2:B:211:GLN:HB3	2.20	0.41
2:B:66:GLU:O	2:B:68:TYR:N	2.54	0.41
2:B:231:GLN:H	2:B:231:GLN:HG2	1.55	0.41
3:C:120:ARG:C	3:C:122:LEU:H	2.22	0.41
1:A:264:ARG:NH1	1:A:286:GLU:OE2	2.53	0.41
2:B:181:THR:CG2	2:B:196:MET:HE2	2.50	0.41
2:B:270:LYS:C	2:B:270:LYS:CD	2.88	0.41
3:C:181:LEU:O	3:C:184:THR:N	2.54	0.41
1:A:91:ARG:HG3	1:A:91:ARG:HH11	1.86	0.41
1:A:302:ASP:O	1:A:303:THR:OG1	2.39	0.41
2:B:127:CYS:HB2	2:B:166:LEU:HD12	1.84	0.41
1:A:62:ILE:CG1	1:A:386:HIS:CB	2.87	0.41
1:A:246:CYS:SG	1:A:246:CYS:O	2.79	0.41
1:A:250:PRO:HG2	1:A:353:TRP:HA	2.03	0.41
2:B:66:GLU:O	2:B:68:TYR:CZ	2.74	0.41
3:C:97:LEU:O	3:C:126:ILE:HA	2.21	0.41
3:C:219:VAL:O	3:C:219:VAL:HG22	2.20	0.41
1:A:65:VAL:N	1:A:67:PRO:HD3	2.36	0.41
1:A:324:ILE:HD13	1:A:324:ILE:N	2.36	0.41
2:B:221:ILE:CD1	2:B:223:CYS:HB3	2.51	0.41
3:C:49:GLY:HA2	3:C:50:PRO:HA	1.90	0.41
3:C:57:PRO:CG	3:C:79:SER:HB2	2.51	0.41
1:A:17:ALA:HB3	1:A:34:TYR:OH	2.20	0.40
1:A:61:ARG:HA	1:A:150:HIS:HE1	1.85	0.40
1:A:202:LEU:HD23	1:A:365:PHE:CD2	2.56	0.40
1:A:349:VAL:CG1	1:A:383:CYS:SG	3.05	0.40
2:B:46:LYS:N	2:B:47:PRO:HD2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:SER:OG	2:B:172:PRO:HB2	2.21	0.40
2:B:250:ILE:O	2:B:251:LYS:HB2	2.20	0.40
3:C:24:GLN:NE2	3:C:74:THR:CB	2.54	0.40
3:C:78:PHE:CE2	3:C:189:GLN:OE1	2.73	0.40
3:C:248:LYS:CG	3:C:249:PRO:HA	2.44	0.40
1:A:117:PHE:CE2	1:A:193:ILE:CG1	3.03	0.40
1:A:250:PRO:CG	1:A:353:TRP:HA	2.51	0.40
2:B:265:PRO:HG2	2:B:265:PRO:O	2.20	0.40
3:C:47:VAL:HG21	3:C:71:ALA:HB3	2.02	0.40
3:C:85:LEU:HD13	3:C:126:ILE:HD12	2.03	0.40
3:C:165:LYS:HD3	3:C:165:LYS:O	2.21	0.40
1:A:144:VAL:CG2	1:A:145:ALA:N	2.85	0.40
1:A:211:ALA:HB2	1:A:264:ARG:HA	2.04	0.40
2:B:120:ARG:CD	2:B:126:VAL:HG11	2.50	0.40
3:C:9:ILE:HD11	3:C:220:ILE:HD12	2.02	0.40
3:C:129:LEU:HD12	3:C:130:VAL:H	1.80	0.40
3:C:240:GLU:CG	3:C:240:GLU:O	2.69	0.40
1:A:29:VAL:CG2	1:A:30:THR:N	2.85	0.40
1:A:205:HIS:CD2	1:A:377:TYR:HH	2.40	0.40
1:A:283:ARG:CG	1:A:283:ARG:NH1	2.84	0.40
1:A:293:ARG:HD2	1:A:297:ILE:HG21	1.99	0.40
2:B:46:LYS:HG3	2:B:47:PRO:HD3	2.03	0.40
2:B:64:LEU:HA	2:B:64:LEU:HD23	1.83	0.40
2:B:165:ASP:O	2:B:197:LEU:HD23	2.22	0.40
3:C:55:TRP:NE1	3:C:158:VAL:HG23	2.35	0.40
3:C:160:LYS:HG2	3:C:171:TYR:CD2	2.56	0.40
1:A:61:ARG:HA	1:A:150:HIS:CE1	2.57	0.40
1:A:150:HIS:NE2	2:B:57:CYS:SG	2.92	0.40
1:A:199:PRO:HD2	1:A:202:LEU:HD12	2.03	0.40
2:B:56:GLY:C	2:B:58:THR:N	2.74	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	383/386 (99%)	369 (96%)	13 (3%)	1 (0%)	41 73
2	B	226/275 (82%)	216 (96%)	10 (4%)	0	100 100
3	C	278/281 (99%)	271 (98%)	7 (2%)	0	100 100
All	All	887/942 (94%)	856 (96%)	30 (3%)	1 (0%)	54 82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	PRO

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	321/322 (100%)	213 (66%)	108 (34%)	0 1
2	B	194/232 (84%)	122 (63%)	72 (37%)	0 0
3	C	229/230 (100%)	139 (61%)	90 (39%)	0 0
All	All	744/784 (95%)	474 (64%)	270 (36%)	1 0

All (270) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	4	ARG
1	A	12	ARG
1	A	13	GLN
1	A	18	GLU
1	A	21	MET
1	A	26	GLU
1	A	28	ILE
1	A	29	VAL

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Mol	Chain	Res	Type
1	A	33	ARG
1	A	35	PHE
1	A	41	ARG
1	A	45	LYS
1	A	46	MET
1	A	50	LYS
1	A	53	GLU
1	A	58	MET
1	A	61	ARG
1	A	62	ILE
1	A	80	ASP
1	A	84	ILE
1	A	88	LYS
1	A	93	LEU
1	A	94	ARG
1	A	96	LEU
1	A	98	LEU
1	A	108	ILE
1	A	116	ASP
1	A	120	GLU
1	A	121	ASN
1	A	122	LEU
1	A	127	ILE
1	A	130	VAL
1	A	132	GLU
1	A	133	ILE
1	A	135	LYS
1	A	139	TYR
1	A	142	ASP
1	A	149	ILE
1	A	152	SER
1	A	155	ARG
1	A	164	THR
1	A	166	LEU
1	A	168	ARG
1	A	170	ARG
1	A	172	TYR
1	A	174	ARG
1	A	176	LYS
1	A	179	LYS
1	A	181	LYS
1	A	185	HIS

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Mol	Chain	Res	Type
1	A	189	MET
1	A	194	GLU
1	A	195	ASP
1	A	196	LYS
1	A	198	LEU
1	A	200	GLU
1	A	202	LEU
1	A	204	VAL
1	A	213	HIS
1	A	215	ILE
1	A	216	TYR
1	A	219	ARG
1	A	221	LYS
1	A	225	ASP
1	A	228	THR
1	A	231	MET
1	A	237	ASP
1	A	240	GLU
1	A	246	CYS
1	A	252	TYR
1	A	255	ARG
1	A	256	ASN
1	A	262	ARG
1	A	265	MET
1	A	269	GLN
1	A	272	LYS
1	A	276	VAL
1	A	279	GLN
1	A	283	ARG
1	A	288	LYS
1	A	293	ARG
1	A	295	ILE
1	A	297	ILE
1	A	298	LEU
1	A	299	ASP
1	A	301	LEU
1	A	302	ASP
1	A	303	THR
1	A	307	VAL
1	A	308	ARG
1	A	314	ARG
1	A	316	THR

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Mol	Chain	Res	Type
1	A	319	LEU
1	A	324	ILE
1	A	325	GLU
1	A	328	ARG
1	A	334	MET
1	A	341	LYS
1	A	349	VAL
1	A	352	THR
1	A	354	ASN
1	A	357	THR
1	A	358	MET
1	A	369	TYR
1	A	380	CYS
1	A	382	SER
1	A	383	CYS
2	B	46	LYS
2	B	48	ARG
2	B	51	TYR
2	B	53	HIS
2	B	54	LEU
2	B	57	CYS
2	B	60	ASP
2	B	64	LEU
2	B	67	ASN
2	B	68	TYR
2	B	69	ASP
2	B	71	LEU
2	B	75	LEU
2	B	80	ASP
2	B	85	GLN
2	B	87	LEU
2	B	90	LEU
2	B	92	GLU
2	B	93	MET
2	B	95	GLU
2	B	96	MET
2	B	98	LEU
2	B	110	GLU
2	B	113	LEU
2	B	116	LEU
2	B	118	GLU
2	B	120	ARG

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Mol	Chain	Res	Type
2	B	121	GLU
2	B	125	LEU
2	B	127	CYS
2	B	129	PHE
2	B	131	SER
2	B	138	PHE
2	B	140	ARG
2	B	143	ARG
2	B	149	GLN
2	B	153	GLU
2	B	160	ASP
2	B	161	LEU
2	B	165	ASP
2	B	166	LEU
2	B	176	GLU
2	B	177	ILE
2	B	178	ILE
2	B	181	THR
2	B	186	LEU
2	B	188	ASN
2	B	189	ASP
2	B	190	MET
2	B	193	LEU
2	B	209	ASP
2	B	210	LEU
2	B	212	THR
2	B	213	LYS
2	B	216	ASN
2	B	217	GLN
2	B	219	LEU
2	B	231	GLN
2	B	235	LEU
2	B	236	ASP
2	B	239	ASN
2	B	241	ARG
2	B	242	PRO
2	B	243	GLU
2	B	244	LEU
2	B	246	SER
2	B	251	LYS
2	B	259	CYS
2	B	266	GLU

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Mol	Chain	Res	Type
2	B	270	LYS
2	B	271	LYS
2	B	273	LEU
3	C	3	LEU
3	C	5	THR
3	C	16	ASP
3	C	17	ARG
3	C	18	GLU
3	C	19	ILE
3	C	22	LEU
3	C	32	LEU
3	C	33	LEU
3	C	41	ILE
3	C	42	ILE
3	C	56	LYS
3	C	60	MET
3	C	61	VAL
3	C	66	ASP
3	C	68	LEU
3	C	75	LYS
3	C	78	PHE
3	C	84	MET
3	C	89	VAL
3	C	90	ARG
3	C	91	GLN
3	C	92	TYR
3	C	96	LYS
3	C	97	LEU
3	C	104	CYS
3	C	105	GLN
3	C	106	THR
3	C	110	ARG
3	C	111	LYS
3	C	117	PHE
3	C	120	ARG
3	C	124	ASP
3	C	126	ILE
3	C	127	LYS
3	C	128	LEU
3	C	129	LEU
3	C	134	CYS
3	C	135	MET

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Mol	Chain	Res	Type
3	C	136	GLU
3	C	137	ASN
3	C	138	PHE
3	C	141	THR
3	C	149	GLU
3	C	150	LYS
3	C	151	LEU
3	C	155	MET
3	C	156	GLU
3	C	157	LEU
3	C	158	VAL
3	C	159	GLU
3	C	160	LYS
3	C	161	MET
3	C	165	LYS
3	C	167	LYS
3	C	169	TRP
3	C	172	THR
3	C	173	GLN
3	C	174	ASP
3	C	177	LEU
3	C	179	LEU
3	C	182	LYS
3	C	183	GLU
3	C	188	GLU
3	C	193	LYS
3	C	195	CYS
3	C	196	LYS
3	C	217	SER
3	C	219	VAL
3	C	220	ILE
3	C	222	ARG
3	C	230	PHE
3	C	232	GLN
3	C	238	LEU
3	C	239	PHE
3	C	240	GLU
3	C	242	LYS
3	C	248	LYS
3	C	251	LEU
3	C	253	LEU
3	C	254	LEU

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Mol	Chain	Res	Type
3	C	255	GLU
3	C	261	LYS
3	C	262	LYS
3	C	266	GLU
3	C	267	LYS
3	C	273	LYS
3	C	274	GLU
3	C	277	LEU
3	C	281	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	70	HIS
1	A	101	HIS
1	A	102	HIS
1	A	121	ASN
1	A	256	ASN
1	A	279	GLN
1	A	280	HIS
1	A	354	ASN
1	A	366	HIS
2	B	53	HIS
2	B	67	ASN
2	B	85	GLN
2	B	114	HIS
2	B	146	GLN
2	B	147	GLN
2	B	149	GLN
2	B	187	ASN
2	B	188	ASN
2	B	194	GLN
2	B	216	ASN
2	B	217	GLN
2	B	231	GLN
2	B	239	ASN
3	C	20	GLN
3	C	24	GLN
3	C	91	GLN
3	C	105	GLN
3	C	185	HIS

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Mol	Chain	Res	Type
3	C	189	GLN
3	C	268	ASN

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)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

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	$\#\|Z\| > 2$
9	FAD	C	1283	-	53,58,58	1.27	6 (11%)	68,89,89	1.44	12 (17%)
7	SF4	C	1282	3	0,12,12	-	-	-		
7	SF4	B	1274	2	0,12,12	-	-	-		
7	SF4	B	1276	2	0,12,12	-	-	-		
7	SF4	B	1275	2	0,12,12	-	-	-		

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
9	FAD	C	1283	-	-	14/30/50/50	0/6/6/6
7	SF4	C	1282	3	-	-	0/6/5/5
7	SF4	B	1274	2	-	-	0/6/5/5
7	SF4	B	1276	2	-	-	0/6/5/5
7	SF4	B	1275	2	-	-	0/6/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1283	FAD	C9A-C5X	4.19	1.48	1.41
9	C	1283	FAD	C4-N3	-2.98	1.33	1.38
9	C	1283	FAD	C5X-N5	-2.69	1.34	1.39
9	C	1283	FAD	C2B-C1B	-2.54	1.49	1.53
9	C	1283	FAD	C8-C7	2.34	1.46	1.40
9	C	1283	FAD	C2-N3	-2.19	1.33	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	1283	FAD	N3A-C2A-N1A	-3.19	123.69	128.68
9	C	1283	FAD	C4A-C5A-N7A	-3.02	106.25	109.40
9	C	1283	FAD	C4-C4X-N5	2.77	122.17	118.23
9	C	1283	FAD	C3B-C2B-C1B	2.76	105.13	100.98
9	C	1283	FAD	O2-C2-N1	-2.66	117.41	121.83
9	C	1283	FAD	O4-C4-C4X	-2.57	119.79	126.60
9	C	1283	FAD	C4X-C10-N1	-2.48	118.97	124.73
9	C	1283	FAD	C10-N1-C2	2.36	121.63	116.90
9	C	1283	FAD	C4X-C4-N3	2.32	119.08	113.19
9	C	1283	FAD	P-O3P-PA	-2.30	124.93	132.83
9	C	1283	FAD	C4X-C10-N10	2.27	119.81	116.48
9	C	1283	FAD	C4-N3-C2	-2.17	121.64	125.64

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	1283	FAD	C5B-O5B-PA-O2A
9	C	1283	FAD	C2'-C1'-N10-C10
9	C	1283	FAD	C2'-C3'-C4'-O4'
9	C	1283	FAD	O3'-C3'-C4'-O4'
9	C	1283	FAD	C3'-C4'-C5'-O5'
9	C	1283	FAD	O4'-C4'-C5'-O5'

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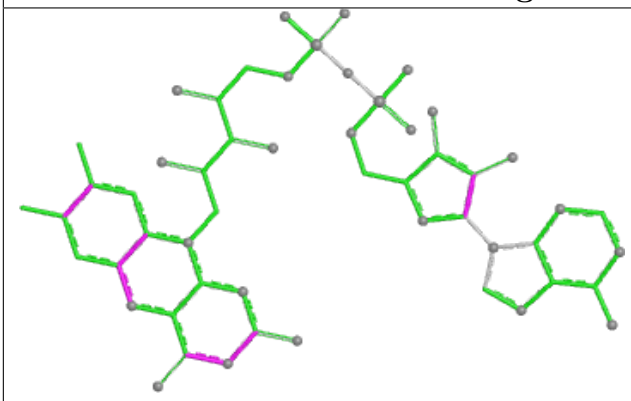
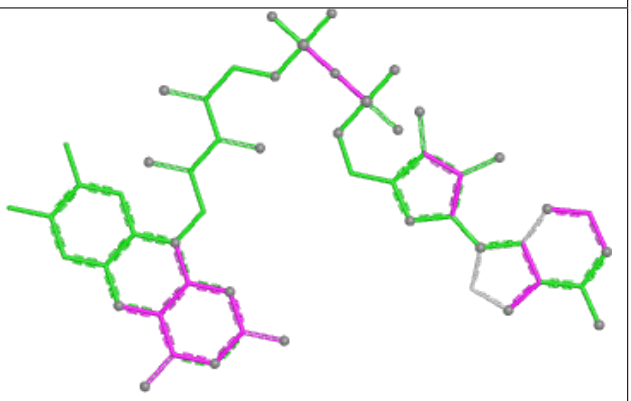
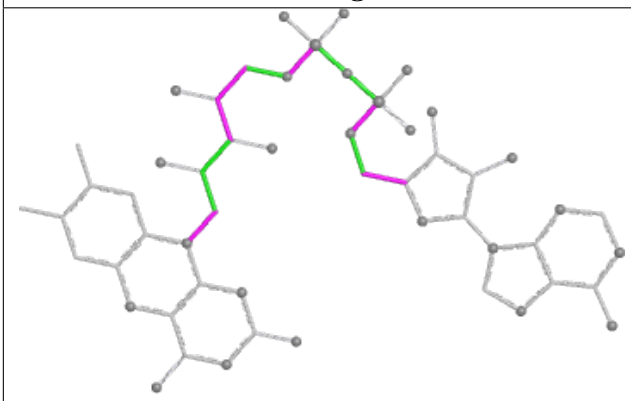
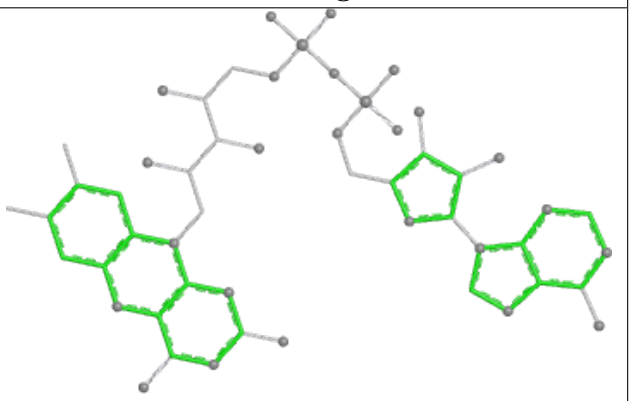
Mol	Chain	Res	Type	Atoms
9	C	1283	FAD	O4B-C4B-C5B-O5B
9	C	1283	FAD	C3B-C4B-C5B-O5B
9	C	1283	FAD	O3'-C3'-C4'-C5'
9	C	1283	FAD	C2'-C3'-C4'-C5'
9	C	1283	FAD	C5B-O5B-PA-O3P
9	C	1283	FAD	C5B-O5B-PA-O1A
9	C	1283	FAD	C5'-O5'-P-O1P
9	C	1283	FAD	C5'-O5'-P-O2P

There are no ring outliers.

5 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	1283	FAD	13	0
7	C	1282	SF4	6	0
7	B	1274	SF4	2	0
7	B	1276	SF4	3	0
7	B	1275	SF4	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand FAD C 1283	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

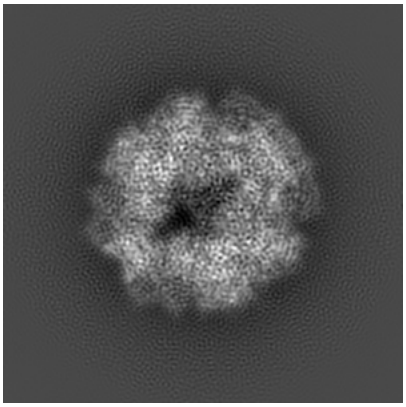
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2513. These allow visual inspection of the internal detail of the map and identification of artifacts.

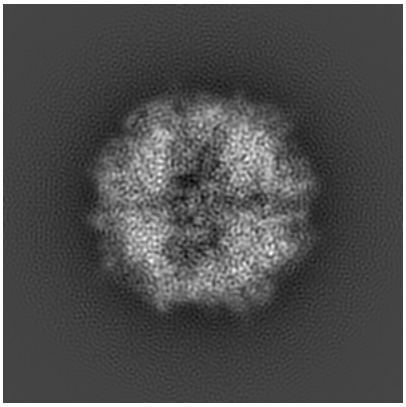
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

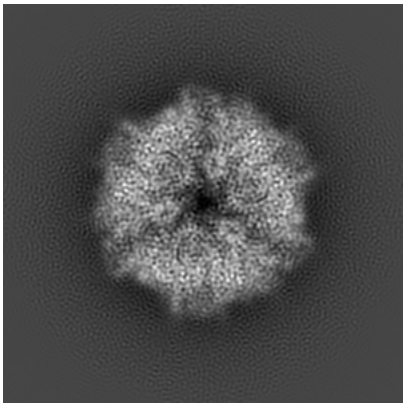
6.1.1 Primary map



X



Y

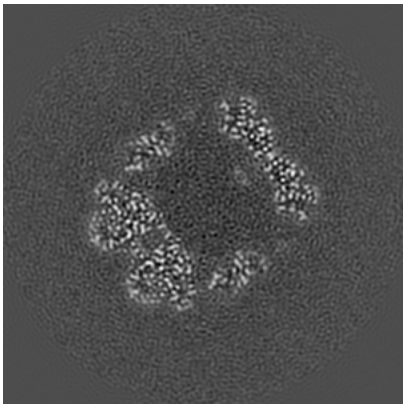


Z

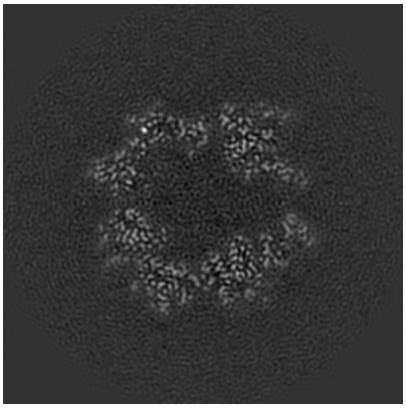
The images above show the map projected in three orthogonal directions.

6.2 Central slices

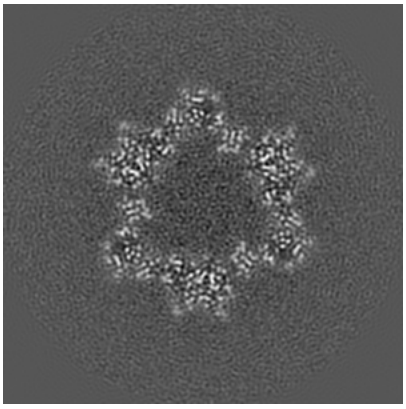
6.2.1 Primary map



X Index: 112



Y Index: 112

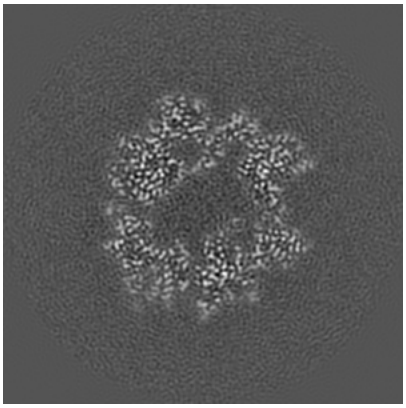


Z Index: 112

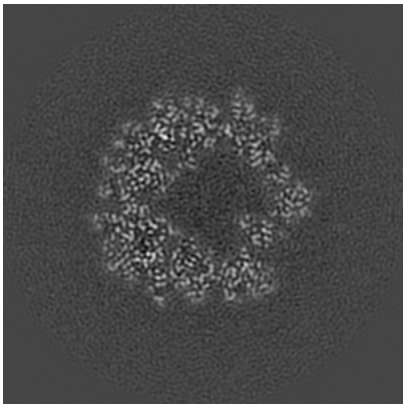
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

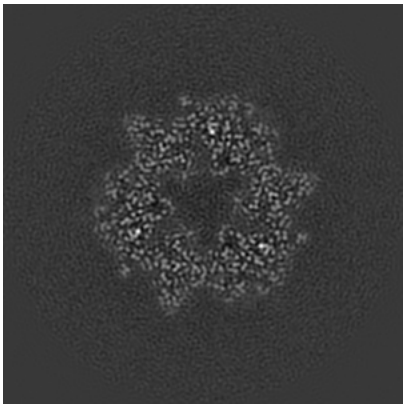
6.3.1 Primary map



X Index: 129



Y Index: 125

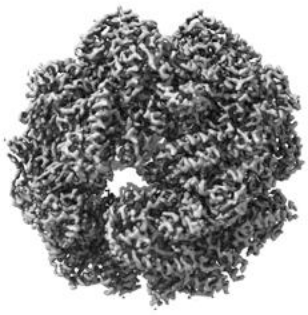


Z Index: 132

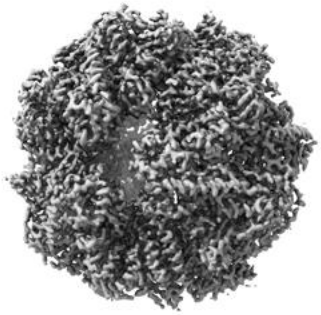
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

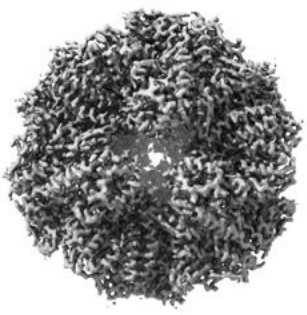
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

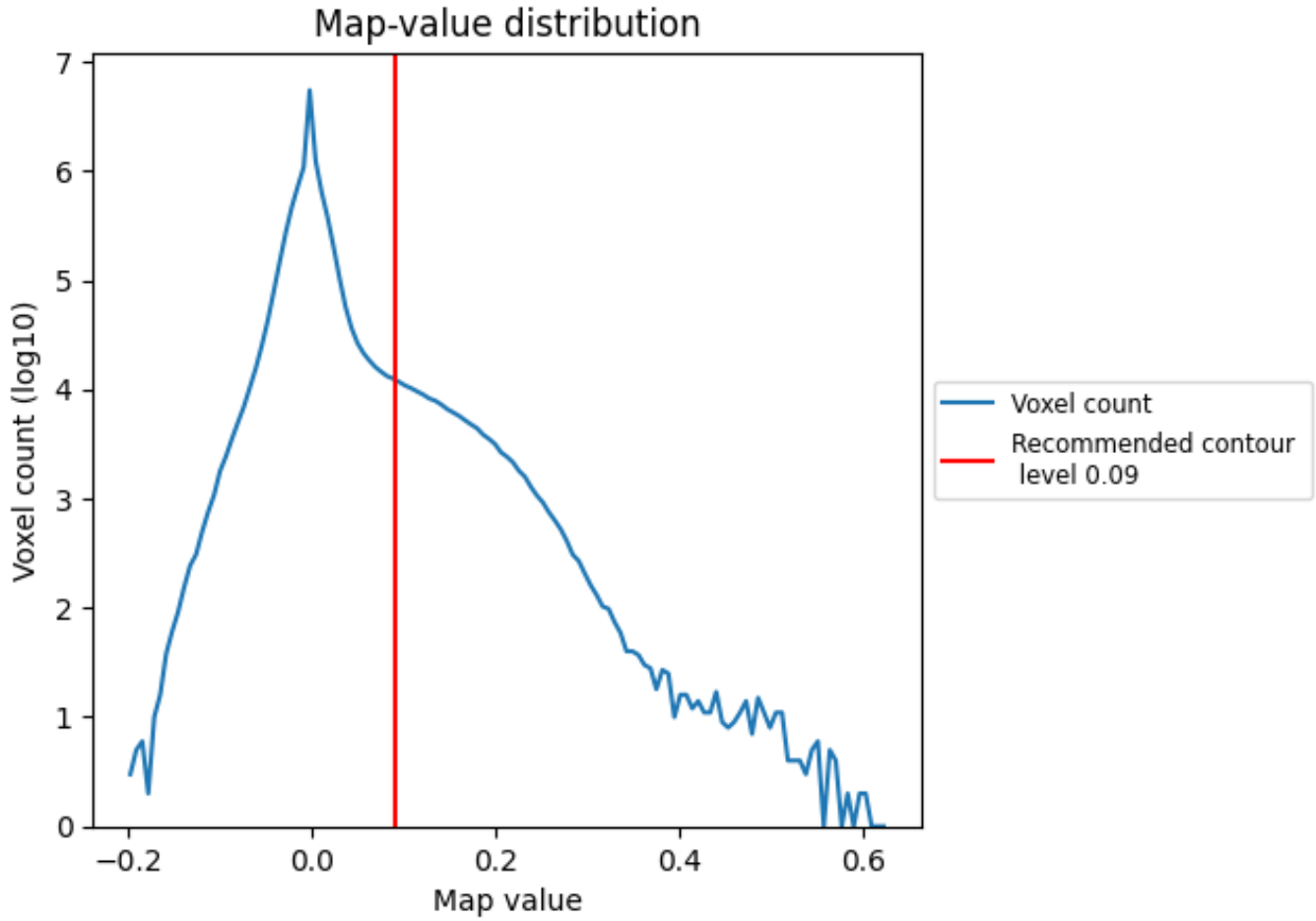
6.5 Mask visualisation (i)

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

7 Map analysis

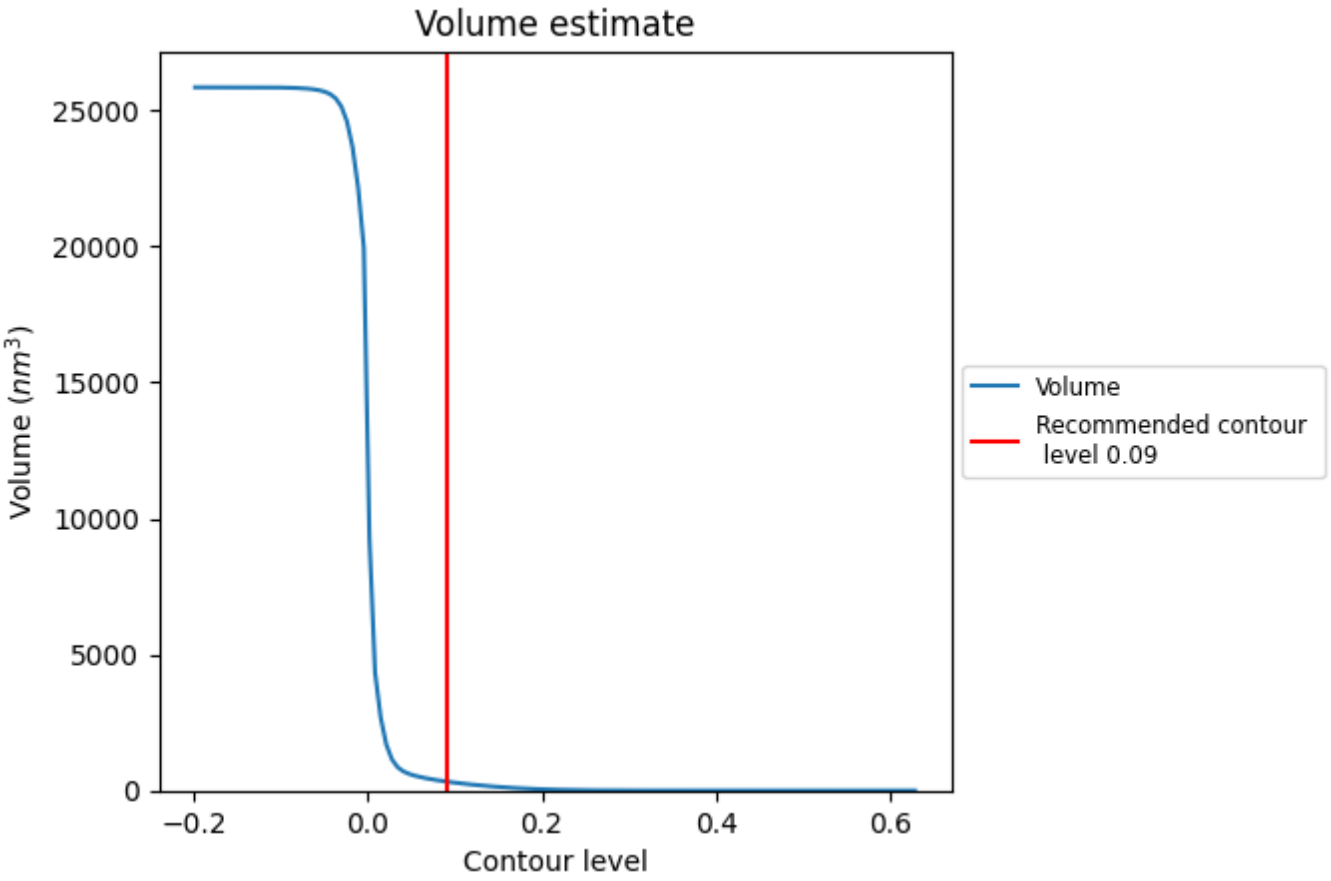
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

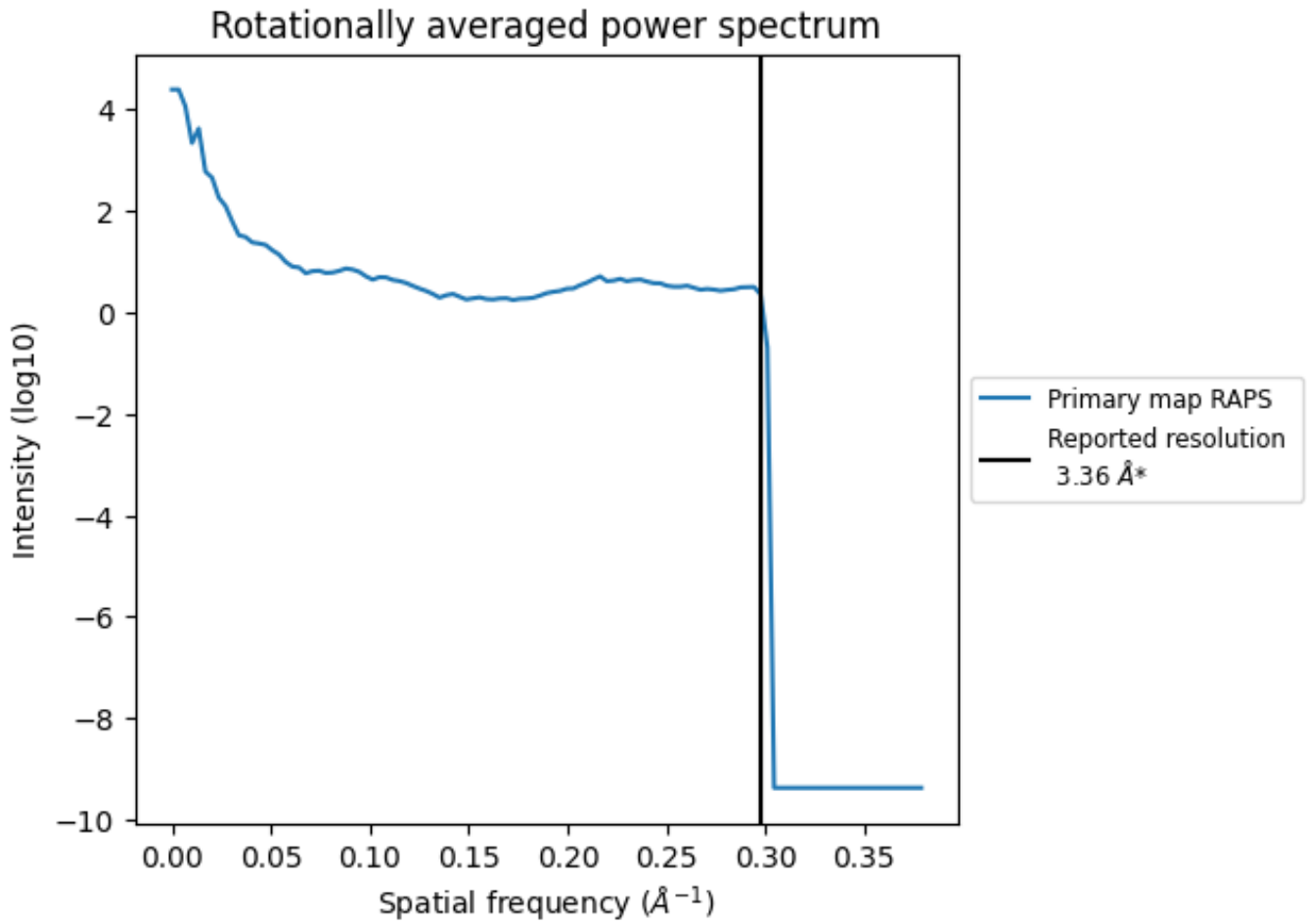
7.2 Volume estimate



The volume at the recommended contour level is 333 nm^3; this corresponds to an approximate mass of 301 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 0.298 Å^{-1}

8 Fourier-Shell correlation (i)

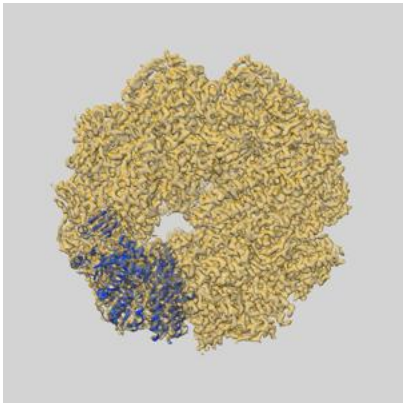
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

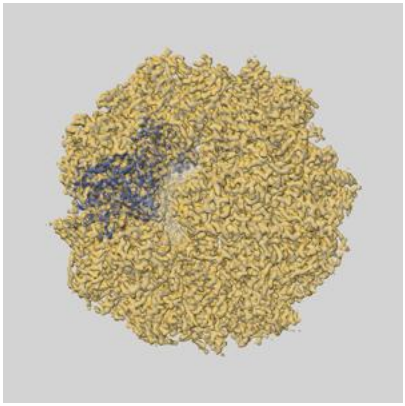
This section contains information regarding the fit between EMDB map EMD-2513 and PDB model 4CI0. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlays

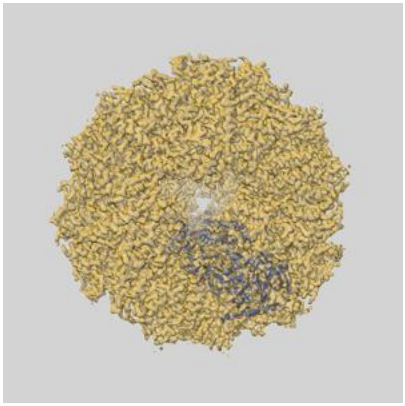
9.1.1 Map-model overlay



X

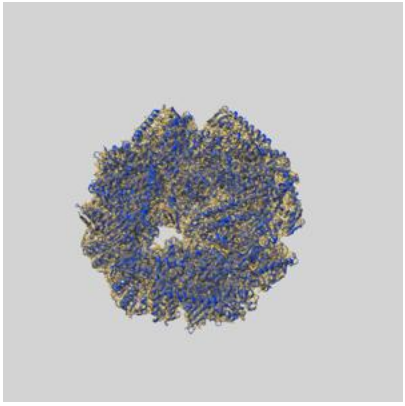


Y

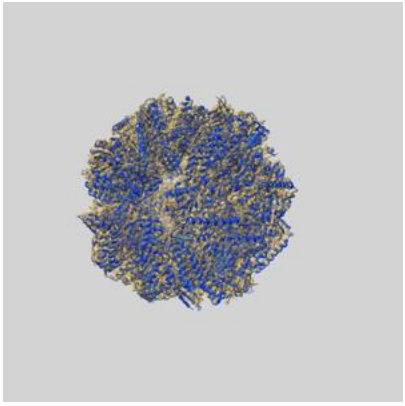


Z

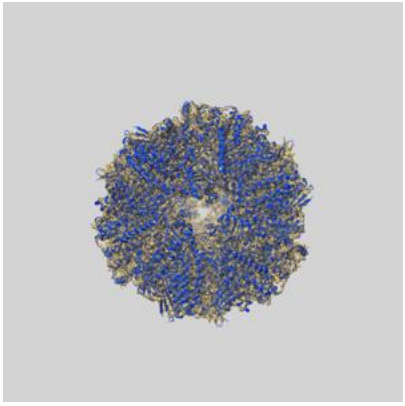
9.1.2 Map-model assembly overlay



X



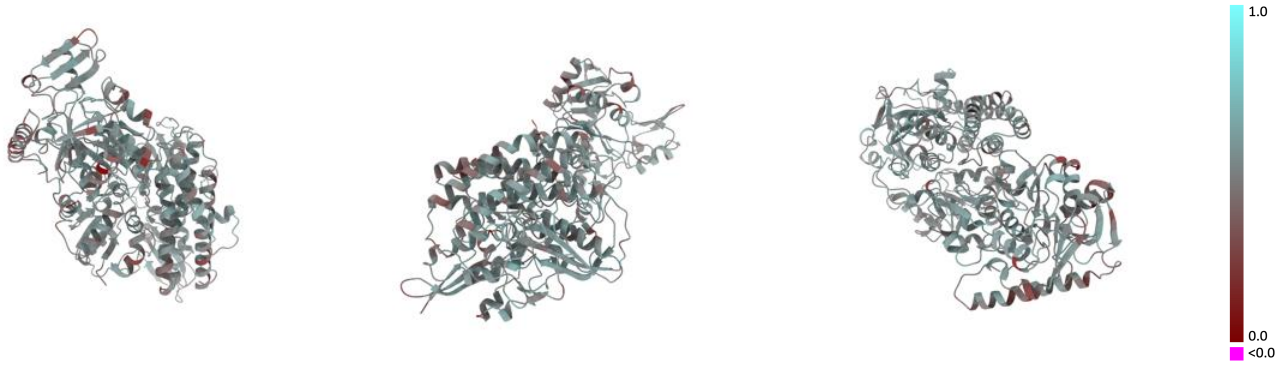
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.09 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.

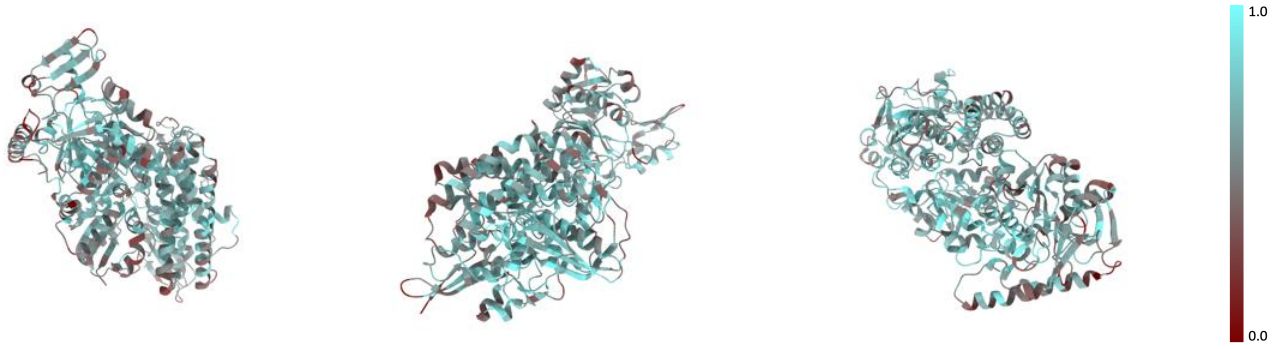
9.2 Q-score mapped to coordinate model (i)



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.

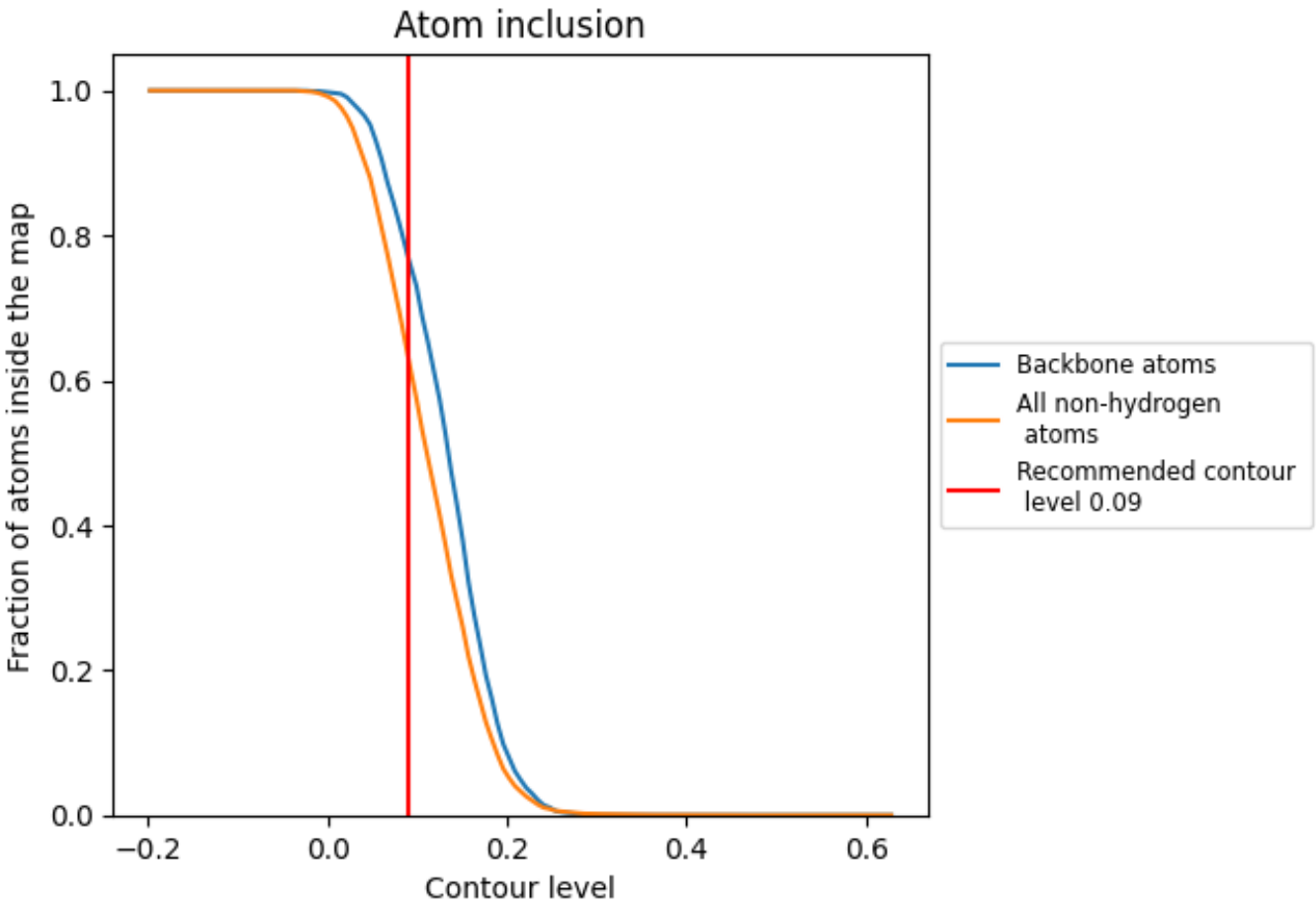
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.09).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 63% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6298	0.5110
A	0.6368	0.5200
B	0.6590	0.5140
C	0.5971	0.4970