Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 02:36 pm GMT

PDB ID	:	2C9F
EMDB ID	:	EMD-1178
Title	:	THE QUASI-ATOMIC MODEL OF THE ADENOVIRUS TYPE 3 PENTON DODECAHEDRON
Authors	:	Fuschiotti, P.; Schoehn, G.; Fender, P.; Fabry, C.M.S.; Hewat, E.A.; Chroboczek, J.; Ruigrok, R.W.H.; Conway, J.F.
Deposited on	:	2005-12-12
Resolution	:	16.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

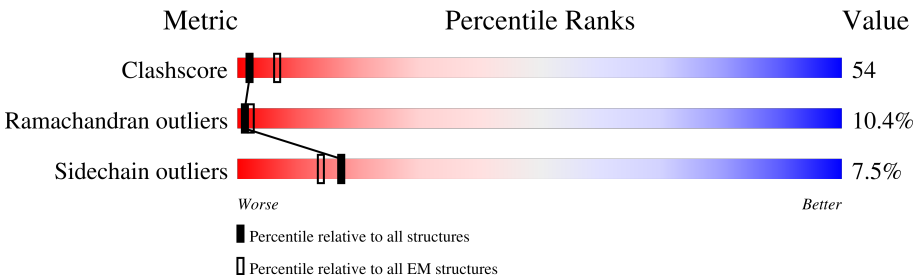
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 16.50 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	523	17%; 30%, 42%, 11%, •, 16%
1	B	523	17%; 30%, 43%, 11%, 16%
1	C	523	16%; 30%, 43%, 11%, •, 16%
1	D	523	16%; 31%, 42%, 11%, •, 16%
1	E	523	16%; 30%, 43%, 11%, •, 16%
2	S	19	53%; 21%, 26%, 5%, 47%
2	T	19	53%; 26%, 21%, 5%, 47%
2	U	19	53%; 21%, 26%, 5%, 47%

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Mol	Chain	Length	Quality of chain
2	V	19	53% 21% 26% 5% 47%
2	W	19	53% 26% 21% 5% 47%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18025 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 PENTON PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	440	3519	2227	608	672	12	0	0
1	B	440	3519	2227	608	672	12	0	0
1	C	440	3519	2227	608	672	12	0	0
1	D	440	3519	2227	608	672	12	0	0
1	E	440	3519	2227	608	672	12	0	0

- Molecule 2 is a protein called FIBER.

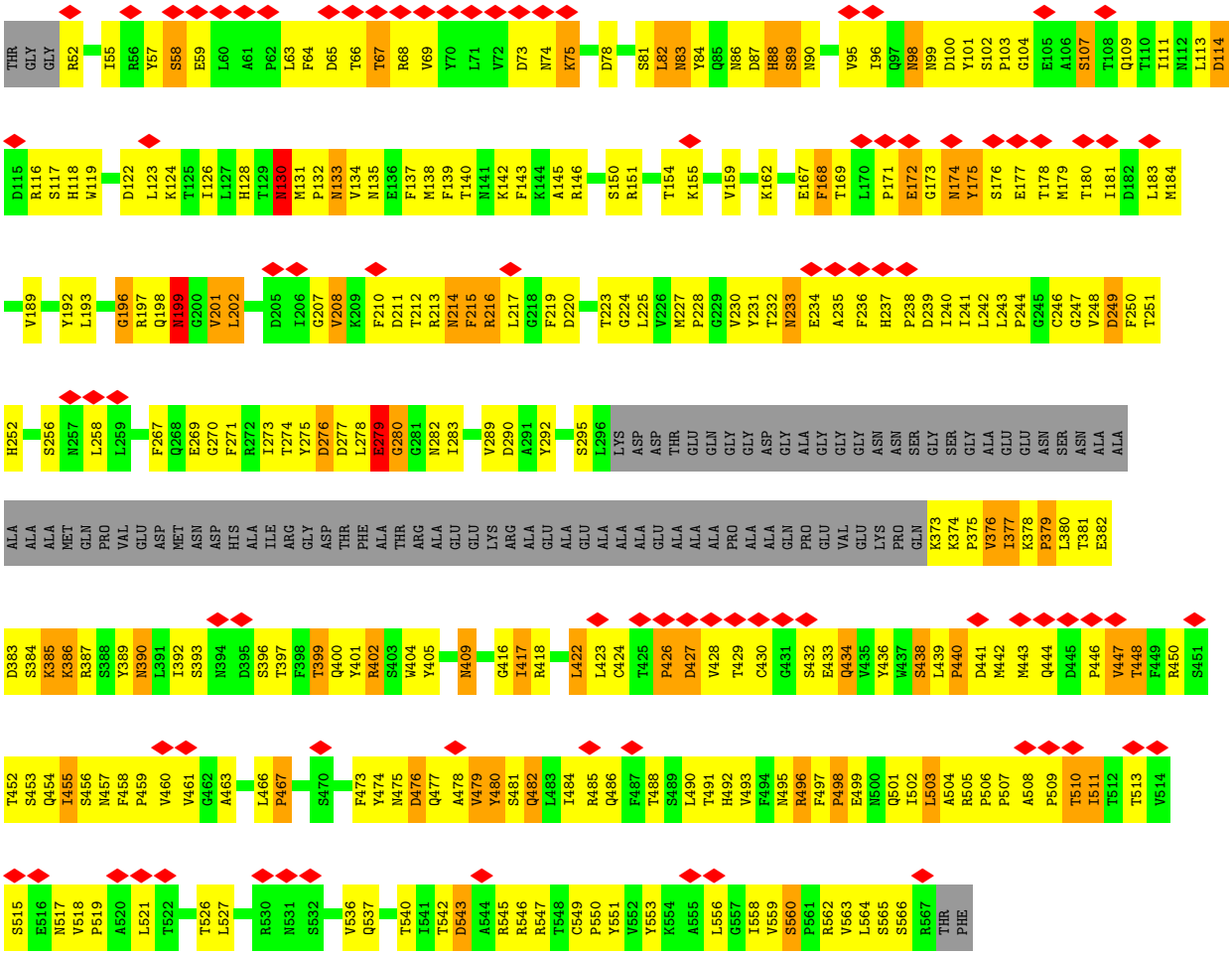
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	S	10	86	58	11	17	0	0
2	T	10	86	58	11	17	0	0
2	U	10	86	58	11	17	0	0
2	V	10	86	58	11	17	0	0
2	W	10	86	58	11	17	0	0

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.

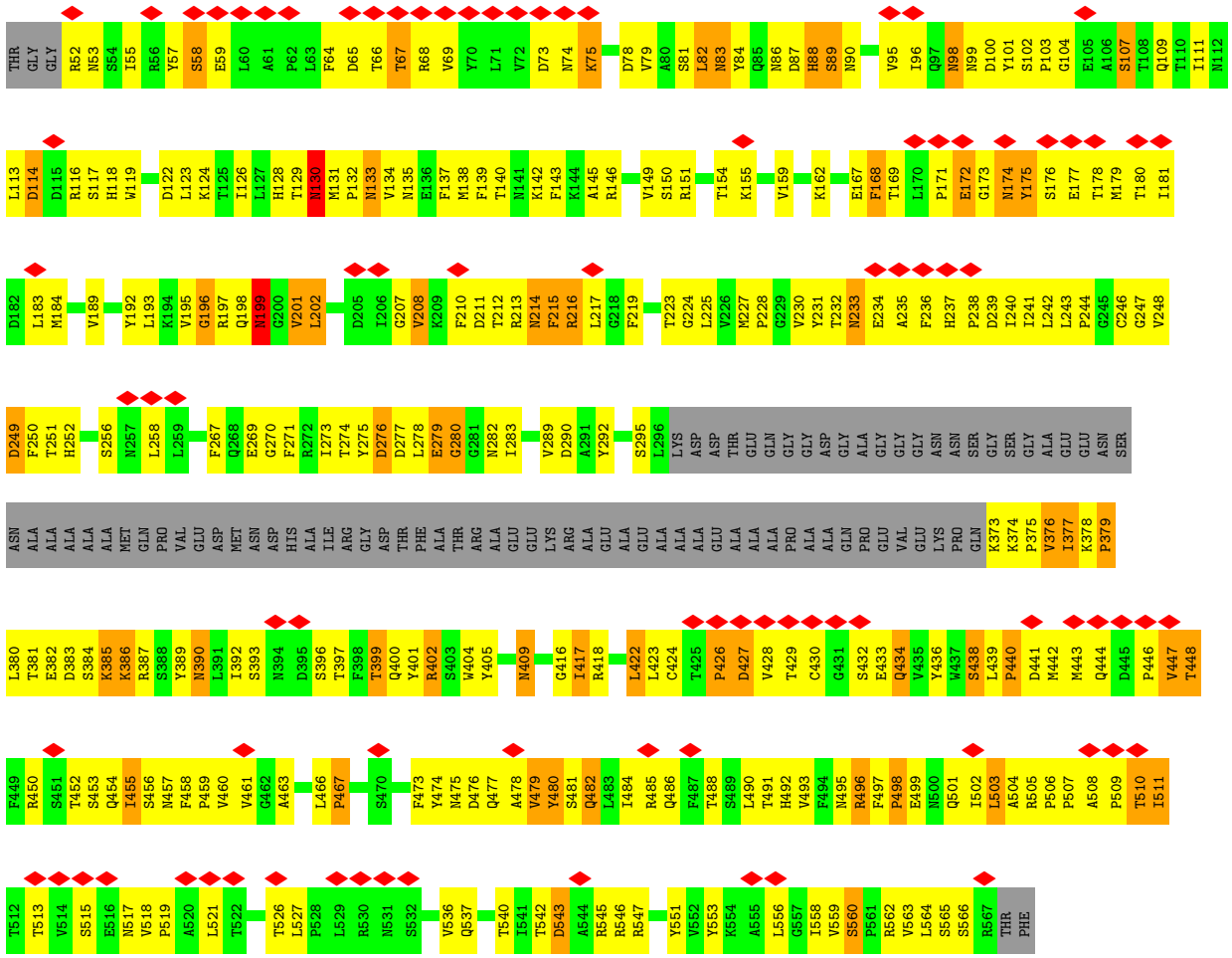
- Molecule 1: PENTON PROTEIN

Chain A: 17% 30% 42% 11% • 16%



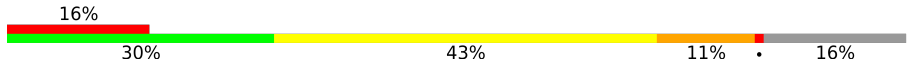
- Molecule 1: PENTON PROTEIN

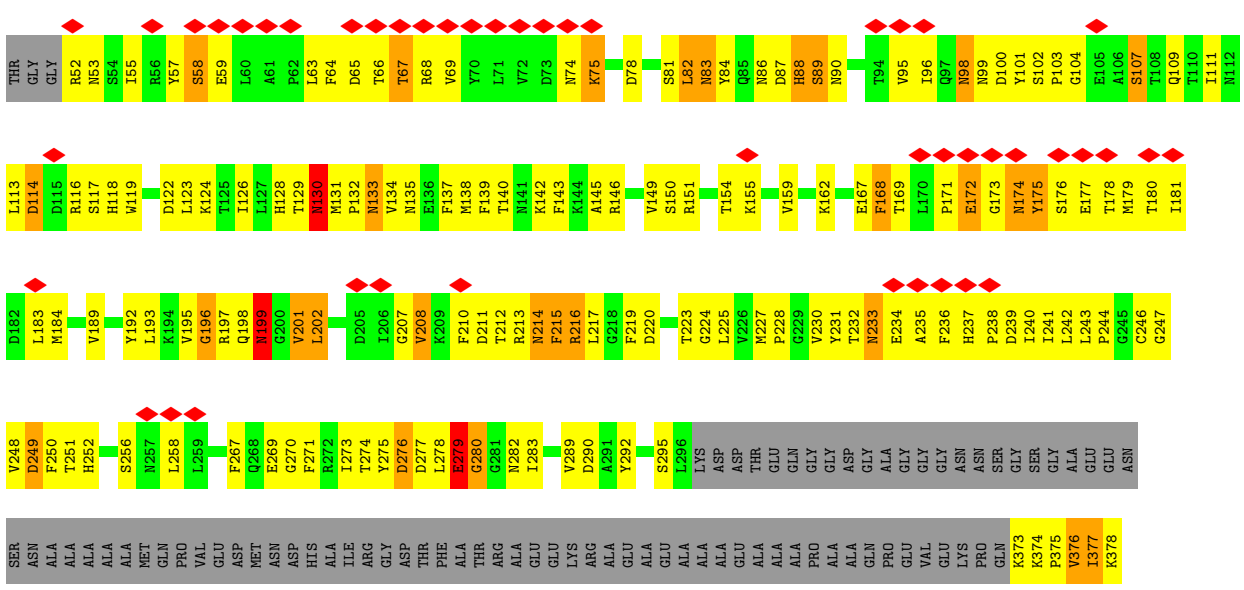
Chain B: 17% 30% 43% 11% 16%

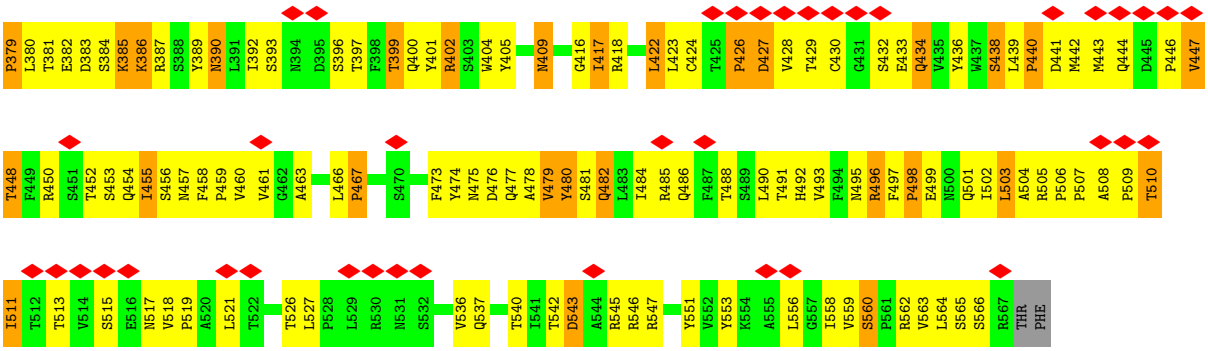


- Molecule 1: PENTON PROTEIN

Chain C:

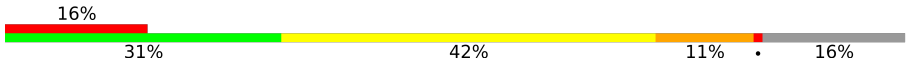


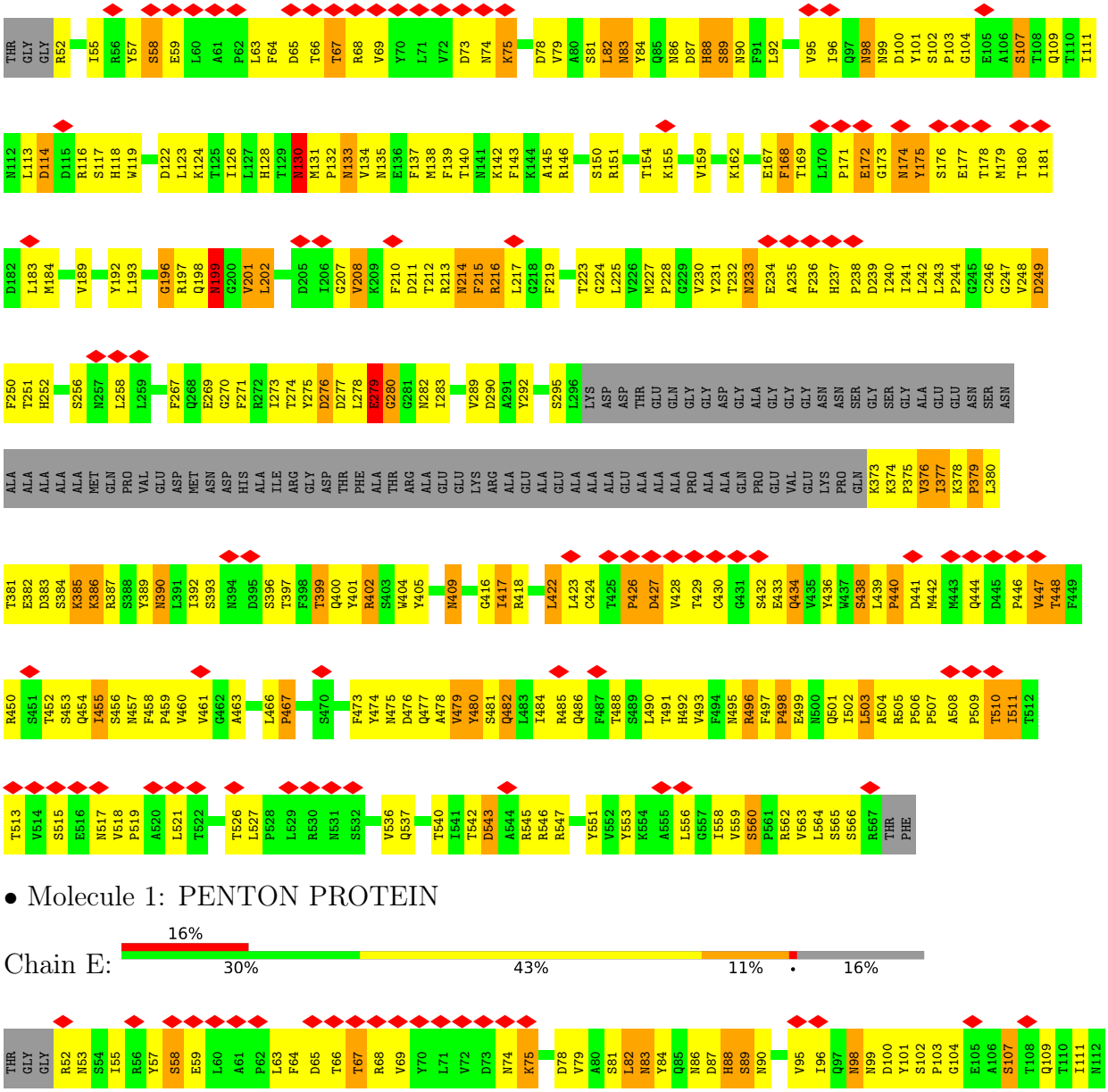




• Molecule 1: PENTON PROTEIN

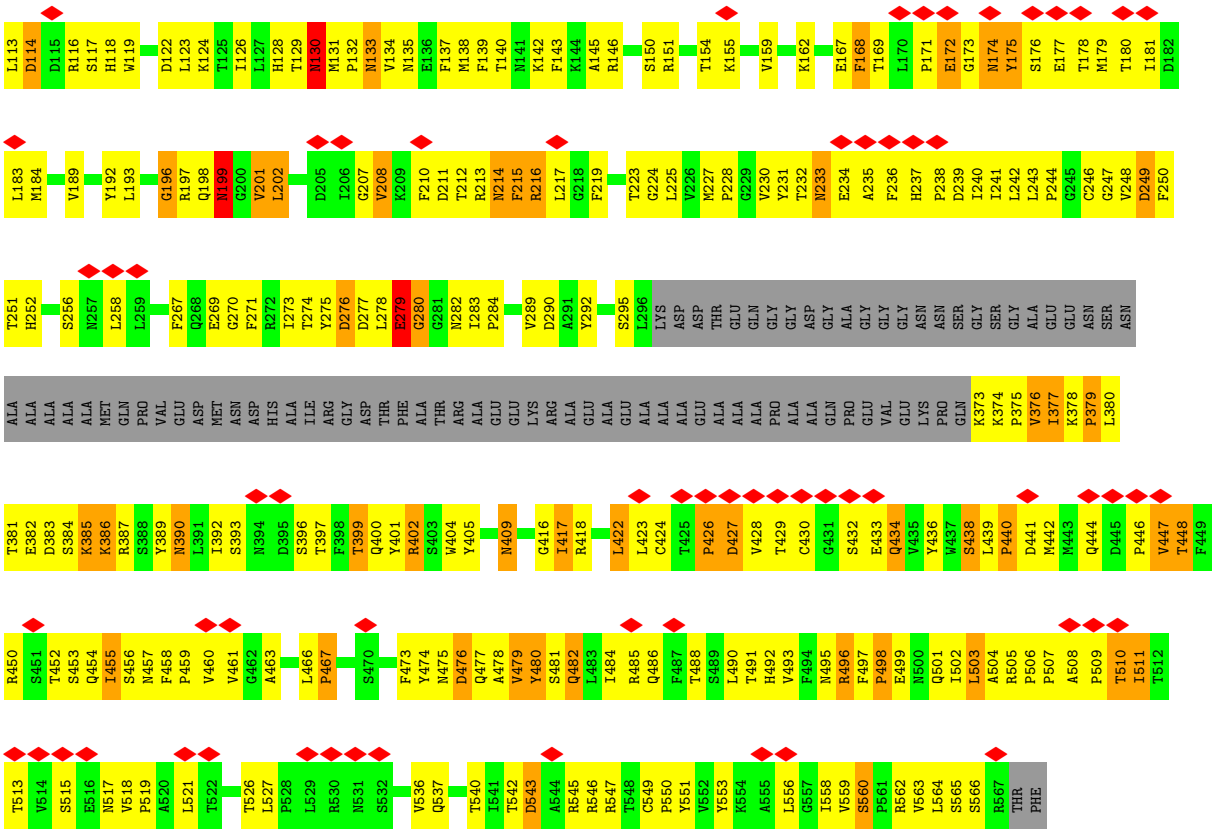
Chain D:





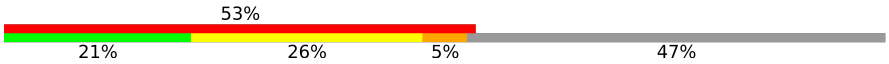
• Molecule 1: PENTON PROTEIN

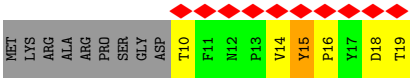
Chain E:



- Molecule 2: FIBER

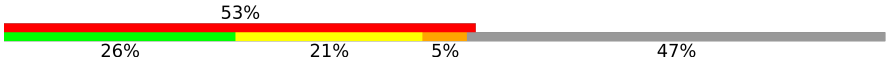
Chain S:

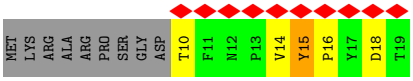




- Molecule 2: FIBER

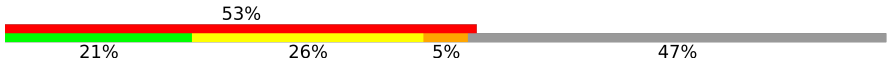
Chain T:

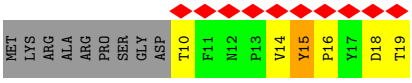




- Molecule 2: FIBER

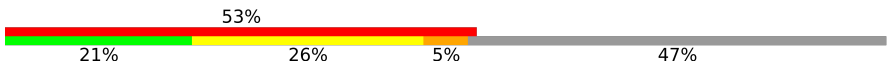
Chain U:

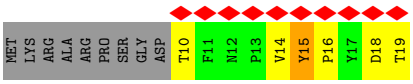




- Molecule 2: FIBER

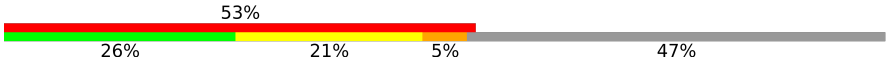
Chain V:

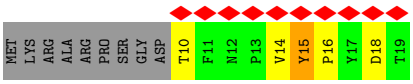




- Molecule 2: FIBER

Chain W:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	1849	Depositor
Resolution determination method	Not provided	
CTF correction method	AMPLITUDE, PHASE	Depositor
Microscope	FEI/PHILIPS CM200T	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	40930	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	509.000	Depositor
Minimum map value	-335.000	Depositor
Average map value	3.055	Depositor
Map value standard deviation	52.415	Depositor
Recommended contour level	91.9	Depositor
Map size (Å)	382.23, 382.23, 382.23	wwPDB
Map dimensions	279, 279, 279	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.61	0/3602	0.81	1/4904 (0.0%)
1	B	0.61	0/3602	0.81	1/4904 (0.0%)
1	C	0.61	0/3602	0.81	1/4904 (0.0%)
1	D	0.61	0/3602	0.81	1/4904 (0.0%)
1	E	0.61	0/3602	0.81	1/4904 (0.0%)
2	S	0.66	0/90	0.69	0/125
2	T	0.66	0/90	0.69	0/125
2	U	0.67	0/90	0.68	0/125
2	V	0.66	0/90	0.69	0/125
2	W	0.66	0/90	0.69	0/125
All	All	0.61	0/18460	0.81	5/25145 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	480	TYR	N-CA-C	-7.27	91.37	111.00
1	A	480	TYR	N-CA-C	-7.26	91.40	111.00
1	D	480	TYR	N-CA-C	-7.26	91.40	111.00
1	B	480	TYR	N-CA-C	-7.25	91.44	111.00
1	E	480	TYR	N-CA-C	-7.24	91.46	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3519	0	3452	425	0
1	B	3519	0	3452	410	0
1	C	3519	0	3452	414	0
1	D	3519	0	3452	420	0
1	E	3519	0	3452	425	0
2	S	86	0	73	19	0
2	T	86	0	73	16	0
2	U	86	0	73	19	0
2	V	86	0	73	17	0
2	W	86	0	73	18	0
All	All	18025	0	17625	1930	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 54.

All (1930) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ARG:NH1	1:B:560:SER:HB3	1.68	1.09
1:D:68:ARG:NH1	1:D:560:SER:HB3	1.68	1.09
1:C:68:ARG:NH1	1:C:560:SER:HB3	1.68	1.09
1:A:68:ARG:NH1	1:A:560:SER:HB3	1.68	1.08
1:E:68:ARG:NH1	1:E:560:SER:HB3	1.68	1.08
1:B:197:ARG:HE	1:B:198:GLN:HE21	1.05	1.03
1:A:477:GLN:O	1:A:481:SER:HB2	1.59	1.03
1:E:477:GLN:O	1:E:481:SER:HB2	1.59	1.02
1:D:466:LEU:HD12	1:D:467:PRO:HD2	1.41	1.02
1:D:477:GLN:O	1:D:481:SER:HB2	1.59	1.01
1:D:197:ARG:HE	1:D:198:GLN:NE2	1.59	1.01
1:E:197:ARG:HE	1:E:198:GLN:NE2	1.59	1.01
1:A:197:ARG:HE	1:A:198:GLN:HE21	1.05	1.01
1:B:197:ARG:HE	1:B:198:GLN:NE2	1.59	1.01
1:B:477:GLN:O	1:B:481:SER:HB2	1.59	1.01
1:C:466:LEU:HD12	1:C:467:PRO:HD2	1.41	1.01
1:A:68:ARG:HG2	1:A:68:ARG:HH11	1.26	1.00
1:A:488:THR:CG2	1:B:479:VAL:HG12	1.91	1.00
1:C:197:ARG:HE	1:C:198:GLN:NE2	1.59	1.00
1:C:477:GLN:O	1:C:481:SER:HB2	1.59	1.00
1:B:466:LEU:HD12	1:B:467:PRO:HD2	1.41	1.00
1:E:481:SER:O	1:E:485:ARG:N	1.95	1.00
1:A:481:SER:O	1:A:485:ARG:N	1.95	1.00
1:C:68:ARG:HG2	1:C:68:ARG:HH11	1.26	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:SER:O	1:B:485:ARG:N	1.95	1.00
1:D:68:ARG:HG2	1:D:68:ARG:HH11	1.26	1.00
1:E:466:LEU:HD12	1:E:467:PRO:HD2	1.41	0.99
1:B:68:ARG:HG2	1:B:68:ARG:HH11	1.26	0.99
1:A:197:ARG:HE	1:A:198:GLN:NE2	1.59	0.99
1:C:481:SER:O	1:C:485:ARG:N	1.95	0.99
1:E:68:ARG:HH11	1:E:68:ARG:HG2	1.25	0.99
1:D:481:SER:O	1:D:485:ARG:N	1.95	0.99
1:A:466:LEU:HD12	1:A:467:PRO:HD2	1.41	0.98
1:C:197:ARG:HE	1:C:198:GLN:HE21	1.05	0.98
1:D:490:LEU:HB2	1:E:230:VAL:HG11	1.45	0.98
1:A:479:VAL:HG12	1:E:488:THR:CG2	1.94	0.98
1:A:484:ILE:HG21	1:B:480:TYR:CE1	1.97	0.98
1:A:479:VAL:HG12	1:E:488:THR:HG23	1.46	0.97
1:C:488:THR:HG23	1:D:479:VAL:HG12	1.45	0.97
1:C:490:LEU:HB2	1:D:230:VAL:HG11	1.47	0.97
1:D:484:ILE:HG21	1:E:480:TYR:CE1	1.99	0.97
1:E:477:GLN:O	1:E:481:SER:CB	2.13	0.97
1:C:477:GLN:O	1:C:481:SER:CB	2.13	0.97
1:D:477:GLN:O	1:D:481:SER:CB	2.13	0.97
1:A:488:THR:HG23	1:B:479:VAL:HG12	1.46	0.96
1:A:477:GLN:O	1:A:481:SER:CB	2.13	0.96
1:B:477:GLN:O	1:B:481:SER:CB	2.13	0.95
1:A:480:TYR:CE1	1:E:484:ILE:HG21	2.00	0.95
1:C:488:THR:CG2	1:D:479:VAL:HG12	1.97	0.95
1:D:488:THR:CG2	1:E:479:VAL:HG12	1.96	0.95
1:A:230:VAL:HG11	1:E:490:LEU:HB2	1.48	0.95
1:E:197:ARG:HE	1:E:198:GLN:HE21	1.05	0.95
1:D:132:PRO:HA	1:D:175:TYR:OH	1.67	0.94
1:D:488:THR:HG23	1:E:479:VAL:HG12	1.49	0.94
1:D:197:ARG:HE	1:D:198:GLN:HE21	1.05	0.94
1:E:132:PRO:HA	1:E:175:TYR:OH	1.67	0.94
1:D:230:VAL:HG13	1:D:501:GLN:NE2	1.83	0.94
1:B:230:VAL:HG13	1:B:501:GLN:NE2	1.83	0.93
1:C:230:VAL:HG13	1:C:501:GLN:NE2	1.83	0.93
1:E:230:VAL:HG13	1:E:501:GLN:NE2	1.83	0.93
1:B:132:PRO:HA	1:B:175:TYR:OH	1.67	0.92
1:C:132:PRO:HA	1:C:175:TYR:OH	1.67	0.92
1:A:230:VAL:HG13	1:A:501:GLN:NE2	1.83	0.92
1:A:132:PRO:HA	1:A:175:TYR:OH	1.67	0.91
1:E:68:ARG:HH12	1:E:560:SER:HB3	1.36	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:ILE:CG2	1:B:480:TYR:CE1	2.54	0.91
1:D:274:THR:HG22	1:D:276:ASP:H	1.37	0.90
1:E:274:THR:HG22	1:E:276:ASP:H	1.37	0.90
1:C:68:ARG:HH12	1:C:560:SER:HB3	1.36	0.89
1:B:274:THR:HG22	1:B:276:ASP:H	1.37	0.89
1:B:83:ASN:HA	1:B:86:ASN:HD22	1.38	0.89
1:D:83:ASN:HA	1:D:86:ASN:HD22	1.38	0.88
1:A:68:ARG:HH12	1:A:560:SER:HB3	1.36	0.88
1:C:275:TYR:CE1	1:C:402:ARG:HD3	2.09	0.88
1:B:275:TYR:CE1	1:B:402:ARG:HD3	2.09	0.87
1:C:83:ASN:HA	1:C:86:ASN:HD22	1.38	0.87
1:A:275:TYR:CE1	1:A:402:ARG:HD3	2.09	0.87
1:A:377:ILE:O	1:A:379:PRO:HD3	1.75	0.87
1:C:274:THR:HG22	1:C:276:ASP:H	1.37	0.87
1:C:377:ILE:O	1:C:379:PRO:HD3	1.75	0.87
1:A:217:LEU:HB2	1:A:232:THR:HG21	1.57	0.87
1:E:83:ASN:HA	1:E:86:ASN:HD22	1.38	0.87
1:B:377:ILE:O	1:B:379:PRO:HD3	1.75	0.87
1:D:217:LEU:HB2	1:D:232:THR:HG21	1.56	0.87
1:A:274:THR:HG22	1:A:276:ASP:H	1.37	0.87
1:B:217:LEU:HB2	1:B:232:THR:HG21	1.57	0.87
1:D:275:TYR:CE1	1:D:402:ARG:HD3	2.09	0.87
1:D:68:ARG:HH12	1:D:560:SER:HB3	1.36	0.87
1:E:275:TYR:CE1	1:E:402:ARG:HD3	2.09	0.86
1:C:484:ILE:HG21	1:D:480:TYR:CE1	2.10	0.86
1:A:83:ASN:HA	1:A:86:ASN:HD22	1.38	0.86
1:C:100:ASP:OD2	1:D:450:ARG:NH1	2.09	0.86
1:D:377:ILE:O	1:D:379:PRO:HD3	1.75	0.86
1:E:377:ILE:O	1:E:379:PRO:HD3	1.75	0.86
1:B:68:ARG:HH12	1:B:560:SER:HB3	1.36	0.86
1:B:100:ASP:OD2	1:C:450:ARG:NH1	2.09	0.85
1:E:217:LEU:HB2	1:E:232:THR:HG21	1.57	0.85
1:A:473:PHE:O	1:A:511:ILE:HA	1.77	0.85
1:C:217:LEU:HB2	1:C:232:THR:HG21	1.57	0.85
1:D:473:PHE:O	1:D:511:ILE:HA	1.77	0.85
1:D:442:MET:HE3	1:D:559:VAL:HG21	1.58	0.85
1:E:526:THR:HG21	1:E:562:ARG:HH21	1.42	0.84
1:C:526:THR:HG21	1:C:562:ARG:HH21	1.42	0.84
1:E:473:PHE:O	1:E:511:ILE:HA	1.77	0.84
1:E:442:MET:HE3	1:E:559:VAL:HG21	1.60	0.84
1:A:484:ILE:HG21	1:B:480:TYR:CD1	2.12	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:526:THR:HG21	1:B:562:ARG:HH21	1.42	0.84
1:C:473:PHE:O	1:C:511:ILE:HA	1.77	0.83
1:D:526:THR:HG21	1:D:562:ARG:HH21	1.42	0.83
1:B:473:PHE:O	1:B:511:ILE:HA	1.77	0.83
1:A:526:THR:HG21	1:A:562:ARG:HH21	1.42	0.82
1:A:488:THR:HG23	1:B:479:VAL:O	1.78	0.82
1:C:485:ARG:NE	1:D:234:GLU:OE2	2.12	0.82
1:B:542:THR:CG2	1:B:546:ARG:HA	2.10	0.81
1:C:67:THR:HG21	1:D:447:VAL:HG22	1.61	0.81
1:D:542:THR:CG2	1:D:546:ARG:HA	2.10	0.81
1:A:484:ILE:CG2	1:B:480:TYR:CD1	2.63	0.81
1:A:490:LEU:HB2	1:B:230:VAL:HG11	1.62	0.81
1:C:542:THR:CG2	1:C:546:ARG:HA	2.10	0.81
1:B:488:THR:HG23	1:C:479:VAL:HG12	1.62	0.81
1:D:485:ARG:NE	1:E:234:GLU:OE2	2.12	0.81
1:E:197:ARG:NE	1:E:198:GLN:HE21	1.80	0.80
1:C:197:ARG:NE	1:C:198:GLN:HE21	1.80	0.80
1:E:542:THR:CG2	1:E:546:ARG:HA	2.10	0.80
1:A:542:THR:CG2	1:A:546:ARG:HA	2.10	0.80
1:C:490:LEU:CB	1:D:230:VAL:HG11	2.11	0.80
1:D:490:LEU:CB	1:E:230:VAL:HG11	2.12	0.80
1:A:197:ARG:NE	1:A:198:GLN:HE21	1.80	0.80
1:A:234:GLU:OE2	1:E:485:ARG:NE	2.14	0.80
1:B:197:ARG:NE	1:B:198:GLN:HE21	1.80	0.79
1:A:480:TYR:CE1	1:E:484:ILE:CG2	2.65	0.79
1:B:466:LEU:HD12	1:B:467:PRO:CD	2.12	0.79
1:D:197:ARG:NE	1:D:198:GLN:HE21	1.80	0.79
1:E:466:LEU:HD12	1:E:467:PRO:CD	2.12	0.79
1:C:466:LEU:HD12	1:C:467:PRO:CD	2.12	0.79
1:D:104:GLY:O	1:D:107:SER:HB3	1.83	0.79
1:D:68:ARG:NH1	1:D:68:ARG:HG2	1.97	0.79
1:A:466:LEU:HD12	1:A:467:PRO:CD	2.12	0.78
1:D:466:LEU:HD12	1:D:467:PRO:CD	2.12	0.78
1:E:104:GLY:O	1:E:107:SER:HB3	1.83	0.78
1:A:401:TYR:CD1	1:A:502:ILE:HG12	2.19	0.78
1:D:100:ASP:OD2	1:E:450:ARG:NH1	2.15	0.78
1:D:230:VAL:HG13	1:D:501:GLN:HE22	1.47	0.78
1:A:230:VAL:HG11	1:E:490:LEU:CB	2.13	0.78
1:D:401:TYR:CD1	1:D:502:ILE:HG12	2.19	0.78
1:E:401:TYR:CD1	1:E:502:ILE:HG12	2.19	0.78
1:A:104:GLY:O	1:A:107:SER:HB3	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:LEU:HB2	1:A:232:THR:CG2	2.14	0.77
1:B:104:GLY:O	1:B:107:SER:HB3	1.83	0.77
1:C:217:LEU:HB2	1:C:232:THR:CG2	2.14	0.77
1:E:68:ARG:NH1	1:E:68:ARG:HG2	1.97	0.77
1:A:230:VAL:HG13	1:A:501:GLN:HE22	1.47	0.77
1:B:488:THR:CG2	1:C:479:VAL:HG12	2.14	0.77
1:B:401:TYR:CD1	1:B:502:ILE:HG12	2.19	0.77
1:C:104:GLY:O	1:C:107:SER:HB3	1.83	0.77
1:C:401:TYR:CD1	1:C:502:ILE:HG12	2.19	0.77
1:D:217:LEU:HB2	1:D:232:THR:CG2	2.14	0.77
1:A:480:TYR:CD1	1:E:484:ILE:HG21	2.19	0.77
1:C:230:VAL:HG13	1:C:501:GLN:HE22	1.47	0.77
1:B:145:ALA:HB3	1:B:168:PHE:HE1	1.50	0.77
1:D:484:ILE:CG2	1:E:480:TYR:CE1	2.66	0.77
1:B:217:LEU:HB2	1:B:232:THR:CG2	2.14	0.76
1:D:145:ALA:HB3	1:D:168:PHE:HE1	1.50	0.76
1:E:376:VAL:HG23	1:E:377:ILE:N	2.01	0.76
1:E:217:LEU:HB2	1:E:232:THR:CG2	2.14	0.76
1:C:376:VAL:HG23	1:C:377:ILE:N	2.01	0.76
1:E:145:ALA:HB3	1:E:168:PHE:HE1	1.50	0.76
1:E:230:VAL:HG13	1:E:501:GLN:HE22	1.47	0.76
1:A:67:THR:HG21	1:B:447:VAL:HG22	1.65	0.76
1:B:376:VAL:HG23	1:B:377:ILE:N	2.01	0.76
1:C:145:ALA:HB3	1:C:168:PHE:HE1	1.50	0.76
1:B:111:ILE:HD13	1:C:447:VAL:HG11	1.67	0.76
1:C:135:ASN:HA	1:C:172:GLU:HG2	1.68	0.76
1:A:145:ALA:HB3	1:A:168:PHE:HE1	1.50	0.76
1:A:376:VAL:HG23	1:A:377:ILE:N	2.01	0.76
1:D:135:ASN:HA	1:D:172:GLU:HG2	1.68	0.76
1:D:376:VAL:HG23	1:D:377:ILE:N	2.01	0.76
1:B:96:ILE:HG22	1:B:98:ASN:H	1.51	0.75
1:B:230:VAL:HG13	1:B:501:GLN:HE22	1.47	0.75
1:B:134:VAL:HG13	1:B:140:THR:O	1.87	0.75
1:B:542:THR:HG22	1:B:546:ARG:HA	1.69	0.75
1:D:134:VAL:HG13	1:D:140:THR:O	1.87	0.75
1:A:96:ILE:HG22	1:A:98:ASN:H	1.51	0.75
1:B:526:THR:HG21	1:B:562:ARG:NH2	2.02	0.75
1:A:135:ASN:HA	1:A:172:GLU:HG2	1.68	0.75
1:A:526:THR:HG21	1:A:562:ARG:NH2	2.02	0.75
1:B:146:ARG:O	1:B:246:CYS:HB2	1.87	0.75
1:B:135:ASN:HA	1:B:172:GLU:HG2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:ARG:NH1	1:C:68:ARG:HG2	1.97	0.74
1:C:96:ILE:HG22	1:C:98:ASN:H	1.51	0.74
1:E:135:ASN:HA	1:E:172:GLU:HG2	1.68	0.74
1:C:551:TYR:CE2	1:D:422:LEU:HD21	2.22	0.74
1:A:277:ASP:HB3	1:A:417:ILE:HD11	1.70	0.74
1:B:277:ASP:HB3	1:B:417:ILE:HD11	1.70	0.74
1:D:146:ARG:O	1:D:246:CYS:HB2	1.87	0.74
1:D:484:ILE:HG21	1:E:480:TYR:CD1	2.22	0.74
1:E:146:ARG:O	1:E:246:CYS:HB2	1.87	0.74
1:E:526:THR:HG21	1:E:562:ARG:NH2	2.02	0.74
1:E:542:THR:HG22	1:E:546:ARG:HA	1.68	0.74
1:A:134:VAL:HG13	1:A:140:THR:O	1.87	0.74
1:C:134:VAL:HG13	1:C:140:THR:O	1.87	0.74
1:C:146:ARG:O	1:C:246:CYS:HB2	1.87	0.74
1:D:542:THR:HG22	1:D:546:ARG:HA	1.69	0.74
1:E:134:VAL:HG13	1:E:140:THR:O	1.87	0.74
1:D:96:ILE:HG22	1:D:98:ASN:H	1.51	0.74
1:D:510:THR:O	1:D:511:ILE:HB	1.88	0.73
1:A:542:THR:HG22	1:A:546:ARG:HA	1.69	0.73
1:C:277:ASP:HB3	1:C:417:ILE:HD11	1.70	0.73
1:D:277:ASP:HB3	1:D:417:ILE:HD11	1.70	0.73
1:E:277:ASP:HB3	1:E:417:ILE:HD11	1.70	0.73
1:D:526:THR:HG21	1:D:562:ARG:NH2	2.02	0.73
1:A:510:THR:O	1:A:511:ILE:HB	1.88	0.73
1:B:510:THR:O	1:B:511:ILE:HB	1.88	0.73
1:C:526:THR:HG21	1:C:562:ARG:NH2	2.02	0.73
1:A:146:ARG:O	1:A:246:CYS:HB2	1.87	0.73
1:A:450:ARG:NH1	1:E:100:ASP:OD2	2.22	0.73
1:C:542:THR:HG22	1:C:546:ARG:HA	1.69	0.73
1:A:447:VAL:HG22	1:E:67:THR:HG21	1.70	0.72
1:A:488:THR:HG22	1:B:479:VAL:HG12	1.70	0.72
1:B:484:ILE:HG21	1:C:480:TYR:CE1	2.24	0.72
2:U:10:THR:O	2:U:10:THR:HG22	1.89	0.72
2:V:10:THR:O	2:V:10:THR:HG22	1.89	0.72
1:E:96:ILE:HG22	1:E:98:ASN:H	1.51	0.72
1:C:510:THR:O	1:C:511:ILE:HB	1.88	0.72
1:B:154:THR:HG22	1:B:155:LYS:HG3	1.71	0.72
1:C:193:LEU:HD11	1:C:496:ARG:HH12	1.54	0.72
1:A:193:LEU:HD11	1:A:496:ARG:HH12	1.54	0.72
1:D:193:LEU:HD11	1:D:496:ARG:HH12	1.54	0.72
2:T:10:THR:HG22	2:T:10:THR:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:PHE:O	1:C:216:ARG:HB2	1.89	0.72
1:A:488:THR:CG2	1:B:479:VAL:CG1	2.66	0.72
1:B:68:ARG:NH1	1:B:68:ARG:HG2	1.97	0.72
1:B:214:ASN:C	1:B:214:ASN:HD22	1.93	0.72
1:A:214:ASN:C	1:A:214:ASN:HD22	1.93	0.71
1:C:111:ILE:HD13	1:D:447:VAL:HG11	1.71	0.71
1:D:154:THR:HG22	1:D:155:LYS:HG3	1.72	0.71
1:B:215:PHE:O	1:B:216:ARG:HB2	1.89	0.71
1:C:154:THR:HG22	1:C:155:LYS:HG3	1.72	0.71
1:E:214:ASN:C	1:E:214:ASN:HD22	1.93	0.71
1:E:154:THR:HG22	1:E:155:LYS:HG3	1.72	0.71
1:B:193:LEU:HD11	1:B:496:ARG:HH12	1.54	0.71
1:B:275:TYR:CZ	1:B:402:ARG:HD3	2.26	0.71
1:C:484:ILE:HG21	1:D:480:TYR:CD1	2.25	0.71
1:C:275:TYR:CZ	1:C:402:ARG:HD3	2.26	0.71
1:E:510:THR:O	1:E:511:ILE:HB	1.88	0.71
1:A:422:LEU:HD23	1:A:423:LEU:N	2.06	0.71
1:B:274:THR:HG22	1:B:276:ASP:N	2.06	0.71
1:D:214:ASN:C	1:D:214:ASN:HD22	1.93	0.71
1:E:193:LEU:HD11	1:E:496:ARG:HH12	1.54	0.71
1:D:215:PHE:O	1:D:216:ARG:HB2	1.90	0.70
2:W:10:THR:HG22	2:W:10:THR:O	1.89	0.70
1:C:502:ILE:HG22	1:C:503:LEU:N	2.06	0.70
1:D:275:TYR:CZ	1:D:402:ARG:HD3	2.26	0.70
1:D:422:LEU:HD23	1:D:423:LEU:N	2.06	0.70
1:E:376:VAL:O	1:E:378:LYS:N	2.25	0.70
1:A:275:TYR:CZ	1:A:402:ARG:HD3	2.26	0.70
1:A:488:THR:HG22	1:B:479:VAL:CG1	2.21	0.70
2:S:10:THR:O	2:S:10:THR:HG22	1.89	0.70
1:A:479:VAL:O	1:E:488:THR:HG23	1.91	0.70
1:C:376:VAL:O	1:C:378:LYS:N	2.25	0.70
1:E:376:VAL:HG23	1:E:377:ILE:H	1.57	0.70
1:A:215:PHE:O	1:A:216:ARG:HB2	1.89	0.70
1:B:376:VAL:O	1:B:378:LYS:N	2.25	0.70
1:C:214:ASN:HD22	1:C:214:ASN:C	1.93	0.70
1:D:376:VAL:O	1:D:378:LYS:N	2.24	0.70
1:A:154:THR:HG22	1:A:155:LYS:HG3	1.72	0.70
1:B:422:LEU:HD23	1:B:423:LEU:N	2.06	0.70
1:C:442:MET:HE3	1:C:559:VAL:HG21	1.73	0.70
1:C:484:ILE:CG2	1:D:480:TYR:CE1	2.75	0.70
1:A:98:ASN:HD22	1:A:99:ASN:N	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:422:LEU:HD23	1:E:423:LEU:N	2.06	0.70
1:A:376:VAL:O	1:A:378:LYS:N	2.25	0.69
1:B:98:ASN:HD22	1:B:99:ASN:N	1.90	0.69
1:C:422:LEU:HD23	1:C:423:LEU:N	2.06	0.69
1:A:479:VAL:CG1	1:E:488:THR:CG2	2.70	0.69
1:A:502:ILE:HG22	1:A:503:LEU:N	2.06	0.69
1:D:98:ASN:HD22	1:D:99:ASN:N	1.90	0.69
1:A:485:ARG:NE	1:B:234:GLU:OE2	2.25	0.69
1:B:376:VAL:HG23	1:B:377:ILE:H	1.57	0.69
1:D:274:THR:HG22	1:D:276:ASP:N	2.06	0.69
1:A:68:ARG:NH1	1:A:68:ARG:HG2	1.97	0.69
1:A:376:VAL:HG23	1:A:377:ILE:H	1.57	0.69
1:C:98:ASN:HD22	1:C:99:ASN:N	1.90	0.69
1:A:274:THR:HG22	1:A:276:ASP:N	2.06	0.69
1:B:442:MET:HE3	1:B:559:VAL:HG21	1.75	0.69
1:E:98:ASN:HD22	1:E:99:ASN:N	1.90	0.69
1:E:274:THR:HG22	1:E:276:ASP:N	2.06	0.69
1:E:275:TYR:CZ	1:E:402:ARG:HD3	2.26	0.69
1:E:283:ILE:O	1:E:399:THR:HG23	1.93	0.69
1:A:442:MET:HE3	1:A:559:VAL:HG21	1.73	0.69
1:B:490:LEU:HB2	1:C:230:VAL:HG11	1.74	0.69
1:B:502:ILE:HG22	1:B:503:LEU:N	2.06	0.69
1:C:488:THR:CG2	1:D:479:VAL:CG1	2.71	0.69
1:E:215:PHE:O	1:E:216:ARG:HB2	1.89	0.69
1:B:283:ILE:O	1:B:399:THR:HG23	1.93	0.69
1:C:455:ILE:HD12	1:C:456:SER:H	1.58	0.69
1:D:67:THR:HG21	1:E:447:VAL:HG22	1.73	0.69
1:C:376:VAL:HG23	1:C:377:ILE:H	1.57	0.69
1:A:83:ASN:HA	1:A:86:ASN:ND2	2.09	0.68
1:A:283:ILE:O	1:A:399:THR:HG23	1.93	0.68
1:A:211:ASP:OD1	1:A:213:ARG:HG2	1.94	0.68
1:C:211:ASP:OD1	1:C:213:ARG:HG2	1.93	0.68
1:C:274:THR:HG22	1:C:276:ASP:N	2.05	0.68
1:C:283:ILE:O	1:C:399:THR:HG23	1.93	0.68
1:D:488:THR:HG23	1:E:479:VAL:O	1.93	0.68
1:E:502:ILE:HG22	1:E:503:LEU:N	2.06	0.68
1:D:211:ASP:OD1	1:D:213:ARG:HG2	1.93	0.68
1:E:83:ASN:HA	1:E:86:ASN:ND2	2.09	0.68
1:E:426:PRO:O	1:E:427:ASP:HB3	1.93	0.68
1:A:497:PHE:HD1	1:A:503:LEU:HB3	1.59	0.68
1:B:426:PRO:O	1:B:427:ASP:HB3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:455:ILE:HD12	1:D:456:SER:H	1.58	0.68
1:D:502:ILE:HG22	1:D:503:LEU:N	2.06	0.68
1:B:455:ILE:HD12	1:B:456:SER:H	1.58	0.68
1:A:480:TYR:CD1	1:E:484:ILE:CG2	2.77	0.67
1:B:83:ASN:HA	1:B:86:ASN:ND2	2.09	0.67
1:C:556:LEU:HD21	1:D:434:GLN:HG2	1.75	0.67
1:D:426:PRO:O	1:D:427:ASP:HB3	1.94	0.67
1:E:455:ILE:HD12	1:E:456:SER:H	1.58	0.67
1:A:455:ILE:HD12	1:A:456:SER:H	1.59	0.67
1:B:274:THR:HG22	1:B:275:TYR:N	2.10	0.67
1:D:283:ILE:O	1:D:399:THR:HG23	1.93	0.67
1:E:497:PHE:HD1	1:E:503:LEU:HB3	1.59	0.67
1:A:422:LEU:HD21	1:E:551:TYR:CE2	2.30	0.67
1:B:214:ASN:HD21	1:B:216:ARG:HB3	1.60	0.67
1:A:183:LEU:HD21	1:B:236:PHE:HE2	1.59	0.67
1:B:211:ASP:OD1	1:B:213:ARG:HG2	1.93	0.67
1:C:214:ASN:HD21	1:C:216:ARG:HB3	1.60	0.67
1:C:497:PHE:HD1	1:C:503:LEU:HB3	1.59	0.67
1:D:130:ASN:HA	1:D:517:ASN:CG	2.16	0.67
1:D:215:PHE:HB3	1:D:283:ILE:HG23	1.77	0.67
1:D:217:LEU:CB	1:D:232:THR:HG21	2.24	0.67
1:C:274:THR:HG22	1:C:275:TYR:N	2.10	0.67
1:E:211:ASP:OD1	1:E:213:ARG:HG2	1.94	0.67
1:E:214:ASN:HD21	1:E:216:ARG:HB3	1.60	0.66
1:A:217:LEU:CB	1:A:232:THR:HG21	2.25	0.66
1:B:145:ALA:HB3	1:B:168:PHE:CE1	2.31	0.66
1:C:215:PHE:HB3	1:C:283:ILE:HG23	1.77	0.66
1:C:217:LEU:CB	1:C:232:THR:HG21	2.24	0.66
1:D:497:PHE:HD1	1:D:503:LEU:HB3	1.59	0.66
1:E:130:ASN:HA	1:E:517:ASN:CG	2.16	0.66
1:A:426:PRO:O	1:A:427:ASP:HB3	1.94	0.66
1:C:83:ASN:HA	1:C:86:ASN:ND2	2.09	0.66
1:E:215:PHE:HB3	1:E:283:ILE:HG23	1.77	0.66
1:E:217:LEU:CB	1:E:232:THR:HG21	2.25	0.66
1:B:497:PHE:HD1	1:B:503:LEU:HB3	1.59	0.66
1:C:426:PRO:O	1:C:427:ASP:HB3	1.94	0.66
1:A:145:ALA:HB3	1:A:168:PHE:CE1	2.31	0.66
1:D:551:TYR:CE2	1:E:422:LEU:HD21	2.31	0.66
1:D:376:VAL:HG23	1:D:377:ILE:H	1.57	0.66
1:D:133:ASN:HB2	1:D:175:TYR:CD2	2.32	0.65
1:A:130:ASN:HA	1:A:517:ASN:CG	2.16	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:488:THR:CG2	1:E:479:VAL:CG1	2.73	0.65
1:A:274:THR:HG22	1:A:275:TYR:N	2.10	0.65
1:A:438:SER:HB3	1:A:459:PRO:O	1.97	0.65
1:A:214:ASN:HD21	1:A:216:ARG:HB3	1.60	0.65
1:A:438:SER:C	1:A:440:PRO:HD3	2.17	0.65
1:C:133:ASN:HB2	1:C:175:TYR:CD2	2.32	0.65
1:C:130:ASN:HA	1:C:517:ASN:CG	2.16	0.65
1:D:274:THR:HG22	1:D:275:TYR:N	2.10	0.65
1:D:485:ARG:NH1	1:D:505:ARG:NH2	2.44	0.65
1:E:274:THR:HG22	1:E:275:TYR:N	2.10	0.65
1:E:438:SER:C	1:E:440:PRO:HD3	2.17	0.65
1:A:490:LEU:CB	1:B:230:VAL:HG11	2.27	0.65
1:B:438:SER:C	1:B:440:PRO:HD3	2.17	0.65
1:C:207:GLY:O	1:C:208:VAL:HB	1.97	0.65
1:B:133:ASN:HB2	1:B:175:TYR:CD2	2.32	0.65
1:B:217:LEU:CB	1:B:232:THR:HG21	2.24	0.65
1:E:133:ASN:HB2	1:E:175:TYR:CD2	2.31	0.65
1:B:130:ASN:HA	1:B:517:ASN:CG	2.16	0.65
1:B:224:GLY:O	1:B:225:LEU:HD23	1.97	0.65
1:B:485:ARG:NH1	1:B:505:ARG:NH2	2.44	0.65
1:A:215:PHE:HB3	1:A:283:ILE:HG23	1.77	0.65
1:B:207:GLY:O	1:B:208:VAL:HB	1.97	0.65
1:C:438:SER:C	1:C:440:PRO:HD3	2.17	0.65
1:E:442:MET:CE	1:E:559:VAL:HG21	2.27	0.65
1:A:485:ARG:NH1	1:A:505:ARG:NH2	2.44	0.65
1:E:207:GLY:O	1:E:208:VAL:HB	1.97	0.65
1:E:485:ARG:NH1	1:E:505:ARG:NH2	2.44	0.65
1:A:224:GLY:O	1:A:225:LEU:HD23	1.97	0.64
1:D:214:ASN:HD21	1:D:216:ARG:HB3	1.60	0.64
1:D:484:ILE:CG2	1:E:480:TYR:CD1	2.80	0.64
1:C:145:ALA:HB3	1:C:168:PHE:CE1	2.31	0.64
1:D:224:GLY:O	1:D:225:LEU:HD23	1.97	0.64
2:W:18:ASP:OD1	2:W:18:ASP:O	2.15	0.64
1:A:442:MET:CE	1:A:559:VAL:HG21	2.27	0.64
1:B:215:PHE:HB3	1:B:283:ILE:HG23	1.77	0.64
1:C:485:ARG:NH1	1:C:505:ARG:NH2	2.44	0.64
2:V:18:ASP:OD1	2:V:18:ASP:O	2.15	0.64
1:A:133:ASN:HB2	1:A:175:TYR:CD2	2.32	0.64
1:B:511:ILE:HG22	1:B:511:ILE:O	1.97	0.64
1:E:145:ALA:HB3	1:E:168:PHE:CE1	2.31	0.64
2:S:18:ASP:OD1	2:S:18:ASP:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:PHE:HD1	1:C:118:HIS:NE2	1.95	0.64
1:C:496:ARG:HD3	2:U:14:VAL:HG12	1.80	0.64
1:D:83:ASN:HA	1:D:86:ASN:ND2	2.09	0.64
1:D:442:MET:CE	1:D:559:VAL:HG21	2.28	0.64
1:C:434:GLN:NE2	1:C:436:TYR:HE2	1.96	0.64
1:D:145:ALA:HB3	1:D:168:PHE:CE1	2.31	0.64
1:D:496:ARG:HD3	2:V:14:VAL:HG12	1.80	0.64
2:T:18:ASP:OD1	2:T:18:ASP:O	2.15	0.64
2:U:18:ASP:O	2:U:18:ASP:OD1	2.15	0.64
1:B:67:THR:HG21	1:C:447:VAL:HG22	1.80	0.64
1:B:442:MET:CE	1:B:559:VAL:HG21	2.28	0.64
1:C:488:THR:HG23	1:D:479:VAL:O	1.97	0.64
1:D:438:SER:C	1:D:440:PRO:HD3	2.17	0.64
1:B:438:SER:HB3	1:B:459:PRO:O	1.97	0.64
1:C:466:LEU:CD1	1:C:467:PRO:HD2	2.24	0.64
1:E:210:PHE:HD2	1:E:240:ILE:HG22	1.63	0.64
1:E:434:GLN:NE2	1:E:436:TYR:HE2	1.96	0.64
1:C:442:MET:CE	1:C:559:VAL:HG21	2.28	0.64
1:E:224:GLY:O	1:E:225:LEU:HD23	1.97	0.64
1:E:511:ILE:O	1:E:511:ILE:HG22	1.97	0.64
1:C:511:ILE:O	1:C:511:ILE:HG22	1.97	0.64
1:D:438:SER:HB3	1:D:459:PRO:O	1.97	0.64
1:E:466:LEU:CD1	1:E:467:PRO:HD2	2.24	0.64
1:A:210:PHE:HD2	1:A:240:ILE:HG22	1.63	0.63
1:A:434:GLN:NE2	1:A:436:TYR:HE2	1.96	0.63
1:A:542:THR:HG21	1:A:546:ARG:HA	1.80	0.63
1:B:68:ARG:NE	1:C:527:LEU:HD21	2.12	0.63
1:D:511:ILE:HG22	1:D:511:ILE:O	1.97	0.63
1:B:496:ARG:HD3	2:T:14:VAL:HG12	1.80	0.63
1:C:210:PHE:HD2	1:C:240:ILE:HG22	1.63	0.63
1:C:224:GLY:O	1:C:225:LEU:HD23	1.97	0.63
1:D:434:GLN:NE2	1:D:436:TYR:HE2	1.96	0.63
1:E:134:VAL:HA	1:E:140:THR:OG1	1.98	0.63
1:E:438:SER:HB3	1:E:459:PRO:O	1.97	0.63
1:A:207:GLY:O	1:A:208:VAL:HB	1.97	0.63
1:C:558:ILE:HD11	1:D:463:ALA:HB3	1.79	0.63
1:A:134:VAL:HA	1:A:140:THR:OG1	1.99	0.63
1:D:207:GLY:O	1:D:208:VAL:HB	1.97	0.63
1:D:228:PRO:HG3	2:U:15:TYR:CE1	2.34	0.63
1:A:111:ILE:HD13	1:B:447:VAL:HG11	1.81	0.63
1:A:511:ILE:HG22	1:A:511:ILE:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:PRO:O	1:E:174:ASN:ND2	2.32	0.63
1:A:496:ARG:HD3	2:S:14:VAL:HG12	1.80	0.63
1:B:484:ILE:CG2	1:C:480:TYR:CE1	2.82	0.63
1:E:138:MET:O	1:E:139:PHE:HB2	1.98	0.63
1:C:542:THR:HG21	1:C:546:ARG:HA	1.80	0.63
1:A:100:ASP:OD2	1:B:450:ARG:NH1	2.32	0.63
1:B:434:GLN:NE2	1:B:436:TYR:HE2	1.96	0.63
1:C:134:VAL:HA	1:C:140:THR:OG1	1.99	0.63
1:D:485:ARG:HH21	1:E:234:GLU:CD	2.02	0.63
1:D:134:VAL:HA	1:D:140:THR:OG1	1.98	0.62
1:B:138:MET:O	1:B:139:PHE:HB2	1.99	0.62
1:B:542:THR:HG21	1:B:546:ARG:HA	1.80	0.62
1:C:138:MET:O	1:C:139:PHE:HB2	1.99	0.62
1:D:171:PRO:O	1:D:174:ASN:ND2	2.32	0.62
1:D:210:PHE:HD2	1:D:240:ILE:HG22	1.63	0.62
1:A:171:PRO:O	1:A:174:ASN:ND2	2.32	0.62
1:D:556:LEU:HD21	1:E:434:GLN:HG2	1.80	0.62
1:B:74:ASN:OD1	1:C:434:GLN:OE1	2.17	0.62
1:B:134:VAL:HA	1:B:140:THR:OG1	1.98	0.62
1:A:479:VAL:HG12	1:A:479:VAL:O	2.00	0.62
1:C:438:SER:HB3	1:C:459:PRO:O	1.97	0.62
1:E:159:VAL:HG23	1:E:159:VAL:O	2.00	0.62
1:E:211:ASP:OD1	1:E:212:THR:N	2.31	0.62
1:A:551:TYR:CE2	1:B:422:LEU:HD21	2.35	0.62
1:C:171:PRO:O	1:C:174:ASN:ND2	2.32	0.62
1:D:138:MET:O	1:D:139:PHE:HB2	1.98	0.62
1:B:177:GLU:HG3	1:B:178:THR:N	2.15	0.62
1:D:154:THR:HG22	1:D:155:LYS:N	2.14	0.62
1:E:154:THR:HG22	1:E:155:LYS:N	2.14	0.62
1:E:496:ARG:HD3	2:W:14:VAL:HG12	1.80	0.62
1:B:159:VAL:O	1:B:159:VAL:HG23	2.00	0.62
1:B:210:PHE:HD2	1:B:240:ILE:HG22	1.63	0.62
1:D:542:THR:HG21	1:D:546:ARG:HA	1.80	0.62
1:E:177:GLU:HG3	1:E:178:THR:N	2.15	0.62
1:A:177:GLU:HG3	1:A:178:THR:N	2.15	0.62
1:A:383:ASP:OD1	1:A:387:ARG:HD2	2.00	0.62
1:C:475:ASN:C	1:C:477:GLN:N	2.54	0.62
1:E:542:THR:HG21	1:E:546:ARG:HA	1.80	0.62
1:A:154:THR:HG22	1:A:155:LYS:N	2.14	0.61
1:B:171:PRO:O	1:B:174:ASN:ND2	2.32	0.61
1:B:479:VAL:HG12	1:B:479:VAL:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:475:ASN:C	1:D:477:GLN:H	2.03	0.61
1:A:159:VAL:HG23	1:A:159:VAL:O	2.00	0.61
1:C:479:VAL:HG12	1:C:479:VAL:O	2.00	0.61
1:D:292:TYR:CD1	1:D:376:VAL:HG12	2.35	0.61
1:E:475:ASN:C	1:E:477:GLN:H	2.03	0.61
1:A:466:LEU:CD1	1:A:467:PRO:HD2	2.24	0.61
1:C:177:GLU:HG3	1:C:178:THR:N	2.15	0.61
1:C:292:TYR:CD1	1:C:376:VAL:HG12	2.35	0.61
1:C:383:ASP:OD1	1:C:387:ARG:HD2	2.00	0.61
1:C:154:THR:HG22	1:C:155:LYS:N	2.14	0.61
1:D:466:LEU:CD1	1:D:467:PRO:HD2	2.24	0.61
1:B:154:THR:HG22	1:B:155:LYS:N	2.14	0.61
1:D:177:GLU:HG3	1:D:178:THR:N	2.15	0.61
1:A:138:MET:O	1:A:139:PHE:HB2	1.98	0.61
1:D:376:VAL:CG2	1:D:377:ILE:H	2.14	0.61
1:D:383:ASP:OD1	1:D:387:ARG:HD2	2.00	0.61
1:A:428:VAL:HG21	1:A:515:SER:N	2.16	0.61
1:A:475:ASN:C	1:A:477:GLN:N	2.53	0.61
1:C:99:ASN:HB3	1:D:450:ARG:NH2	2.16	0.61
1:E:479:VAL:HG12	1:E:479:VAL:O	2.00	0.61
1:A:292:TYR:CD1	1:A:376:VAL:HG12	2.35	0.61
1:A:479:VAL:CG1	1:E:488:THR:HG22	2.31	0.61
1:D:159:VAL:HG23	1:D:159:VAL:O	2.00	0.61
1:D:428:VAL:HG21	1:D:515:SER:N	2.16	0.61
1:B:292:TYR:CD1	1:B:376:VAL:HG12	2.35	0.61
1:B:428:VAL:HG21	1:B:515:SER:N	2.16	0.61
1:C:183:LEU:HD21	1:D:236:PHE:HE2	1.65	0.61
1:C:428:VAL:HG21	1:C:515:SER:N	2.16	0.61
1:D:495:ASN:O	1:D:497:PHE:N	2.34	0.61
1:E:383:ASP:OD1	1:E:387:ARG:HD2	2.00	0.61
1:E:475:ASN:C	1:E:477:GLN:N	2.53	0.61
1:A:447:VAL:HG11	1:E:111:ILE:HD13	1.83	0.60
1:A:495:ASN:O	1:A:497:PHE:N	2.34	0.60
1:D:479:VAL:HG12	1:D:479:VAL:O	2.00	0.60
1:A:236:PHE:HE2	1:E:183:LEU:HD21	1.66	0.60
1:B:383:ASP:OD1	1:B:387:ARG:HD2	2.00	0.60
1:B:475:ASN:C	1:B:477:GLN:H	2.03	0.60
1:C:376:VAL:CG2	1:C:377:ILE:H	2.14	0.60
1:C:484:ILE:CG2	1:D:480:TYR:CD1	2.83	0.60
1:B:376:VAL:CG2	1:B:377:ILE:H	2.14	0.60
1:C:159:VAL:HG23	1:C:159:VAL:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:273:ILE:HG23	1:D:273:ILE:O	2.02	0.60
1:E:292:TYR:CD1	1:E:376:VAL:HG12	2.35	0.60
1:E:478:ALA:HB1	1:E:508:ALA:HB3	1.83	0.60
1:E:479:VAL:HA	1:E:482:GLN:HB3	1.83	0.60
1:B:273:ILE:O	1:B:273:ILE:HG23	2.02	0.60
1:C:68:ARG:NE	1:D:527:LEU:HD21	2.16	0.60
1:A:57:TYR:O	1:A:58:SER:C	2.40	0.60
1:A:173:GLY:O	1:A:175:TYR:CD1	2.55	0.60
1:B:479:VAL:HA	1:B:482:GLN:HB3	1.83	0.60
1:C:67:THR:HG21	1:D:447:VAL:CG2	2.29	0.60
1:C:495:ASN:O	1:C:497:PHE:N	2.35	0.60
1:D:475:ASN:C	1:D:477:GLN:N	2.53	0.60
1:A:478:ALA:HB1	1:A:508:ALA:HB3	1.83	0.60
1:A:479:VAL:HA	1:A:482:GLN:HB3	1.83	0.60
1:A:491:THR:HB	1:A:493:VAL:HG23	1.84	0.60
1:B:488:THR:HG23	1:C:479:VAL:O	2.02	0.60
1:C:57:TYR:O	1:C:58:SER:C	2.40	0.60
1:C:479:VAL:HA	1:C:482:GLN:HB3	1.83	0.60
1:C:491:THR:HB	1:C:493:VAL:HG23	1.84	0.60
1:D:479:VAL:HA	1:D:482:GLN:HB3	1.83	0.60
1:D:488:THR:HG22	1:E:479:VAL:HG12	1.82	0.60
1:E:173:GLY:O	1:E:175:TYR:CD1	2.55	0.60
1:E:495:ASN:O	1:E:497:PHE:N	2.35	0.60
1:A:376:VAL:CG2	1:A:377:ILE:N	2.65	0.60
1:A:497:PHE:N	1:A:497:PHE:CD2	2.69	0.60
1:B:475:ASN:C	1:B:477:GLN:N	2.53	0.60
1:B:478:ALA:HB1	1:B:508:ALA:HB3	1.83	0.60
1:C:475:ASN:C	1:C:477:GLN:H	2.03	0.60
1:E:52:ARG:N	1:E:116:ARG:HH12	2.00	0.60
1:A:475:ASN:C	1:A:477:GLN:H	2.03	0.60
1:B:173:GLY:O	1:B:175:TYR:CD1	2.55	0.60
1:C:488:THR:HG22	1:D:479:VAL:HG12	1.84	0.60
1:D:211:ASP:OD1	1:D:212:THR:N	2.31	0.60
1:C:52:ARG:N	1:C:116:ARG:HH12	2.00	0.59
1:C:173:GLY:O	1:C:175:TYR:CD1	2.55	0.59
1:E:273:ILE:O	1:E:273:ILE:HG23	2.02	0.59
1:E:428:VAL:HG21	1:E:515:SER:N	2.16	0.59
1:B:52:ARG:N	1:B:116:ARG:HH12	2.00	0.59
1:B:497:PHE:CD2	1:B:497:PHE:N	2.69	0.59
1:D:57:TYR:O	1:D:58:SER:C	2.40	0.59
1:D:173:GLY:O	1:D:175:TYR:CD1	2.55	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:PHE:CD2	1:D:240:ILE:HG22	2.37	0.59
1:D:233:ASN:OD1	1:D:507:PRO:HG3	2.02	0.59
1:D:278:LEU:HD22	1:D:404:TRP:HA	1.84	0.59
1:E:376:VAL:CG2	1:E:377:ILE:N	2.65	0.59
1:B:387:ARG:HG2	1:B:387:ARG:HH11	1.68	0.59
1:D:491:THR:HB	1:D:493:VAL:HG23	1.84	0.59
1:C:273:ILE:HG23	1:C:273:ILE:O	2.02	0.59
1:C:536:VAL:HG23	1:C:536:VAL:O	2.02	0.59
1:E:233:ASN:OD1	1:E:507:PRO:HG3	2.02	0.59
1:B:57:TYR:O	1:B:58:SER:C	2.40	0.59
1:C:237:HIS:CD2	1:C:238:PRO:O	2.56	0.59
1:C:278:LEU:HD22	1:C:404:TRP:HA	1.84	0.59
1:E:237:HIS:CD2	1:E:238:PRO:O	2.56	0.59
1:A:237:HIS:CD2	1:A:238:PRO:O	2.56	0.59
1:A:479:VAL:HG12	1:E:488:THR:HG22	1.80	0.59
1:B:495:ASN:O	1:B:497:PHE:N	2.34	0.59
1:C:211:ASP:OD1	1:C:212:THR:N	2.31	0.59
1:D:208:VAL:HG22	1:D:242:LEU:CD2	2.33	0.59
1:E:491:THR:HB	1:E:493:VAL:HG23	1.83	0.59
1:E:536:VAL:HG23	1:E:536:VAL:O	2.02	0.59
1:A:376:VAL:CG2	1:A:377:ILE:H	2.14	0.59
1:B:536:VAL:HG23	1:B:536:VAL:O	2.02	0.59
1:C:208:VAL:HG22	1:C:242:LEU:CD2	2.33	0.59
1:C:488:THR:HG22	1:D:479:VAL:CG1	2.33	0.59
1:C:490:LEU:HB2	1:D:230:VAL:CG1	2.28	0.59
1:C:497:PHE:N	1:C:497:PHE:CD2	2.69	0.59
1:D:111:ILE:HD13	1:E:447:VAL:HG11	1.82	0.59
1:D:478:ALA:HB1	1:D:508:ALA:HB3	1.83	0.59
1:A:211:ASP:OD1	1:A:212:THR:N	2.31	0.59
1:A:536:VAL:HG23	1:A:536:VAL:O	2.02	0.59
1:B:210:PHE:CD2	1:B:240:ILE:HG22	2.37	0.59
1:B:409:ASN:OD1	1:B:409:ASN:N	2.36	0.59
1:E:57:TYR:O	1:E:58:SER:C	2.40	0.59
1:A:210:PHE:CD2	1:A:240:ILE:HG22	2.37	0.59
1:D:376:VAL:CG2	1:D:377:ILE:N	2.65	0.59
1:E:208:VAL:HG22	1:E:242:LEU:CD2	2.33	0.59
1:E:376:VAL:CG2	1:E:377:ILE:H	2.14	0.59
1:B:278:LEU:HD22	1:B:404:TRP:HA	1.84	0.59
1:D:475:ASN:HB3	1:E:474:TYR:CE2	2.38	0.59
1:E:122:ASP:OD1	1:E:526:THR:HG22	2.03	0.59
1:E:433:GLU:OE1	1:E:433:GLU:HA	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ASN:OD1	1:A:507:PRO:HG3	2.03	0.58
1:C:210:PHE:CD2	1:C:240:ILE:HG22	2.37	0.58
1:C:376:VAL:CG2	1:C:377:ILE:N	2.65	0.58
1:D:536:VAL:O	1:D:536:VAL:HG23	2.02	0.58
1:A:52:ARG:N	1:A:116:ARG:HH12	2.00	0.58
1:A:208:VAL:HG22	1:A:242:LEU:CD2	2.33	0.58
1:A:278:LEU:HD22	1:A:404:TRP:HA	1.84	0.58
1:B:433:GLU:OE1	1:B:433:GLU:HA	2.03	0.58
1:B:477:GLN:O	1:B:481:SER:N	2.36	0.58
1:C:478:ALA:HB1	1:C:508:ALA:HB3	1.83	0.58
1:A:295:SER:OG	1:A:375:PRO:HD3	2.03	0.58
1:B:233:ASN:OD1	1:B:507:PRO:HG3	2.02	0.58
1:B:491:THR:HB	1:B:493:VAL:HG23	1.84	0.58
1:C:409:ASN:OD1	1:C:409:ASN:N	2.36	0.58
1:D:57:TYR:CD2	1:E:448:THR:HG22	2.39	0.58
1:D:183:LEU:HD21	1:E:236:PHE:HE2	1.67	0.58
1:D:496:ARG:O	2:V:16:PRO:HD3	2.03	0.58
1:A:68:ARG:NE	1:B:527:LEU:HD21	2.18	0.58
1:A:234:GLU:CD	1:E:485:ARG:HH21	2.06	0.58
1:A:433:GLU:OE1	1:A:433:GLU:HA	2.03	0.58
1:A:434:GLN:HG2	1:E:556:LEU:HD21	1.83	0.58
1:A:477:GLN:O	1:A:481:SER:N	2.36	0.58
1:A:556:LEU:HD21	1:B:434:GLN:HG2	1.86	0.58
1:B:274:THR:CG2	1:B:275:TYR:N	2.67	0.58
1:B:376:VAL:CG2	1:B:377:ILE:N	2.65	0.58
1:E:387:ARG:HH11	1:E:387:ARG:HG2	1.67	0.58
1:A:387:ARG:HG2	1:A:387:ARG:HH11	1.67	0.58
1:A:401:TYR:HD1	1:A:502:ILE:HG12	1.69	0.58
1:A:409:ASN:OD1	1:A:409:ASN:N	2.36	0.58
1:A:474:TYR:CE2	1:E:475:ASN:HB3	2.38	0.58
1:B:122:ASP:OD1	1:B:526:THR:HG22	2.03	0.58
1:D:237:HIS:CD2	1:D:238:PRO:O	2.56	0.58
1:D:295:SER:OG	1:D:375:PRO:HD3	2.03	0.58
1:D:558:ILE:HD11	1:E:463:ALA:HB3	1.86	0.58
1:E:210:PHE:CD2	1:E:240:ILE:HG22	2.37	0.58
1:E:497:PHE:N	1:E:497:PHE:CD2	2.69	0.58
1:A:98:ASN:HD22	1:A:98:ASN:C	2.06	0.58
1:A:496:ARG:O	2:S:16:PRO:HD3	2.03	0.58
1:B:401:TYR:HD1	1:B:502:ILE:HG12	1.69	0.58
1:C:295:SER:OG	1:C:375:PRO:HD3	2.03	0.58
1:C:433:GLU:HA	1:C:433:GLU:OE1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:GLN:O	1:C:481:SER:N	2.36	0.58
1:D:52:ARG:N	1:D:116:ARG:HH12	2.00	0.58
1:E:477:GLN:O	1:E:481:SER:N	2.36	0.58
1:A:274:THR:CG2	1:A:275:TYR:N	2.67	0.58
1:C:387:ARG:HG2	1:C:387:ARG:HH11	1.68	0.58
1:D:387:ARG:HG2	1:D:387:ARG:HH11	1.67	0.58
1:C:233:ASN:OD1	1:C:507:PRO:HG3	2.02	0.58
1:C:496:ARG:O	2:U:16:PRO:HD3	2.03	0.58
1:D:98:ASN:HD22	1:D:98:ASN:C	2.06	0.58
2:S:15:TYR:HD2	2:S:16:PRO:N	2.02	0.58
1:B:211:ASP:OD1	1:B:212:THR:N	2.31	0.58
1:B:237:HIS:CD2	1:B:238:PRO:O	2.56	0.58
1:C:122:ASP:OD1	1:C:526:THR:HG22	2.04	0.58
1:D:274:THR:CG2	1:D:275:TYR:N	2.67	0.58
1:D:433:GLU:OE1	1:D:433:GLU:HA	2.03	0.58
1:A:502:ILE:O	1:A:504:ALA:N	2.36	0.58
1:B:295:SER:OG	1:B:375:PRO:HD3	2.03	0.58
1:E:278:LEU:HD22	1:E:404:TRP:HA	1.84	0.58
1:C:274:THR:CG2	1:C:275:TYR:N	2.67	0.57
1:D:439:LEU:N	1:D:440:PRO:HD3	2.19	0.57
1:D:477:GLN:O	1:D:481:SER:N	2.36	0.57
1:D:496:ARG:C	1:D:497:PHE:HD2	2.07	0.57
1:E:98:ASN:HD22	1:E:98:ASN:C	2.06	0.57
1:E:295:SER:OG	1:E:375:PRO:HD3	2.03	0.57
2:T:15:TYR:HD2	2:T:16:PRO:N	2.02	0.57
2:W:15:TYR:HD2	2:W:16:PRO:N	2.02	0.57
1:B:99:ASN:HB3	1:C:450:ARG:NH2	2.19	0.57
1:B:496:ARG:O	2:T:16:PRO:HD3	2.03	0.57
1:C:502:ILE:O	1:C:504:ALA:N	2.37	0.57
1:D:122:ASP:OD1	1:D:526:THR:HG22	2.03	0.57
1:D:498:PRO:HG2	1:D:499:GLU:OE2	2.04	0.57
1:E:496:ARG:O	2:W:16:PRO:HD3	2.03	0.57
1:A:475:ASN:HB3	1:B:474:TYR:CE2	2.39	0.57
1:A:496:ARG:C	1:A:497:PHE:HD2	2.08	0.57
1:A:498:PRO:HG2	1:A:499:GLU:OE2	2.04	0.57
1:A:518:VAL:HG23	1:A:519:PRO:HD2	1.87	0.57
1:B:208:VAL:HG22	1:B:242:LEU:CD2	2.33	0.57
1:B:484:ILE:HG21	1:C:480:TYR:CD1	2.39	0.57
1:D:497:PHE:N	1:D:497:PHE:CD2	2.69	0.57
1:E:409:ASN:OD1	1:E:409:ASN:N	2.36	0.57
1:E:502:ILE:O	1:E:504:ALA:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:518:VAL:HG23	1:E:519:PRO:HD2	1.87	0.57
1:A:122:ASP:OD1	1:A:526:THR:HG22	2.03	0.57
1:C:475:ASN:HB3	1:D:474:TYR:CE2	2.39	0.57
1:D:214:ASN:C	1:D:214:ASN:ND2	2.58	0.57
1:A:484:ILE:HG23	1:B:480:TYR:CE1	2.40	0.57
1:B:466:LEU:CD1	1:B:467:PRO:HD2	2.24	0.57
1:C:175:TYR:CD1	1:C:175:TYR:N	2.72	0.57
1:C:496:ARG:C	1:C:497:PHE:HD2	2.07	0.57
1:D:502:ILE:O	1:D:504:ALA:N	2.37	0.57
1:B:100:ASP:CG	1:C:450:ARG:HH12	2.07	0.57
1:B:175:TYR:H	1:B:175:TYR:HD1	1.52	0.57
1:B:498:PRO:HG2	1:B:499:GLU:OE2	2.05	0.57
1:C:485:ARG:HH21	1:D:234:GLU:CD	2.08	0.57
1:C:498:PRO:HG2	1:C:499:GLU:OE2	2.04	0.57
1:E:496:ARG:C	1:E:497:PHE:CD2	2.78	0.57
1:E:496:ARG:C	1:E:497:PHE:HD2	2.08	0.57
2:U:15:TYR:HD2	2:U:16:PRO:N	2.02	0.57
1:A:273:ILE:HG23	1:A:273:ILE:O	2.02	0.57
1:B:175:TYR:CD1	1:B:175:TYR:N	2.72	0.57
1:B:496:ARG:C	1:B:497:PHE:HD2	2.07	0.57
1:B:502:ILE:O	1:B:504:ALA:N	2.37	0.57
1:E:258:LEU:CD1	1:E:428:VAL:HA	2.35	0.57
1:E:498:PRO:HG2	1:E:499:GLU:OE2	2.05	0.57
1:A:88:HIS:ND1	1:A:553:TYR:O	2.38	0.57
1:A:496:ARG:C	1:A:497:PHE:CD2	2.78	0.57
1:B:490:LEU:CB	1:C:230:VAL:HG11	2.34	0.57
1:C:214:ASN:C	1:C:214:ASN:ND2	2.58	0.57
1:E:274:THR:CG2	1:E:275:TYR:N	2.67	0.57
2:S:15:TYR:HD2	2:S:16:PRO:CD	2.18	0.57
2:U:15:TYR:HD2	2:U:16:PRO:CD	2.18	0.57
2:V:15:TYR:HD2	2:V:16:PRO:N	2.02	0.57
1:A:175:TYR:CD1	1:A:175:TYR:N	2.72	0.57
1:B:88:HIS:ND1	1:B:553:TYR:O	2.38	0.57
1:B:258:LEU:CD1	1:B:428:VAL:HA	2.35	0.57
1:A:99:ASN:HB3	1:B:450:ARG:NH2	2.20	0.56
1:A:258:LEU:CD1	1:A:428:VAL:HA	2.35	0.56
1:B:429:THR:O	1:B:430:CYS:HB2	2.05	0.56
1:B:496:ARG:C	1:B:497:PHE:CD2	2.78	0.56
1:C:68:ARG:NH1	1:C:68:ARG:CG	2.67	0.56
1:E:401:TYR:HD1	1:E:502:ILE:HG12	1.69	0.56
1:A:175:TYR:HD1	1:A:175:TYR:H	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:ALA:HB3	1:E:558:ILE:HD11	1.88	0.56
1:B:98:ASN:HD22	1:B:98:ASN:C	2.06	0.56
1:D:88:HIS:ND1	1:D:553:TYR:O	2.38	0.56
1:D:409:ASN:OD1	1:D:409:ASN:N	2.36	0.56
1:A:130:ASN:HA	1:A:517:ASN:ND2	2.21	0.56
1:A:151:ARG:HB3	1:A:201:VAL:H	1.70	0.56
1:B:461:VAL:HB	1:B:527:LEU:HD13	1.87	0.56
1:C:98:ASN:HD22	1:C:98:ASN:C	2.06	0.56
1:C:258:LEU:CD1	1:C:428:VAL:HA	2.35	0.56
1:C:496:ARG:C	1:C:497:PHE:CD2	2.78	0.56
1:D:461:VAL:HB	1:D:527:LEU:HD13	1.88	0.56
1:D:488:THR:HG22	1:E:479:VAL:CG1	2.34	0.56
1:E:69:VAL:CG2	1:E:559:VAL:HB	2.36	0.56
1:E:151:ARG:HB3	1:E:201:VAL:H	1.70	0.56
1:E:175:TYR:CD1	1:E:175:TYR:N	2.72	0.56
1:E:439:LEU:N	1:E:440:PRO:HD3	2.19	0.56
2:V:15:TYR:HD2	2:V:16:PRO:CD	2.18	0.56
1:C:130:ASN:HA	1:C:517:ASN:ND2	2.21	0.56
1:C:439:LEU:N	1:C:440:PRO:HD3	2.19	0.56
1:A:429:THR:O	1:A:430:CYS:HB2	2.05	0.56
1:D:429:THR:O	1:D:430:CYS:HB2	2.05	0.56
1:D:496:ARG:C	1:D:497:PHE:CD2	2.78	0.56
1:E:130:ASN:HA	1:E:517:ASN:ND2	2.21	0.56
1:E:214:ASN:C	1:E:214:ASN:ND2	2.58	0.56
1:A:128:HIS:CE1	1:B:432:SER:HG	2.24	0.56
1:A:214:ASN:C	1:A:214:ASN:ND2	2.58	0.56
1:A:243:LEU:HG	1:A:401:TYR:HE2	1.71	0.56
1:B:154:THR:CG2	1:B:155:LYS:N	2.69	0.56
1:C:86:ASN:HB3	1:C:90:ASN:O	2.06	0.56
1:C:132:PRO:HD2	1:C:551:TYR:CE2	2.41	0.56
1:C:151:ARG:HB3	1:C:201:VAL:H	1.70	0.56
1:C:461:VAL:HB	1:C:527:LEU:HD13	1.88	0.56
1:D:132:PRO:HD2	1:D:551:TYR:CE2	2.41	0.56
1:D:154:THR:CG2	1:D:155:LYS:N	2.69	0.56
1:D:258:LEU:CD1	1:D:428:VAL:HA	2.35	0.56
1:E:429:THR:O	1:E:430:CYS:HB2	2.05	0.56
1:B:86:ASN:HB3	1:B:90:ASN:O	2.06	0.56
1:B:130:ASN:HA	1:B:517:ASN:ND2	2.21	0.56
1:B:439:LEU:N	1:B:440:PRO:HD3	2.19	0.56
1:C:69:VAL:CG2	1:C:559:VAL:HB	2.36	0.56
1:D:67:THR:OG1	1:D:68:ARG:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:ASN:HA	1:D:517:ASN:ND2	2.21	0.56
1:E:86:ASN:HB3	1:E:90:ASN:O	2.06	0.56
1:E:132:PRO:HD2	1:E:551:TYR:CE2	2.41	0.56
2:W:18:ASP:O	2:W:18:ASP:CG	2.44	0.56
1:A:67:THR:OG1	1:B:447:VAL:HG23	2.06	0.56
1:A:86:ASN:HB3	1:A:90:ASN:O	2.06	0.56
1:A:154:THR:CG2	1:A:155:LYS:N	2.69	0.56
1:A:447:VAL:CG2	1:E:67:THR:HG21	2.36	0.56
1:B:132:PRO:HD2	1:B:551:TYR:CE2	2.41	0.56
1:D:150:SER:HB3	1:D:199:ASN:HD22	1.71	0.56
1:D:518:VAL:HG23	1:D:519:PRO:HD2	1.87	0.56
1:E:279:GLU:O	1:E:280:GLY:O	2.24	0.56
1:A:69:VAL:CG2	1:A:559:VAL:HB	2.36	0.56
1:A:179:MET:HE3	1:A:485:ARG:HH22	1.71	0.56
1:C:243:LEU:HG	1:C:401:TYR:HE2	1.71	0.56
1:C:279:GLU:O	1:C:280:GLY:O	2.24	0.56
1:D:151:ARG:HB3	1:D:201:VAL:H	1.70	0.56
1:C:88:HIS:HD2	1:D:267:PHE:CZ	2.24	0.56
1:D:86:ASN:HB3	1:D:90:ASN:O	2.06	0.56
1:E:175:TYR:H	1:E:175:TYR:HD1	1.52	0.56
2:W:15:TYR:HD2	2:W:16:PRO:CD	2.18	0.56
1:B:69:VAL:CG2	1:B:559:VAL:HB	2.36	0.55
1:C:67:THR:OG1	1:C:68:ARG:N	2.39	0.55
1:C:197:ARG:HG3	1:C:198:GLN:HG3	1.88	0.55
1:A:132:PRO:HD2	1:A:551:TYR:CE2	2.41	0.55
1:A:279:GLU:O	1:A:280:GLY:O	2.24	0.55
1:C:150:SER:HB3	1:C:199:ASN:HD22	1.71	0.55
1:E:154:THR:CG2	1:E:155:LYS:N	2.69	0.55
1:E:243:LEU:HG	1:E:401:TYR:HE2	1.71	0.55
2:T:15:TYR:HD2	2:T:16:PRO:CD	2.18	0.55
1:B:65:ASP:O	1:B:66:THR:HB	2.06	0.55
1:B:150:SER:HB3	1:B:199:ASN:HD22	1.71	0.55
1:B:151:ARG:HB3	1:B:201:VAL:H	1.71	0.55
1:B:518:VAL:HG23	1:B:519:PRO:HD2	1.87	0.55
1:A:150:SER:HB3	1:A:199:ASN:HD22	1.71	0.55
1:A:461:VAL:HB	1:A:527:LEU:HD13	1.88	0.55
1:D:69:VAL:CG2	1:D:559:VAL:HB	2.36	0.55
1:D:197:ARG:HG3	1:D:198:GLN:HG3	1.89	0.55
1:E:65:ASP:O	1:E:66:THR:HB	2.06	0.55
2:T:18:ASP:O	2:T:18:ASP:CG	2.44	0.55
1:C:154:THR:CG2	1:C:155:LYS:N	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:518:VAL:HG23	1:C:519:PRO:HD2	1.87	0.55
1:D:65:ASP:O	1:D:66:THR:HB	2.06	0.55
1:D:243:LEU:HG	1:D:401:TYR:HE2	1.71	0.55
2:S:18:ASP:O	2:S:18:ASP:CG	2.44	0.55
1:C:65:ASP:O	1:C:66:THR:HB	2.06	0.55
1:D:175:TYR:HD1	1:D:175:TYR:H	1.52	0.55
1:E:88:HIS:ND1	1:E:553:TYR:O	2.38	0.55
2:U:18:ASP:O	2:U:18:ASP:CG	2.44	0.55
2:V:18:ASP:O	2:V:18:ASP:CG	2.44	0.55
1:A:67:THR:OG1	1:A:68:ARG:N	2.39	0.55
1:A:404:TRP:NE1	1:A:417:ILE:HG21	2.22	0.55
1:C:175:TYR:HD1	1:C:175:TYR:H	1.52	0.55
1:E:150:SER:HB3	1:E:199:ASN:HD22	1.71	0.55
1:B:444:GLN:O	1:B:446:PRO:HD3	2.07	0.55
1:C:444:GLN:O	1:C:446:PRO:HD3	2.07	0.55
1:E:444:GLN:O	1:E:446:PRO:HD3	2.07	0.55
1:E:461:VAL:HB	1:E:527:LEU:HD13	1.88	0.55
1:B:214:ASN:C	1:B:214:ASN:ND2	2.58	0.55
1:D:175:TYR:CD1	1:D:175:TYR:N	2.72	0.55
1:D:401:TYR:HD1	1:D:502:ILE:HG12	1.69	0.55
1:E:279:GLU:O	1:E:280:GLY:C	2.45	0.55
1:A:439:LEU:N	1:A:440:PRO:HD3	2.19	0.55
1:C:429:THR:O	1:C:430:CYS:HB2	2.05	0.55
1:E:67:THR:OG1	1:E:68:ARG:N	2.39	0.55
1:A:444:GLN:O	1:A:446:PRO:HD3	2.07	0.54
1:B:197:ARG:HG3	1:B:198:GLN:HG3	1.89	0.54
1:B:279:GLU:O	1:B:280:GLY:O	2.24	0.54
1:C:375:PRO:O	1:C:377:ILE:N	2.40	0.54
1:A:122:ASP:OD1	1:A:526:THR:CG2	2.56	0.54
1:A:228:PRO:HG3	2:W:15:TYR:CE1	2.42	0.54
1:A:375:PRO:O	1:A:377:ILE:N	2.40	0.54
1:B:67:THR:OG1	1:B:68:ARG:N	2.39	0.54
1:B:122:ASP:OD1	1:B:526:THR:CG2	2.56	0.54
1:B:428:VAL:CG1	1:B:513:THR:HB	2.38	0.54
1:E:197:ARG:HG3	1:E:198:GLN:HG3	1.88	0.54
1:E:375:PRO:O	1:E:377:ILE:N	2.41	0.54
1:B:52:ARG:N	1:B:116:ARG:NH1	2.56	0.54
1:C:171:PRO:HG2	1:C:174:ASN:ND2	2.23	0.54
1:D:279:GLU:O	1:D:280:GLY:C	2.45	0.54
1:E:52:ARG:N	1:E:116:ARG:NH1	2.56	0.54
1:E:495:ASN:O	1:E:498:PRO:HD3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:PRO:O	1:B:377:ILE:N	2.40	0.54
1:C:428:VAL:CG1	1:C:513:THR:HB	2.38	0.54
1:C:542:THR:CG2	1:C:547:ARG:N	2.70	0.54
1:E:404:TRP:NE1	1:E:417:ILE:HG21	2.22	0.54
1:A:495:ASN:O	1:A:498:PRO:HD3	2.08	0.54
1:A:563:VAL:HG12	1:A:564:LEU:N	2.23	0.54
1:B:484:ILE:CG2	1:C:480:TYR:CD1	2.90	0.54
1:B:556:LEU:HD21	1:C:434:GLN:HG2	1.89	0.54
1:C:404:TRP:NE1	1:C:417:ILE:HG21	2.22	0.54
1:D:171:PRO:HG2	1:D:174:ASN:ND2	2.23	0.54
1:D:428:VAL:CG1	1:D:513:THR:HB	2.38	0.54
1:B:495:ASN:O	1:B:498:PRO:HD3	2.08	0.54
1:C:88:HIS:ND1	1:C:553:TYR:O	2.38	0.54
1:D:179:MET:HE3	1:D:485:ARG:HH22	1.72	0.54
1:E:214:ASN:O	1:E:216:ARG:N	2.41	0.54
1:B:243:LEU:HG	1:B:401:TYR:HE2	1.71	0.54
1:B:404:TRP:NE1	1:B:417:ILE:HG21	2.22	0.54
1:D:67:THR:HG21	1:E:447:VAL:CG2	2.37	0.54
1:A:65:ASP:O	1:A:66:THR:HB	2.06	0.54
1:B:542:THR:CG2	1:B:547:ARG:N	2.70	0.54
1:C:122:ASP:OD1	1:C:526:THR:CG2	2.56	0.54
1:D:563:VAL:HG12	1:D:564:LEU:N	2.23	0.54
1:E:428:VAL:CG1	1:E:513:THR:HB	2.38	0.54
1:A:52:ARG:N	1:A:116:ARG:NH1	2.56	0.54
1:A:542:THR:CG2	1:A:547:ARG:N	2.71	0.54
1:B:96:ILE:O	1:C:448:THR:HB	2.07	0.54
1:B:485:ARG:NE	1:C:234:GLU:OE2	2.38	0.54
1:C:214:ASN:O	1:C:216:ARG:N	2.41	0.54
1:D:404:TRP:HE1	1:D:417:ILE:HG21	1.73	0.54
1:E:171:PRO:HG2	1:E:174:ASN:ND2	2.23	0.54
1:E:542:THR:CG2	1:E:547:ARG:N	2.70	0.54
1:B:64:PHE:CD1	1:C:118:HIS:NE2	2.76	0.54
1:B:177:GLU:CG	1:B:178:THR:N	2.71	0.54
1:B:214:ASN:O	1:B:216:ARG:N	2.41	0.54
1:B:243:LEU:HG	1:B:401:TYR:CE2	2.43	0.54
1:C:223:THR:HG21	1:C:227:MET:SD	2.48	0.54
1:A:404:TRP:HE1	1:A:417:ILE:HG21	1.73	0.53
1:B:279:GLU:O	1:B:280:GLY:C	2.45	0.53
1:D:243:LEU:HG	1:D:401:TYR:CE2	2.43	0.53
1:D:279:GLU:O	1:D:280:GLY:O	2.24	0.53
1:D:375:PRO:O	1:D:377:ILE:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:ASP:OD1	1:E:526:THR:CG2	2.55	0.53
1:A:558:ILE:HD11	1:B:463:ALA:HB3	1.90	0.53
1:B:223:THR:HG21	1:B:227:MET:SD	2.49	0.53
1:C:563:VAL:HG12	1:C:564:LEU:N	2.23	0.53
1:D:52:ARG:N	1:D:116:ARG:NH1	2.56	0.53
1:D:122:ASP:OD1	1:D:526:THR:CG2	2.56	0.53
1:D:542:THR:CG2	1:D:547:ARG:N	2.71	0.53
1:E:243:LEU:HG	1:E:401:TYR:CE2	2.44	0.53
1:A:171:PRO:HG2	1:A:174:ASN:ND2	2.23	0.53
1:A:279:GLU:O	1:A:280:GLY:C	2.45	0.53
1:C:228:PRO:HG3	2:T:15:TYR:CE1	2.43	0.53
1:D:404:TRP:NE1	1:D:417:ILE:HG21	2.22	0.53
1:A:197:ARG:HG3	1:A:198:GLN:HG3	1.89	0.53
1:A:214:ASN:O	1:A:216:ARG:N	2.41	0.53
1:A:230:VAL:CG1	1:E:490:LEU:HB2	2.31	0.53
1:A:428:VAL:CG1	1:A:513:THR:HB	2.38	0.53
1:B:214:ASN:ND2	1:B:216:ARG:HB3	2.24	0.53
1:B:404:TRP:HE1	1:B:417:ILE:HG21	1.73	0.53
1:B:563:VAL:HG12	1:B:564:LEU:N	2.23	0.53
1:C:495:ASN:O	1:C:498:PRO:HD3	2.08	0.53
1:A:67:THR:HG21	1:B:447:VAL:CG2	2.37	0.53
1:A:486:GLN:HE22	1:A:495:ASN:ND2	2.07	0.53
1:A:542:THR:HG22	1:A:543:ASP:H	1.74	0.53
1:C:243:LEU:HG	1:C:401:TYR:CE2	2.44	0.53
1:D:214:ASN:O	1:D:216:ARG:N	2.41	0.53
1:D:495:ASN:O	1:D:498:PRO:HD3	2.08	0.53
1:D:542:THR:HG22	1:D:543:ASP:H	1.74	0.53
1:B:488:THR:CG2	1:C:479:VAL:CG1	2.86	0.53
1:B:542:THR:HG22	1:B:543:ASP:H	1.74	0.53
1:C:88:HIS:CD2	1:D:267:PHE:CZ	2.96	0.53
1:C:279:GLU:O	1:C:280:GLY:C	2.45	0.53
1:D:444:GLN:O	1:D:446:PRO:HD3	2.07	0.53
1:E:404:TRP:HE1	1:E:417:ILE:HG21	1.73	0.53
1:A:442:MET:HB2	1:A:537:GLN:OE1	2.08	0.53
1:B:442:MET:HB2	1:B:537:GLN:OE1	2.09	0.53
1:C:177:GLU:CG	1:C:178:THR:N	2.71	0.53
1:C:542:THR:HG22	1:C:543:ASP:H	1.74	0.53
1:D:214:ASN:ND2	1:D:216:ARG:HB3	2.24	0.53
1:D:442:MET:HB2	1:D:537:GLN:OE1	2.09	0.53
1:D:486:GLN:HE22	1:D:495:ASN:ND2	2.07	0.53
1:A:223:THR:HG21	1:A:227:MET:SD	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:TYR:OH	1:B:109:GLN:NE2	2.42	0.53
1:C:52:ARG:N	1:C:116:ARG:NH1	2.56	0.53
1:C:100:ASP:CG	1:D:450:ARG:HH12	2.10	0.53
1:C:486:GLN:HE22	1:C:495:ASN:ND2	2.07	0.53
1:D:376:VAL:C	1:D:378:LYS:N	2.62	0.53
1:E:442:MET:HB2	1:E:537:GLN:OE1	2.08	0.53
1:A:57:TYR:OH	1:A:109:GLN:NE2	2.42	0.53
1:B:376:VAL:C	1:B:378:LYS:N	2.62	0.53
1:B:486:GLN:HE22	1:B:495:ASN:ND2	2.07	0.53
1:D:392:ILE:HA	1:D:400:GLN:HE21	1.74	0.53
1:C:404:TRP:HE1	1:C:417:ILE:HG21	1.73	0.53
1:E:113:LEU:O	1:E:114:ASP:C	2.47	0.53
1:A:113:LEU:O	1:A:114:ASP:C	2.47	0.52
1:B:392:ILE:HA	1:B:400:GLN:HE21	1.74	0.52
1:C:57:TYR:OH	1:C:109:GLN:NE2	2.42	0.52
1:D:223:THR:HG21	1:D:227:MET:SD	2.49	0.52
1:E:151:ARG:HB3	1:E:201:VAL:N	2.24	0.52
1:E:486:GLN:HE22	1:E:495:ASN:ND2	2.07	0.52
1:A:527:LEU:HD21	1:E:68:ARG:NE	2.25	0.52
1:C:113:LEU:O	1:C:114:ASP:C	2.47	0.52
1:C:214:ASN:ND2	1:C:216:ARG:HB3	2.24	0.52
1:D:68:ARG:NH1	1:D:68:ARG:CG	2.67	0.52
1:D:151:ARG:HB3	1:D:201:VAL:N	2.24	0.52
1:D:491:THR:HG23	2:V:15:TYR:CE1	2.45	0.52
1:E:126:ILE:HG12	1:E:521:LEU:HD23	1.91	0.52
1:E:223:THR:HG21	1:E:227:MET:SD	2.49	0.52
1:E:376:VAL:C	1:E:378:LYS:N	2.62	0.52
1:E:392:ILE:HA	1:E:400:GLN:HE21	1.74	0.52
1:E:455:ILE:HA	1:E:458:PHE:CE2	2.44	0.52
1:E:563:VAL:HG12	1:E:564:LEU:N	2.23	0.52
1:A:88:HIS:CD2	1:B:267:PHE:CZ	2.97	0.52
1:B:474:TYR:CD1	1:B:511:ILE:HD11	2.45	0.52
1:D:57:TYR:OH	1:D:109:GLN:NE2	2.42	0.52
1:D:455:ILE:HA	1:D:458:PHE:CE2	2.45	0.52
1:A:474:TYR:CD1	1:A:511:ILE:HD11	2.45	0.52
1:A:491:THR:HG23	2:S:15:TYR:CE1	2.45	0.52
1:B:113:LEU:O	1:B:114:ASP:C	2.47	0.52
1:B:171:PRO:HG2	1:B:174:ASN:ND2	2.23	0.52
1:C:401:TYR:HD1	1:C:502:ILE:HG12	1.68	0.52
1:A:243:LEU:HG	1:A:401:TYR:CE2	2.44	0.52
1:A:455:ILE:HA	1:A:458:PHE:CE2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:TYR:OH	1:E:109:GLN:NE2	2.42	0.52
1:B:128:HIS:CE1	1:C:432:SER:HG	2.27	0.52
1:C:392:ILE:HA	1:C:400:GLN:HE21	1.74	0.52
1:C:442:MET:HB2	1:C:537:GLN:OE1	2.08	0.52
1:D:474:TYR:CD1	1:D:511:ILE:HD11	2.45	0.52
1:D:511:ILE:HD12	1:D:511:ILE:N	2.25	0.52
1:E:231:TYR:HD1	1:E:501:GLN:HB3	1.75	0.52
1:E:511:ILE:HD12	1:E:511:ILE:N	2.25	0.52
1:A:214:ASN:ND2	1:A:216:ARG:HB3	2.24	0.52
1:A:418:ARG:O	1:A:418:ARG:HG2	2.10	0.52
1:A:455:ILE:HD12	1:A:456:SER:N	2.25	0.52
1:B:455:ILE:HA	1:B:458:PHE:CE2	2.44	0.52
1:B:491:THR:HG23	2:T:15:TYR:CE1	2.45	0.52
1:C:178:THR:OG1	1:C:509:PRO:HD2	2.10	0.52
1:C:455:ILE:HA	1:C:458:PHE:CE2	2.44	0.52
1:C:485:ARG:NH1	1:C:505:ARG:HH22	2.07	0.52
1:D:68:ARG:NE	1:E:527:LEU:HD21	2.25	0.52
1:E:177:GLU:CG	1:E:178:THR:N	2.71	0.52
1:E:455:ILE:HD12	1:E:456:SER:N	2.25	0.52
1:A:126:ILE:HG12	1:A:521:LEU:HD23	1.91	0.52
1:A:151:ARG:HB3	1:A:201:VAL:N	2.24	0.52
1:A:177:GLU:CG	1:A:178:THR:N	2.71	0.52
1:C:151:ARG:HB3	1:C:201:VAL:N	2.24	0.52
1:C:556:LEU:C	1:C:556:LEU:HD12	2.30	0.52
1:D:177:GLU:CG	1:D:178:THR:N	2.72	0.52
1:E:214:ASN:ND2	1:E:216:ARG:HB3	2.24	0.52
1:A:231:TYR:HD1	1:A:501:GLN:HB3	1.75	0.52
1:A:448:THR:HG22	1:E:57:TYR:CD2	2.45	0.52
1:C:74:ASN:OD1	1:D:434:GLN:OE1	2.28	0.52
1:C:491:THR:HG23	2:U:15:TYR:CE1	2.45	0.52
1:D:490:LEU:HB2	1:E:230:VAL:CG1	2.29	0.52
1:E:474:TYR:CD1	1:E:511:ILE:HD11	2.45	0.52
1:A:556:LEU:HD12	1:A:556:LEU:C	2.31	0.52
1:B:151:ARG:HB3	1:B:201:VAL:N	2.24	0.52
1:B:277:ASP:O	1:B:417:ILE:HD13	2.10	0.52
1:B:485:ARG:NH1	1:B:505:ARG:HH22	2.07	0.52
1:B:556:LEU:C	1:B:556:LEU:HD12	2.30	0.52
1:C:231:TYR:HD1	1:C:501:GLN:HB3	1.75	0.52
1:C:277:ASP:O	1:C:417:ILE:HD13	2.10	0.52
1:C:474:TYR:CD1	1:C:511:ILE:HD11	2.45	0.52
1:E:228:PRO:HG3	2:V:15:TYR:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:491:THR:HG23	2:W:15:TYR:CE1	2.45	0.52
1:B:228:PRO:HB3	2:S:15:TYR:HE1	1.75	0.51
1:B:231:TYR:HD1	1:B:501:GLN:HB3	1.75	0.51
1:D:113:LEU:O	1:D:114:ASP:C	2.47	0.51
1:E:154:THR:CG2	1:E:155:LYS:HG3	2.41	0.51
1:E:277:ASP:O	1:E:417:ILE:HD13	2.10	0.51
1:A:88:HIS:HD2	1:B:267:PHE:CZ	2.28	0.51
1:C:128:HIS:CE1	1:D:432:SER:HG	2.28	0.51
1:C:511:ILE:N	1:C:511:ILE:HD12	2.25	0.51
1:D:178:THR:OG1	1:D:509:PRO:HD2	2.10	0.51
1:D:277:ASP:O	1:D:417:ILE:HD13	2.10	0.51
1:D:427:ASP:C	1:D:427:ASP:OD1	2.49	0.51
1:A:392:ILE:HA	1:A:400:GLN:HE21	1.74	0.51
1:B:126:ILE:HG12	1:B:521:LEU:HD23	1.91	0.51
1:C:551:TYR:CZ	1:D:422:LEU:HD21	2.45	0.51
1:D:418:ARG:O	1:D:418:ARG:HG2	2.10	0.51
1:E:132:PRO:HA	1:E:175:TYR:CZ	2.45	0.51
1:E:556:LEU:C	1:E:556:LEU:HD12	2.30	0.51
1:A:427:ASP:C	1:A:427:ASP:OD1	2.49	0.51
1:A:497:PHE:CD1	1:A:503:LEU:HB3	2.44	0.51
1:E:387:ARG:HG2	1:E:387:ARG:NH1	2.26	0.51
1:E:418:ARG:HG2	1:E:418:ARG:O	2.10	0.51
1:E:427:ASP:C	1:E:427:ASP:OD1	2.49	0.51
1:A:387:ARG:HG2	1:A:387:ARG:NH1	2.26	0.51
1:B:178:THR:OG1	1:B:509:PRO:HD2	2.10	0.51
1:C:427:ASP:C	1:C:427:ASP:OD1	2.49	0.51
1:D:485:ARG:NH1	1:D:505:ARG:HH22	2.07	0.51
1:A:484:ILE:HG23	1:B:480:TYR:HE1	1.75	0.51
1:C:477:GLN:O	1:C:481:SER:HB3	2.07	0.51
1:D:74:ASN:OD1	1:E:434:GLN:OE1	2.27	0.51
1:D:556:LEU:C	1:D:556:LEU:HD12	2.31	0.51
1:E:542:THR:HG22	1:E:543:ASP:H	1.74	0.51
1:C:130:ASN:C	1:C:130:ASN:HD22	2.14	0.51
1:D:227:MET:HB2	1:D:228:PRO:HD3	1.92	0.51
1:D:477:GLN:O	1:D:481:SER:HB3	2.07	0.51
1:A:178:THR:OG1	1:A:509:PRO:HD2	2.10	0.51
1:B:511:ILE:HD12	1:B:511:ILE:N	2.25	0.51
1:C:132:PRO:HA	1:C:175:TYR:CZ	2.45	0.51
1:D:126:ILE:HG12	1:D:521:LEU:HD23	1.91	0.51
1:E:130:ASN:C	1:E:130:ASN:HD22	2.14	0.51
1:B:427:ASP:C	1:B:427:ASP:OD1	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:TYR:HD1	1:D:376:VAL:HG12	1.75	0.51
1:E:237:HIS:CD2	1:E:423:LEU:HD11	2.46	0.51
1:A:292:TYR:HD1	1:A:376:VAL:HG12	1.75	0.51
1:B:235:ALA:C	1:B:236:PHE:HD1	2.15	0.51
1:C:64:PHE:HD1	1:D:118:HIS:NE2	2.09	0.51
1:C:126:ILE:HG12	1:C:521:LEU:HD23	1.91	0.51
1:C:376:VAL:C	1:C:378:LYS:N	2.62	0.51
1:D:130:ASN:HD22	1:D:130:ASN:C	2.14	0.51
1:E:485:ARG:NH1	1:E:505:ARG:HH22	2.07	0.51
1:A:277:ASP:O	1:A:417:ILE:HD13	2.10	0.50
1:C:67:THR:CG2	1:D:447:VAL:CG2	2.89	0.50
1:C:292:TYR:HD1	1:C:376:VAL:HG12	1.75	0.50
1:D:237:HIS:CD2	1:D:423:LEU:HD11	2.46	0.50
1:E:227:MET:HB2	1:E:228:PRO:HD3	1.92	0.50
1:E:477:GLN:O	1:E:481:SER:HB3	2.07	0.50
1:C:171:PRO:CA	1:D:409:ASN:HD22	2.24	0.50
1:B:228:PRO:HG3	2:S:15:TYR:CE1	2.46	0.50
1:B:497:PHE:HD1	1:B:503:LEU:CB	2.25	0.50
1:B:551:TYR:CE2	1:C:422:LEU:HD21	2.47	0.50
1:E:235:ALA:C	1:E:236:PHE:HD1	2.15	0.50
1:E:422:LEU:HD23	1:E:423:LEU:H	1.76	0.50
1:B:295:SER:CB	1:B:375:PRO:CG	2.90	0.50
1:C:497:PHE:HD1	1:C:503:LEU:CB	2.25	0.50
1:D:154:THR:CG2	1:D:155:LYS:HG3	2.41	0.50
1:A:235:ALA:C	1:A:236:PHE:HD1	2.15	0.50
1:A:511:ILE:HD12	1:A:511:ILE:N	2.25	0.50
1:B:418:ARG:O	1:B:418:ARG:HG2	2.10	0.50
1:C:235:ALA:C	1:C:236:PHE:HD1	2.15	0.50
1:C:237:HIS:CD2	1:C:423:LEU:HD11	2.46	0.50
1:D:64:PHE:HD1	1:E:118:HIS:NE2	2.09	0.50
1:A:130:ASN:C	1:A:130:ASN:HD22	2.14	0.50
1:A:373:LYS:O	1:A:374:LYS:HG3	2.12	0.50
1:B:154:THR:CG2	1:B:155:LYS:HG3	2.40	0.50
1:B:179:MET:HE3	1:B:485:ARG:HH22	1.76	0.50
1:B:237:HIS:CD2	1:B:423:LEU:HD11	2.46	0.50
1:C:227:MET:HB2	1:C:228:PRO:HD3	1.92	0.50
1:C:543:ASP:OD1	1:C:547:ARG:HG2	2.12	0.50
1:D:231:TYR:HD1	1:D:501:GLN:HB3	1.75	0.50
1:E:178:THR:OG1	1:E:509:PRO:HD2	2.10	0.50
2:S:15:TYR:HD2	2:S:16:PRO:HD2	1.77	0.50
2:T:15:TYR:HD2	2:T:16:PRO:HD2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:VAL:HA	1:E:63:LEU:HD12	1.93	0.50
1:B:387:ARG:HG2	1:B:387:ARG:NH1	2.26	0.50
1:B:553:TYR:HE2	1:C:432:SER:N	2.09	0.50
1:C:387:ARG:HG2	1:C:387:ARG:NH1	2.26	0.50
1:C:418:ARG:HG2	1:C:418:ARG:O	2.10	0.50
1:D:132:PRO:HA	1:D:175:TYR:CZ	2.45	0.50
1:D:422:LEU:HD23	1:D:423:LEU:H	1.76	0.50
1:D:543:ASP:OD1	1:D:547:ARG:HG2	2.12	0.50
2:U:15:TYR:HD2	2:U:16:PRO:HD2	1.76	0.50
1:A:237:HIS:CD2	1:A:423:LEU:HD11	2.46	0.50
1:A:485:ARG:NH1	1:A:505:ARG:HH22	2.07	0.50
1:B:132:PRO:HA	1:B:175:TYR:CZ	2.45	0.50
1:B:542:THR:HG22	1:B:543:ASP:N	2.27	0.50
1:C:130:ASN:HD22	1:C:130:ASN:N	2.10	0.50
1:D:228:PRO:CB	2:U:15:TYR:HE1	2.25	0.50
1:E:384:SER:O	1:E:386:LYS:N	2.45	0.50
1:A:497:PHE:HD1	1:A:503:LEU:CB	2.25	0.50
1:D:243:LEU:CD2	1:D:244:PRO:HD3	2.42	0.50
1:D:373:LYS:O	1:D:374:LYS:HG3	2.12	0.50
1:D:484:ILE:CG2	1:E:480:TYR:HE1	2.22	0.50
1:E:295:SER:CB	1:E:375:PRO:CG	2.90	0.50
2:V:15:TYR:HD2	2:V:16:PRO:HD2	1.77	0.50
1:A:376:VAL:C	1:A:378:LYS:N	2.62	0.49
1:B:68:ARG:NH1	1:B:68:ARG:CG	2.67	0.49
1:B:227:MET:HB2	1:B:228:PRO:HD3	1.92	0.49
1:B:292:TYR:HD1	1:B:376:VAL:HG12	1.76	0.49
1:C:151:ARG:CB	1:C:201:VAL:H	2.25	0.49
1:C:173:GLY:O	1:C:175:TYR:CE1	2.65	0.49
1:D:63:LEU:HD12	1:E:447:VAL:HA	1.93	0.49
1:D:243:LEU:CG	1:D:401:TYR:HE2	2.25	0.49
1:D:384:SER:O	1:D:386:LYS:N	2.45	0.49
1:E:131:MET:HA	1:E:551:TYR:CD2	2.47	0.49
1:E:173:GLY:O	1:E:175:TYR:CE1	2.65	0.49
1:A:227:MET:HB2	1:A:228:PRO:HD3	1.92	0.49
1:B:130:ASN:HD22	1:B:130:ASN:C	2.14	0.49
1:B:543:ASP:OD1	1:B:547:ARG:HG2	2.12	0.49
1:D:455:ILE:HD12	1:D:456:SER:N	2.25	0.49
1:E:542:THR:HG22	1:E:543:ASP:N	2.27	0.49
1:C:295:SER:CB	1:C:375:PRO:CG	2.90	0.49
1:D:131:MET:HA	1:D:551:TYR:CD2	2.47	0.49
1:D:197:ARG:HG3	1:D:198:GLN:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:ILE:HD11	1:D:273:ILE:HG21	1.95	0.49
1:D:392:ILE:HD11	1:D:396:SER:OG	2.13	0.49
1:D:542:THR:HG22	1:D:543:ASP:N	2.27	0.49
1:E:201:VAL:O	1:E:201:VAL:HG13	2.12	0.49
2:W:10:THR:O	2:W:10:THR:CG2	2.60	0.49
1:A:74:ASN:OD1	1:B:434:GLN:OE1	2.30	0.49
1:A:173:GLY:O	1:A:175:TYR:CE1	2.65	0.49
1:A:243:LEU:CD2	1:A:244:PRO:HD3	2.42	0.49
1:A:243:LEU:CG	1:A:401:TYR:HE2	2.25	0.49
1:B:98:ASN:C	1:B:98:ASN:ND2	2.66	0.49
1:B:132:PRO:CA	1:B:175:TYR:OH	2.53	0.49
1:B:243:LEU:CG	1:B:401:TYR:HE2	2.25	0.49
1:C:63:LEU:HD12	1:D:447:VAL:HA	1.95	0.49
1:C:98:ASN:C	1:C:98:ASN:ND2	2.66	0.49
1:C:197:ARG:HG3	1:C:198:GLN:N	2.27	0.49
1:C:392:ILE:HD11	1:C:396:SER:OG	2.13	0.49
1:D:295:SER:CB	1:D:375:PRO:CG	2.90	0.49
1:D:491:THR:HG22	1:D:492:HIS:N	2.27	0.49
1:E:197:ARG:HG3	1:E:198:GLN:N	2.27	0.49
1:A:130:ASN:HD22	1:A:130:ASN:N	2.10	0.49
1:A:295:SER:CB	1:A:375:PRO:CG	2.90	0.49
1:A:542:THR:HG22	1:A:543:ASP:N	2.27	0.49
1:B:131:MET:HA	1:B:551:TYR:CD2	2.47	0.49
1:B:201:VAL:O	1:B:201:VAL:HG13	2.12	0.49
1:B:243:LEU:CD2	1:B:244:PRO:HD3	2.42	0.49
1:B:384:SER:O	1:B:386:LYS:N	2.45	0.49
1:B:389:TYR:O	1:B:390:ASN:C	2.51	0.49
1:B:392:ILE:HD11	1:B:396:SER:OG	2.13	0.49
1:B:491:THR:HG22	1:B:492:HIS:N	2.27	0.49
1:C:154:THR:CG2	1:C:155:LYS:HG3	2.41	0.49
1:C:240:ILE:HD11	1:C:273:ILE:HG21	1.95	0.49
1:C:373:LYS:O	1:C:374:LYS:HG3	2.12	0.49
1:C:501:GLN:OE1	1:C:501:GLN:HA	2.12	0.49
1:C:518:VAL:CG2	1:C:519:PRO:HD2	2.43	0.49
1:D:151:ARG:CB	1:D:201:VAL:H	2.25	0.49
1:D:173:GLY:O	1:D:175:TYR:CE1	2.65	0.49
1:D:235:ALA:C	1:D:236:PHE:HD1	2.15	0.49
1:D:387:ARG:HG2	1:D:387:ARG:NH1	2.26	0.49
1:D:501:GLN:OE1	1:D:501:GLN:HA	2.12	0.49
1:D:518:VAL:CG2	1:D:519:PRO:HD2	2.42	0.49
1:E:151:ARG:CB	1:E:201:VAL:H	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ARG:NH1	1:A:68:ARG:CG	2.67	0.49
1:A:131:MET:HA	1:A:551:TYR:CD2	2.47	0.49
1:A:384:SER:O	1:A:386:LYS:N	2.45	0.49
1:A:495:ASN:ND2	1:A:498:PRO:HB3	2.28	0.49
1:B:373:LYS:O	1:B:374:LYS:HG3	2.12	0.49
1:C:243:LEU:CD2	1:C:244:PRO:HD3	2.43	0.49
1:E:68:ARG:NH1	1:E:68:ARG:CG	2.67	0.49
1:E:243:LEU:CG	1:E:401:TYR:HE2	2.25	0.49
1:E:373:LYS:O	1:E:374:LYS:HG3	2.12	0.49
1:E:518:VAL:CG2	1:E:519:PRO:HD2	2.42	0.49
1:B:130:ASN:HD22	1:B:130:ASN:N	2.10	0.49
1:C:131:MET:HA	1:C:551:TYR:CD2	2.47	0.49
1:C:389:TYR:O	1:C:390:ASN:C	2.51	0.49
1:D:98:ASN:C	1:D:98:ASN:ND2	2.66	0.49
1:D:130:ASN:HD22	1:D:130:ASN:N	2.10	0.49
1:A:98:ASN:C	1:A:98:ASN:ND2	2.66	0.49
1:A:151:ARG:CB	1:A:201:VAL:H	2.25	0.49
1:A:240:ILE:HD11	1:A:273:ILE:HG21	1.95	0.49
1:C:243:LEU:CG	1:C:401:TYR:HE2	2.25	0.49
1:C:491:THR:HG22	1:C:492:HIS:N	2.27	0.49
1:C:542:THR:HG22	1:C:543:ASP:N	2.27	0.49
1:D:495:ASN:ND2	1:D:498:PRO:HB3	2.28	0.49
1:A:501:GLN:OE1	1:A:501:GLN:HA	2.12	0.49
1:A:518:VAL:CG2	1:A:519:PRO:HD2	2.43	0.49
1:A:540:THR:HG22	1:A:540:THR:O	2.13	0.49
1:B:249:ASP:C	1:B:249:ASP:OD1	2.51	0.49
1:C:422:LEU:HD23	1:C:423:LEU:H	1.76	0.49
1:C:455:ILE:HD12	1:C:456:SER:N	2.25	0.49
1:D:201:VAL:HG13	1:D:201:VAL:O	2.12	0.49
1:D:497:PHE:HD1	1:D:503:LEU:CB	2.25	0.49
1:E:130:ASN:HD22	1:E:130:ASN:N	2.10	0.49
2:U:10:THR:O	2:U:10:THR:CG2	2.60	0.49
1:B:237:HIS:HD2	1:B:238:PRO:O	1.96	0.49
1:C:201:VAL:HG13	1:C:201:VAL:O	2.12	0.49
1:C:495:ASN:ND2	1:C:498:PRO:HB3	2.28	0.49
1:D:57:TYR:CE2	1:E:448:THR:HG22	2.48	0.49
1:D:237:HIS:HD2	1:D:238:PRO:O	1.96	0.49
1:D:249:ASP:C	1:D:249:ASP:OD1	2.51	0.49
1:E:501:GLN:HA	1:E:501:GLN:OE1	2.12	0.49
1:E:540:THR:O	1:E:540:THR:HG22	2.13	0.49
1:B:173:GLY:O	1:B:175:TYR:CE1	2.65	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ARG:HG3	1:B:198:GLN:N	2.27	0.48
1:E:543:ASP:OD1	1:E:547:ARG:HG2	2.12	0.48
2:W:15:TYR:HD2	2:W:16:PRO:HD2	1.76	0.48
1:A:132:PRO:HA	1:A:175:TYR:CZ	2.45	0.48
1:A:434:GLN:OE1	1:E:74:ASN:OD1	2.30	0.48
1:A:447:VAL:HG23	1:E:67:THR:OG1	2.12	0.48
1:B:518:VAL:CG2	1:B:519:PRO:HD2	2.43	0.48
1:E:243:LEU:CD2	1:E:244:PRO:HD3	2.42	0.48
1:E:491:THR:HG22	1:E:492:HIS:N	2.27	0.48
1:A:154:THR:CG2	1:A:155:LYS:HG3	2.40	0.48
1:A:201:VAL:HG13	1:A:201:VAL:O	2.12	0.48
1:A:392:ILE:HD11	1:A:396:SER:OG	2.13	0.48
1:B:151:ARG:CB	1:B:201:VAL:H	2.26	0.48
1:B:495:ASN:ND2	1:B:498:PRO:HB3	2.28	0.48
1:C:130:ASN:N	1:C:130:ASN:ND2	2.61	0.48
1:D:244:PRO:HA	1:D:275:TYR:CD2	2.49	0.48
1:D:540:THR:O	1:D:540:THR:HG22	2.13	0.48
1:D:553:TYR:HE2	1:E:432:SER:N	2.11	0.48
1:E:392:ILE:HD11	1:E:396:SER:OG	2.13	0.48
1:A:179:MET:HE3	1:A:485:ARG:NH2	2.28	0.48
1:A:197:ARG:HG3	1:A:198:GLN:N	2.27	0.48
1:A:237:HIS:HD2	1:A:238:PRO:O	1.96	0.48
1:A:389:TYR:O	1:A:390:ASN:C	2.51	0.48
1:B:228:PRO:HG3	2:S:15:TYR:CD1	2.48	0.48
1:D:130:ASN:N	1:D:130:ASN:ND2	2.61	0.48
1:E:237:HIS:HD2	1:E:238:PRO:O	1.96	0.48
1:E:292:TYR:HD1	1:E:376:VAL:HG12	1.75	0.48
1:E:495:ASN:ND2	1:E:498:PRO:HB3	2.28	0.48
1:E:497:PHE:O	1:E:499:GLU:N	2.45	0.48
1:A:142:LYS:O	1:A:143:PHE:HB3	2.14	0.48
1:A:477:GLN:O	1:A:481:SER:HB3	2.07	0.48
1:A:543:ASP:OD1	1:A:547:ARG:HG2	2.12	0.48
1:D:497:PHE:O	1:D:499:GLU:N	2.45	0.48
1:B:142:LYS:HD3	1:B:167:GLU:OE2	2.14	0.48
1:B:142:LYS:O	1:B:143:PHE:HB3	2.14	0.48
1:B:497:PHE:CD1	1:B:503:LEU:HB3	2.44	0.48
1:B:501:GLN:OE1	1:B:501:GLN:HA	2.12	0.48
1:C:142:LYS:O	1:C:143:PHE:HB3	2.14	0.48
1:D:74:ASN:O	1:D:75:LYS:C	2.52	0.48
1:D:142:LYS:O	1:D:143:PHE:HB3	2.14	0.48
1:E:179:MET:CE	1:E:485:ARG:NH2	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:10:THR:O	2:V:10:THR:CG2	2.60	0.48
1:A:130:ASN:N	1:A:130:ASN:ND2	2.61	0.48
1:A:142:LYS:HD3	1:A:167:GLU:OE2	2.14	0.48
1:A:179:MET:CE	1:A:485:ARG:NH2	2.77	0.48
1:A:422:LEU:HD23	1:A:423:LEU:H	1.76	0.48
1:A:491:THR:HG22	1:A:492:HIS:N	2.27	0.48
1:B:455:ILE:HD12	1:B:456:SER:N	2.25	0.48
1:B:491:THR:HG22	1:B:493:VAL:N	2.29	0.48
1:C:74:ASN:O	1:C:75:LYS:C	2.52	0.48
1:C:244:PRO:HA	1:C:275:TYR:CD2	2.49	0.48
1:C:249:ASP:C	1:C:249:ASP:OD1	2.52	0.48
1:C:497:PHE:CD1	1:C:503:LEU:HB3	2.44	0.48
1:A:244:PRO:HA	1:A:275:TYR:CD2	2.49	0.48
1:A:249:ASP:C	1:A:249:ASP:OD1	2.52	0.48
1:B:75:LYS:O	1:B:78:ASP:OD1	2.32	0.48
1:B:211:ASP:HA	1:B:506:PRO:CG	2.44	0.48
1:C:193:LEU:HD22	1:C:197:ARG:NH1	2.29	0.48
1:C:384:SER:O	1:C:386:LYS:N	2.45	0.48
1:C:540:THR:O	1:C:540:THR:HG22	2.13	0.48
1:D:179:MET:CE	1:D:485:ARG:NH2	2.77	0.48
1:E:142:LYS:O	1:E:143:PHE:HB3	2.14	0.48
1:E:491:THR:HG22	1:E:493:VAL:N	2.29	0.48
1:A:118:HIS:NE2	1:E:64:PHE:HD1	2.12	0.48
1:B:87:ASP:O	1:B:89:SER:N	2.46	0.48
1:C:179:MET:CE	1:C:485:ARG:NH2	2.77	0.48
1:D:454:GLN:O	1:D:456:SER:N	2.47	0.48
1:E:145:ALA:HA	1:E:248:VAL:HA	1.96	0.48
1:E:240:ILE:HD11	1:E:273:ILE:HG21	1.95	0.48
1:E:244:PRO:HA	1:E:275:TYR:CD2	2.49	0.48
1:E:269:GLU:HG3	1:E:269:GLU:O	2.14	0.48
1:A:239:ASP:HB3	1:A:405:TYR:HB2	1.96	0.48
1:A:454:GLN:O	1:A:456:SER:N	2.47	0.48
1:B:193:LEU:HD22	1:B:197:ARG:NH1	2.29	0.48
1:B:215:PHE:CE1	1:B:241:ILE:HD11	2.49	0.48
1:B:240:ILE:HD11	1:B:273:ILE:HG21	1.95	0.48
1:B:542:THR:HG22	1:B:547:ARG:H	1.79	0.48
1:C:171:PRO:HA	1:D:409:ASN:HD22	1.79	0.48
1:D:228:PRO:HG3	2:U:15:TYR:CD1	2.49	0.48
1:E:130:ASN:N	1:E:130:ASN:ND2	2.61	0.48
1:E:389:TYR:O	1:E:390:ASN:C	2.51	0.48
1:B:74:ASN:O	1:B:75:LYS:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ALA:HA	1:B:248:VAL:HA	1.96	0.47
1:B:183:LEU:HD21	1:C:236:PHE:HE2	1.78	0.47
1:B:244:PRO:HA	1:B:275:TYR:CD2	2.49	0.47
1:C:491:THR:HG22	1:C:493:VAL:N	2.29	0.47
1:C:497:PHE:O	1:C:499:GLU:N	2.46	0.47
1:D:215:PHE:CE1	1:D:241:ILE:HD11	2.49	0.47
1:E:75:LYS:O	1:E:78:ASP:OD1	2.32	0.47
1:E:454:GLN:O	1:E:456:SER:N	2.47	0.47
1:B:540:THR:O	1:B:540:THR:HG22	2.13	0.47
1:C:75:LYS:O	1:C:78:ASP:OD1	2.32	0.47
1:D:193:LEU:HD22	1:D:197:ARG:NH1	2.29	0.47
1:D:211:ASP:HA	1:D:506:PRO:CG	2.44	0.47
1:D:383:ASP:C	1:D:384:SER:O	2.52	0.47
1:D:461:VAL:HB	1:D:527:LEU:CD1	2.44	0.47
1:E:142:LYS:HD3	1:E:167:GLU:OE2	2.14	0.47
1:E:249:ASP:C	1:E:249:ASP:OD1	2.51	0.47
1:A:269:GLU:O	1:A:269:GLU:HG3	2.14	0.47
1:A:450:ARG:NH2	1:E:99:ASN:HB3	2.29	0.47
1:A:491:THR:HG22	1:A:493:VAL:N	2.29	0.47
1:B:142:LYS:HG2	1:B:169:THR:HG22	1.97	0.47
1:B:179:MET:CE	1:B:485:ARG:NH2	2.77	0.47
1:B:180:THR:HG21	1:B:258:LEU:CD2	2.44	0.47
1:C:180:THR:HG21	1:C:258:LEU:CD2	2.44	0.47
1:E:497:PHE:CD1	1:E:503:LEU:HB3	2.44	0.47
1:A:74:ASN:O	1:A:75:LYS:C	2.52	0.47
1:B:422:LEU:HD23	1:B:423:LEU:H	1.76	0.47
1:A:171:PRO:HA	1:B:409:ASN:HD22	1.80	0.47
1:A:211:ASP:HA	1:A:506:PRO:CG	2.44	0.47
1:A:277:ASP:O	1:A:279:GLU:N	2.46	0.47
1:B:269:GLU:HG3	1:B:269:GLU:O	2.14	0.47
1:C:102:SER:O	1:C:103:PRO:C	2.52	0.47
1:C:131:MET:SD	1:C:138:MET:HG3	2.55	0.47
1:D:142:LYS:HD3	1:D:167:GLU:OE2	2.14	0.47
1:D:145:ALA:HA	1:D:248:VAL:HA	1.96	0.47
1:D:179:MET:HE3	1:D:485:ARG:NH2	2.29	0.47
1:D:180:THR:HG21	1:D:258:LEU:CD2	2.44	0.47
1:D:389:TYR:O	1:D:390:ASN:C	2.51	0.47
1:E:74:ASN:O	1:E:75:LYS:C	2.52	0.47
1:E:179:MET:HE3	1:E:485:ARG:HH22	1.78	0.47
1:E:180:THR:HG21	1:E:258:LEU:CD2	2.44	0.47
1:E:211:ASP:HA	1:E:506:PRO:CG	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:TYR:HD1	1:A:511:ILE:HD11	1.80	0.47
1:B:130:ASN:N	1:B:130:ASN:ND2	2.61	0.47
1:B:488:THR:HG22	1:C:479:VAL:CG1	2.45	0.47
1:C:215:PHE:CE1	1:C:241:ILE:HD11	2.49	0.47
1:C:237:HIS:HD2	1:C:238:PRO:O	1.96	0.47
1:D:142:LYS:HG2	1:D:169:THR:HG22	1.97	0.47
1:D:491:THR:HG22	1:D:493:VAL:N	2.29	0.47
1:B:96:ILE:O	1:C:448:THR:CB	2.63	0.47
1:B:383:ASP:C	1:B:384:SER:O	2.52	0.47
1:B:434:GLN:NE2	1:B:436:TYR:CE2	2.81	0.47
1:C:142:LYS:HD3	1:C:167:GLU:OE2	2.14	0.47
1:C:142:LYS:HG2	1:C:169:THR:HG22	1.97	0.47
1:C:211:ASP:HA	1:C:506:PRO:CG	2.44	0.47
1:C:454:GLN:O	1:C:456:SER:N	2.47	0.47
1:C:553:TYR:HE2	1:D:432:SER:N	2.12	0.47
1:E:142:LYS:HG2	1:E:169:THR:HG22	1.97	0.47
1:A:75:LYS:O	1:A:78:ASP:OD1	2.32	0.47
1:A:215:PHE:CE1	1:A:241:ILE:HD11	2.50	0.47
1:B:497:PHE:O	1:B:499:GLU:N	2.46	0.47
1:C:83:ASN:CA	1:C:86:ASN:HD22	2.21	0.47
1:D:289:VAL:HG13	1:D:290:ASP:N	2.30	0.47
1:D:542:THR:CG2	1:D:547:ARG:H	2.28	0.47
1:E:98:ASN:C	1:E:98:ASN:ND2	2.66	0.47
1:A:497:PHE:O	1:A:499:GLU:N	2.46	0.47
1:B:131:MET:SD	1:B:138:MET:HG3	2.55	0.47
1:B:454:GLN:O	1:B:456:SER:N	2.47	0.47
1:C:269:GLU:HG3	1:C:269:GLU:O	2.14	0.47
1:A:78:ASP:HB2	1:A:82:LEU:HD12	1.97	0.47
1:A:180:THR:HG21	1:A:258:LEU:CD2	2.44	0.47
1:A:193:LEU:HD22	1:A:197:ARG:NH1	2.29	0.47
1:A:461:VAL:HB	1:A:527:LEU:CD1	2.45	0.47
1:A:485:ARG:CZ	1:A:505:ARG:HH22	2.28	0.47
1:B:542:THR:CG2	1:B:547:ARG:H	2.28	0.47
1:C:88:HIS:HD2	1:D:267:PHE:HZ	1.63	0.47
1:D:78:ASP:HB2	1:D:82:LEU:HD12	1.97	0.47
1:D:132:PRO:CA	1:D:175:TYR:OH	2.53	0.47
1:D:542:THR:HG22	1:D:547:ARG:H	1.79	0.47
1:E:78:ASP:HB2	1:E:82:LEU:HD12	1.97	0.47
1:E:542:THR:HG22	1:E:547:ARG:H	1.79	0.47
1:A:145:ALA:HA	1:A:248:VAL:HA	1.96	0.46
1:A:432:SER:HG	1:E:128:HIS:CE1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:VAL:HG12	1:B:448:THR:HG23	1.97	0.46
1:D:131:MET:SD	1:D:138:MET:HG3	2.55	0.46
1:E:87:ASP:O	1:E:89:SER:N	2.46	0.46
1:E:239:ASP:HB3	1:E:405:TYR:HB2	1.96	0.46
1:E:289:VAL:HG13	1:E:290:ASP:N	2.30	0.46
1:E:461:VAL:HB	1:E:527:LEU:CD1	2.44	0.46
1:A:96:ILE:O	1:B:448:THR:HB	2.16	0.46
1:B:231:TYR:CD1	1:B:501:GLN:HB3	2.51	0.46
1:C:67:THR:OG1	1:D:447:VAL:HG23	2.14	0.46
1:C:542:THR:HG22	1:C:547:ARG:H	1.79	0.46
1:D:75:LYS:O	1:D:78:ASP:OD1	2.32	0.46
1:D:239:ASP:HB3	1:D:405:TYR:HB2	1.96	0.46
1:D:269:GLU:HG3	1:D:269:GLU:O	2.14	0.46
1:E:193:LEU:HD22	1:E:197:ARG:NH1	2.29	0.46
1:A:485:ARG:HH21	1:B:234:GLU:CD	2.18	0.46
1:A:542:THR:CG2	1:A:547:ARG:H	2.28	0.46
1:A:542:THR:HG22	1:A:547:ARG:H	1.79	0.46
1:B:228:PRO:CB	2:S:15:TYR:HE1	2.28	0.46
1:C:145:ALA:HA	1:C:248:VAL:HA	1.96	0.46
1:C:179:MET:HE2	1:C:485:ARG:NH2	2.30	0.46
1:C:231:TYR:CD1	1:C:501:GLN:HB3	2.51	0.46
1:E:474:TYR:HD1	1:E:511:ILE:HD11	1.80	0.46
1:A:67:THR:CG2	1:B:447:VAL:CG2	2.94	0.46
1:A:434:GLN:NE2	1:A:436:TYR:CE2	2.81	0.46
1:B:474:TYR:HD1	1:B:511:ILE:HD11	1.80	0.46
1:C:78:ASP:HB2	1:C:82:LEU:HD12	1.97	0.46
1:C:289:VAL:HG13	1:C:290:ASP:N	2.30	0.46
1:D:434:GLN:NE2	1:D:436:TYR:CE2	2.81	0.46
1:E:215:PHE:CE1	1:E:241:ILE:HD11	2.50	0.46
1:E:542:THR:CG2	1:E:547:ARG:H	2.28	0.46
1:A:267:PHE:CZ	1:E:88:HIS:HD2	2.34	0.46
1:A:295:SER:CB	1:A:375:PRO:HG2	2.46	0.46
1:B:452:THR:OG1	1:B:453:SER:N	2.49	0.46
1:B:461:VAL:HB	1:B:527:LEU:CD1	2.45	0.46
1:B:558:ILE:HD11	1:C:463:ALA:HB3	1.97	0.46
1:C:295:SER:CB	1:C:375:PRO:HG2	2.46	0.46
1:C:461:VAL:HB	1:C:527:LEU:CD1	2.45	0.46
1:C:542:THR:CG2	1:C:547:ARG:H	2.27	0.46
1:D:87:ASP:O	1:D:89:SER:N	2.46	0.46
1:D:123:LEU:HD13	1:D:559:VAL:HG22	1.98	0.46
1:E:295:SER:CB	1:E:375:PRO:HG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:497:PHE:HD1	1:E:503:LEU:CB	2.25	0.46
1:A:267:PHE:CZ	1:E:88:HIS:CD2	3.04	0.46
1:B:102:SER:O	1:B:103:PRO:C	2.52	0.46
1:B:289:VAL:HG13	1:B:290:ASP:N	2.30	0.46
1:B:477:GLN:OE1	1:B:477:GLN:HA	2.16	0.46
1:C:87:ASP:O	1:C:89:SER:N	2.46	0.46
1:C:452:THR:OG1	1:C:453:SER:N	2.49	0.46
1:C:477:GLN:OE1	1:C:477:GLN:HA	2.16	0.46
1:E:123:LEU:HD13	1:E:559:VAL:HG22	1.98	0.46
2:U:15:TYR:CD2	2:U:16:PRO:HD2	2.51	0.46
1:A:142:LYS:HG2	1:A:169:THR:HG22	1.97	0.46
1:A:447:VAL:HG12	1:A:448:THR:HG23	1.97	0.46
1:B:239:ASP:HB3	1:B:405:TYR:HB2	1.96	0.46
1:B:295:SER:CB	1:B:375:PRO:HG2	2.46	0.46
1:B:477:GLN:O	1:B:481:SER:HB3	2.07	0.46
1:C:474:TYR:HD1	1:C:511:ILE:HD11	1.80	0.46
1:E:447:VAL:HG12	1:E:448:THR:HG23	1.97	0.46
1:E:485:ARG:CZ	1:E:505:ARG:HH22	2.28	0.46
1:A:376:VAL:C	1:A:378:LYS:H	2.19	0.46
1:A:553:TYR:HE2	1:B:432:SER:N	2.14	0.46
1:C:239:ASP:HB3	1:C:405:TYR:HB2	1.96	0.46
1:C:242:LEU:HD22	1:C:247:GLY:HA2	1.98	0.46
1:C:485:ARG:CZ	1:C:505:ARG:HH22	2.28	0.46
1:D:485:ARG:CZ	1:D:505:ARG:HH22	2.29	0.46
1:B:243:LEU:HD23	1:B:243:LEU:HA	1.82	0.46
1:B:485:ARG:CZ	1:B:505:ARG:HH22	2.28	0.46
1:D:217:LEU:HD23	1:D:217:LEU:HA	1.74	0.46
1:D:477:GLN:OE1	1:D:477:GLN:HA	2.15	0.46
1:E:131:MET:SD	1:E:138:MET:HG3	2.55	0.46
1:E:452:THR:OG1	1:E:453:SER:N	2.49	0.46
1:E:477:GLN:OE1	1:E:477:GLN:HA	2.16	0.46
2:W:15:TYR:CD2	2:W:16:PRO:HD2	2.50	0.46
1:A:132:PRO:CA	1:A:175:TYR:OH	2.53	0.46
1:B:243:LEU:HD21	1:B:401:TYR:CE2	2.51	0.46
1:D:295:SER:CB	1:D:375:PRO:HG2	2.46	0.46
1:E:102:SER:O	1:E:103:PRO:C	2.52	0.46
1:E:135:ASN:OD1	1:E:135:ASN:C	2.55	0.46
1:E:242:LEU:HD22	1:E:247:GLY:HA2	1.98	0.46
1:E:250:PHE:O	1:E:252:HIS:N	2.49	0.46
1:A:102:SER:O	1:A:103:PRO:C	2.53	0.45
1:A:131:MET:SD	1:A:138:MET:HG3	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:LEU:HD22	1:B:247:GLY:HA2	1.98	0.45
1:B:277:ASP:O	1:B:279:GLU:N	2.46	0.45
1:C:123:LEU:HD13	1:C:559:VAL:HG22	1.98	0.45
1:D:102:SER:O	1:D:103:PRO:C	2.52	0.45
1:D:231:TYR:CD1	1:D:501:GLN:HB3	2.51	0.45
1:D:545:ARG:O	1:D:546:ARG:HB2	2.16	0.45
1:E:231:TYR:CD1	1:E:501:GLN:HB3	2.51	0.45
1:A:63:LEU:HD12	1:B:447:VAL:HA	1.98	0.45
1:A:225:LEU:CD2	1:A:397:THR:HB	2.47	0.45
1:A:385:LYS:HZ2	2:S:16:PRO:HB3	1.82	0.45
1:C:237:HIS:HE1	1:C:424:CYS:O	2.00	0.45
1:C:243:LEU:HD21	1:C:401:TYR:CE2	2.51	0.45
1:C:556:LEU:CD2	1:D:434:GLN:HG2	2.44	0.45
1:D:135:ASN:C	1:D:135:ASN:OD1	2.55	0.45
1:D:497:PHE:CD1	1:D:503:LEU:HB3	2.44	0.45
1:E:243:LEU:HD21	1:E:401:TYR:CE2	2.51	0.45
2:S:15:TYR:CD2	2:S:16:PRO:HD2	2.51	0.45
2:T:15:TYR:CD2	2:T:16:PRO:HD2	2.51	0.45
1:A:64:PHE:O	1:A:65:ASP:HB2	2.17	0.45
1:A:432:SER:N	1:E:553:TYR:HE2	2.14	0.45
1:A:477:GLN:OE1	1:A:477:GLN:HA	2.16	0.45
1:B:207:GLY:O	1:B:208:VAL:CB	2.64	0.45
1:B:491:THR:HG23	2:T:15:TYR:CZ	2.52	0.45
1:C:223:THR:HG22	1:C:225:LEU:HB2	1.99	0.45
1:D:474:TYR:HD1	1:D:511:ILE:HD11	1.80	0.45
1:A:123:LEU:HD13	1:A:559:VAL:HG22	1.98	0.45
1:A:289:VAL:HG13	1:A:290:ASP:N	2.30	0.45
1:B:135:ASN:C	1:B:135:ASN:OD1	2.55	0.45
1:C:243:LEU:HA	1:C:243:LEU:HD23	1.82	0.45
1:C:250:PHE:O	1:C:252:HIS:N	2.49	0.45
1:C:295:SER:HB3	1:C:375:PRO:HG2	1.98	0.45
1:C:545:ARG:O	1:C:546:ARG:HB2	2.16	0.45
1:D:79:VAL:HG13	1:E:267:PHE:HD2	1.82	0.45
1:D:223:THR:HG22	1:D:225:LEU:HB2	1.99	0.45
1:D:243:LEU:HD21	1:D:401:TYR:CE2	2.51	0.45
1:D:250:PHE:O	1:D:252:HIS:N	2.49	0.45
1:D:452:THR:OG1	1:D:453:SER:N	2.49	0.45
1:E:177:GLU:HG3	1:E:178:THR:H	1.82	0.45
1:A:243:LEU:HD21	1:A:401:TYR:CE2	2.51	0.45
1:B:64:PHE:O	1:B:65:ASP:HB2	2.17	0.45
1:B:78:ASP:HB2	1:B:82:LEU:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:LEU:HD22	1:D:247:GLY:HA2	1.98	0.45
1:D:485:ARG:NH2	1:E:234:GLU:OE1	2.50	0.45
1:A:223:THR:HG22	1:A:225:LEU:HB2	1.99	0.45
1:A:250:PHE:O	1:A:252:HIS:N	2.49	0.45
1:A:439:LEU:N	1:A:440:PRO:CD	2.79	0.45
1:B:439:LEU:N	1:B:440:PRO:CD	2.79	0.45
1:C:129:THR:HB	1:C:130:ASN:H	1.63	0.45
1:C:225:LEU:CD2	1:C:397:THR:HB	2.47	0.45
1:C:447:VAL:HG12	1:C:448:THR:HG23	1.97	0.45
1:D:64:PHE:O	1:D:65:ASP:HB2	2.17	0.45
1:D:502:ILE:C	1:D:504:ALA:H	2.20	0.45
1:E:225:LEU:CD2	1:E:397:THR:HB	2.47	0.45
1:E:382:GLU:HA	1:E:387:ARG:O	2.17	0.45
1:A:228:PRO:CB	2:W:15:TYR:HE1	2.29	0.45
1:A:491:THR:HG23	2:S:15:TYR:CZ	2.52	0.45
1:A:502:ILE:C	1:A:504:ALA:H	2.20	0.45
1:D:295:SER:HB3	1:D:375:PRO:HG2	1.99	0.45
1:D:447:VAL:HG12	1:D:448:THR:HG23	1.97	0.45
1:D:491:THR:HG23	2:V:15:TYR:CZ	2.52	0.45
1:E:376:VAL:O	1:E:377:ILE:C	2.55	0.45
2:V:15:TYR:CD2	2:V:16:PRO:HD2	2.51	0.45
1:A:177:GLU:CG	1:A:178:THR:H	2.30	0.45
1:B:123:LEU:HD13	1:B:559:VAL:HG22	1.98	0.45
1:B:223:THR:HG22	1:B:225:LEU:HB2	1.99	0.45
1:B:231:TYR:H	1:B:501:GLN:HE21	1.65	0.45
1:C:135:ASN:C	1:C:135:ASN:OD1	2.55	0.45
1:D:100:ASP:CG	1:E:450:ARG:HH12	2.19	0.45
1:D:376:VAL:C	1:D:378:LYS:H	2.19	0.45
1:D:382:GLU:HA	1:D:387:ARG:O	2.17	0.45
1:E:129:THR:HB	1:E:130:ASN:H	1.63	0.45
1:E:439:LEU:N	1:E:440:PRO:CD	2.79	0.45
1:A:64:PHE:HD1	1:B:118:HIS:NE2	2.15	0.45
1:A:171:PRO:CA	1:B:409:ASN:HD22	2.30	0.45
1:A:417:ILE:HD12	1:A:417:ILE:HA	1.80	0.45
1:B:295:SER:HB3	1:B:375:PRO:HG2	1.98	0.45
1:B:382:GLU:HA	1:B:387:ARG:O	2.17	0.45
1:C:381:THR:O	1:C:381:THR:CG2	2.65	0.45
1:D:225:LEU:CD2	1:D:397:THR:HB	2.47	0.45
1:D:237:HIS:HE1	1:D:424:CYS:O	2.00	0.45
1:E:545:ARG:O	1:E:546:ARG:HB2	2.17	0.45
1:A:242:LEU:HD22	1:A:247:GLY:HA2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:SER:HB3	1:A:375:PRO:HG2	1.98	0.45
1:A:474:TYR:CD1	1:A:511:ILE:CD1	3.00	0.45
1:A:480:TYR:HE1	1:E:484:ILE:CG2	2.24	0.45
1:A:545:ARG:O	1:A:546:ARG:HB2	2.16	0.45
1:B:177:GLU:CG	1:B:178:THR:H	2.30	0.45
1:B:225:LEU:CD2	1:B:397:THR:HB	2.47	0.45
1:B:446:PRO:HG2	1:B:460:VAL:O	2.17	0.45
1:B:545:ARG:O	1:B:546:ARG:HB2	2.17	0.45
1:C:376:VAL:C	1:C:378:LYS:H	2.19	0.45
1:C:474:TYR:CD1	1:C:511:ILE:CD1	3.00	0.45
1:E:376:VAL:C	1:E:378:LYS:H	2.19	0.45
1:A:231:TYR:CD1	1:A:501:GLN:HB3	2.50	0.44
1:E:237:HIS:HE1	1:E:424:CYS:O	2.00	0.44
1:E:381:THR:HG22	1:E:382:GLU:HG3	1.99	0.44
1:E:502:ILE:C	1:E:504:ALA:H	2.20	0.44
1:A:237:HIS:HE1	1:A:424:CYS:O	2.00	0.44
1:A:381:THR:HG22	1:A:382:GLU:HG3	1.99	0.44
1:A:446:PRO:HG2	1:A:460:VAL:O	2.17	0.44
1:A:452:THR:OG1	1:A:453:SER:N	2.49	0.44
1:B:171:PRO:O	1:B:172:GLU:O	2.36	0.44
1:B:237:HIS:HE1	1:B:424:CYS:O	1.99	0.44
1:C:202:LEU:N	1:C:202:LEU:HD23	2.33	0.44
1:D:171:PRO:O	1:D:172:GLU:O	2.36	0.44
1:E:392:ILE:HG13	1:E:393:SER:N	2.32	0.44
1:A:88:HIS:HD2	1:B:267:PHE:HZ	1.63	0.44
1:A:382:GLU:HA	1:A:387:ARG:O	2.17	0.44
1:B:376:VAL:O	1:B:377:ILE:C	2.55	0.44
1:B:502:ILE:C	1:B:504:ALA:H	2.20	0.44
1:C:485:ARG:NH2	1:D:234:GLU:OE1	2.49	0.44
1:D:392:ILE:HG13	1:D:393:SER:N	2.32	0.44
1:E:458:PHE:O	1:E:546:ARG:NH2	2.50	0.44
1:E:506:PRO:HA	1:E:507:PRO:HD3	1.81	0.44
1:A:267:PHE:HB3	1:E:79:VAL:HG13	2.00	0.44
1:A:383:ASP:C	1:A:384:SER:O	2.52	0.44
1:A:466:LEU:HA	1:A:467:PRO:HD3	1.78	0.44
1:B:250:PHE:O	1:B:252:HIS:N	2.49	0.44
1:B:458:PHE:O	1:B:546:ARG:NH2	2.50	0.44
1:C:171:PRO:O	1:C:172:GLU:O	2.36	0.44
1:C:177:GLU:CG	1:C:178:THR:H	2.30	0.44
1:D:79:VAL:HG13	1:E:267:PHE:CD2	2.52	0.44
1:E:64:PHE:O	1:E:65:ASP:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:231:TYR:H	1:E:501:GLN:HE21	1.65	0.44
1:E:446:PRO:HG2	1:E:460:VAL:O	2.17	0.44
1:A:69:VAL:HG22	1:A:559:VAL:HB	2.00	0.44
1:A:202:LEU:N	1:A:202:LEU:HD23	2.33	0.44
1:A:244:PRO:HA	1:A:275:TYR:CE2	2.53	0.44
1:A:381:THR:O	1:A:381:THR:CG2	2.65	0.44
1:D:128:HIS:CE1	1:E:432:SER:HG	2.36	0.44
1:D:177:GLU:CG	1:D:178:THR:H	2.30	0.44
1:E:207:GLY:HA3	1:E:246:CYS:SG	2.58	0.44
1:E:244:PRO:HA	1:E:275:TYR:CE2	2.53	0.44
1:A:171:PRO:O	1:A:172:GLU:O	2.36	0.44
1:B:376:VAL:C	1:B:378:LYS:H	2.19	0.44
1:B:474:TYR:CD1	1:B:511:ILE:CD1	3.00	0.44
1:C:64:PHE:O	1:C:65:ASP:HB2	2.17	0.44
1:C:383:ASP:C	1:C:384:SER:O	2.52	0.44
1:C:446:PRO:HG2	1:C:460:VAL:O	2.17	0.44
1:C:502:ILE:C	1:C:504:ALA:H	2.20	0.44
1:D:79:VAL:HG13	1:E:267:PHE:HB3	1.99	0.44
1:D:99:ASN:HB3	1:E:450:ARG:NH2	2.32	0.44
1:D:202:LEU:N	1:D:202:LEU:HD23	2.33	0.44
1:E:177:GLU:CG	1:E:178:THR:H	2.30	0.44
1:E:295:SER:HB3	1:E:375:PRO:HG2	1.98	0.44
1:E:474:TYR:CD1	1:E:511:ILE:CD1	3.01	0.44
1:E:491:THR:HG23	2:W:15:TYR:CZ	2.52	0.44
1:A:207:GLY:HA3	1:A:246:CYS:SG	2.58	0.44
1:B:113:LEU:HB3	1:B:119:TRP:CE2	2.53	0.44
1:B:244:PRO:HA	1:B:275:TYR:CE2	2.53	0.44
1:B:385:LYS:HZ2	2:T:16:PRO:HB3	1.82	0.44
1:C:385:LYS:HZ2	2:U:16:PRO:HB3	1.83	0.44
1:A:113:LEU:HB3	1:A:119:TRP:CE2	2.53	0.44
1:A:189:VAL:O	1:A:192:TYR:N	2.51	0.44
1:C:57:TYR:CD2	1:D:448:THR:HG22	2.53	0.44
1:C:382:GLU:HA	1:C:387:ARG:O	2.17	0.44
1:C:491:THR:HG23	2:U:15:TYR:CZ	2.52	0.44
1:D:207:GLY:HA3	1:D:246:CYS:SG	2.58	0.44
1:D:244:PRO:HA	1:D:275:TYR:CE2	2.53	0.44
1:D:381:THR:HG22	1:D:382:GLU:HG3	1.99	0.44
1:E:171:PRO:O	1:E:172:GLU:O	2.35	0.44
1:E:202:LEU:N	1:E:202:LEU:HD23	2.33	0.44
1:B:381:THR:O	1:B:381:THR:CG2	2.65	0.44
1:C:69:VAL:HG22	1:C:559:VAL:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:VAL:O	1:C:69:VAL:HG23	2.18	0.44
1:D:556:LEU:CD2	1:E:434:GLN:HG2	2.46	0.44
1:E:69:VAL:HG22	1:E:559:VAL:HB	2.00	0.44
1:E:383:ASP:C	1:E:384:SER:O	2.52	0.44
1:A:135:ASN:C	1:A:135:ASN:OD1	2.55	0.43
1:B:179:MET:HE3	1:B:485:ARG:NH2	2.33	0.43
1:B:189:VAL:O	1:B:192:TYR:N	2.51	0.43
1:C:381:THR:HG22	1:C:382:GLU:HG3	1.99	0.43
1:C:466:LEU:HA	1:C:467:PRO:HD3	1.78	0.43
1:D:67:THR:OG1	1:E:447:VAL:HG23	2.18	0.43
1:D:381:THR:O	1:D:381:THR:CG2	2.65	0.43
1:B:392:ILE:HG13	1:B:393:SER:N	2.32	0.43
1:C:392:ILE:HG13	1:C:393:SER:N	2.32	0.43
1:C:506:PRO:HA	1:C:507:PRO:HD3	1.81	0.43
1:E:189:VAL:O	1:E:192:TYR:N	2.51	0.43
1:E:223:THR:HG22	1:E:225:LEU:HB2	1.99	0.43
1:B:202:LEU:N	1:B:202:LEU:HD23	2.33	0.43
1:D:113:LEU:HB3	1:D:119:TRP:CE2	2.53	0.43
1:D:192:TYR:CD1	1:D:196:GLY:HA3	2.54	0.43
1:D:446:PRO:HG2	1:D:460:VAL:O	2.17	0.43
1:D:458:PHE:O	1:D:546:ARG:NH2	2.50	0.43
1:D:474:TYR:CD1	1:D:511:ILE:CD1	3.00	0.43
1:A:564:LEU:O	1:A:565:SER:HB3	2.19	0.43
1:C:179:MET:HE3	1:C:485:ARG:HH22	1.83	0.43
1:C:542:THR:HG23	1:C:547:ARG:N	2.34	0.43
1:D:131:MET:HA	1:D:132:PRO:HD3	1.80	0.43
1:E:479:VAL:O	1:E:479:VAL:CG1	2.66	0.43
1:B:79:VAL:HG13	1:C:267:PHE:HD2	1.83	0.43
1:C:113:LEU:HB3	1:C:119:TRP:CE2	2.53	0.43
1:C:207:GLY:HA3	1:C:246:CYS:SG	2.58	0.43
1:C:428:VAL:HG13	1:C:513:THR:HB	2.01	0.43
1:D:189:VAL:O	1:D:192:TYR:N	2.51	0.43
1:D:376:VAL:O	1:D:377:ILE:C	2.55	0.43
1:E:75:LYS:HE2	1:E:75:LYS:HB3	1.88	0.43
1:E:96:ILE:HD13	1:E:96:ILE:HA	1.82	0.43
1:E:113:LEU:HB3	1:E:119:TRP:CE2	2.53	0.43
2:U:15:TYR:CD2	2:U:15:TYR:C	2.92	0.43
1:A:376:VAL:O	1:A:377:ILE:C	2.55	0.43
1:B:88:HIS:CD2	1:C:267:PHE:CZ	3.06	0.43
1:B:192:TYR:CD1	1:B:196:GLY:HA3	2.54	0.43
1:C:181:ILE:O	1:C:184:MET:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:564:LEU:O	1:C:565:SER:HB3	2.19	0.43
1:D:428:VAL:HG13	1:D:513:THR:HB	2.01	0.43
1:D:564:LEU:O	1:D:565:SER:HB3	2.19	0.43
1:E:223:THR:CG2	1:E:225:LEU:HB2	2.49	0.43
1:A:83:ASN:CA	1:A:86:ASN:HD22	2.21	0.43
1:A:231:TYR:H	1:A:501:GLN:HE21	1.65	0.43
1:A:392:ILE:HG13	1:A:393:SER:N	2.32	0.43
1:B:69:VAL:O	1:B:69:VAL:HG23	2.18	0.43
1:B:181:ILE:O	1:B:184:MET:HB2	2.19	0.43
1:D:64:PHE:CD1	1:E:118:HIS:NE2	2.86	0.43
1:D:231:TYR:H	1:D:501:GLN:HE21	1.65	0.43
1:E:422:LEU:CD2	1:E:423:LEU:N	2.80	0.43
1:E:428:VAL:HG13	1:E:513:THR:HB	2.00	0.43
1:A:177:GLU:HG3	1:A:178:THR:H	1.82	0.43
1:B:69:VAL:HG22	1:B:559:VAL:HB	2.00	0.43
1:B:126:ILE:HG12	1:B:521:LEU:CD2	2.49	0.43
1:B:381:THR:HG22	1:B:382:GLU:HG3	2.00	0.43
1:C:189:VAL:O	1:C:192:TYR:N	2.51	0.43
1:C:192:TYR:CD1	1:C:196:GLY:HA3	2.54	0.43
1:C:458:PHE:O	1:C:546:ARG:NH2	2.50	0.43
1:E:132:PRO:CA	1:E:175:TYR:OH	2.53	0.43
1:E:474:TYR:HH	1:E:476:ASP:CG	2.21	0.43
1:A:422:LEU:HD21	1:E:551:TYR:CZ	2.53	0.43
1:A:448:THR:HG22	1:E:57:TYR:CE2	2.54	0.43
1:B:207:GLY:HA3	1:B:246:CYS:SG	2.58	0.43
1:B:223:THR:CG2	1:B:225:LEU:HB2	2.49	0.43
1:C:95:VAL:O	1:C:95:VAL:HG12	2.19	0.43
1:C:231:TYR:H	1:C:501:GLN:HE21	1.65	0.43
1:D:385:LYS:HZ2	2:V:16:PRO:HB3	1.83	0.43
1:E:126:ILE:HG12	1:E:521:LEU:CD2	2.49	0.43
1:E:381:THR:O	1:E:381:THR:CG2	2.65	0.43
2:S:15:TYR:CD2	2:S:15:TYR:C	2.92	0.43
1:A:87:ASP:OD1	1:A:89:SER:HB3	2.19	0.43
1:A:192:TYR:CD1	1:A:196:GLY:HA3	2.54	0.43
1:A:223:THR:CG2	1:A:225:LEU:HB2	2.49	0.43
1:A:234:GLU:OE1	1:E:485:ARG:NH2	2.52	0.43
1:A:447:VAL:CG2	1:E:67:THR:CG2	2.97	0.43
1:B:95:VAL:O	1:B:95:VAL:HG12	2.19	0.43
1:C:243:LEU:HD23	1:C:244:PRO:HD3	2.01	0.43
1:D:551:TYR:CZ	1:E:422:LEU:HD21	2.54	0.43
1:E:243:LEU:HD23	1:E:244:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ILE:HD13	1:A:96:ILE:HA	1.82	0.42
1:A:493:VAL:HG21	1:B:232:THR:HB	2.00	0.42
1:B:58:SER:OG	1:B:59:GLU:N	2.52	0.42
1:B:243:LEU:HD23	1:B:244:PRO:HD3	2.01	0.42
1:B:542:THR:HG23	1:B:547:ARG:N	2.34	0.42
1:C:58:SER:OG	1:C:59:GLU:N	2.52	0.42
1:C:96:ILE:O	1:D:448:THR:HB	2.19	0.42
1:C:376:VAL:O	1:C:377:ILE:C	2.55	0.42
1:D:57:TYR:CG	1:E:448:THR:HG22	2.55	0.42
1:A:96:ILE:HG22	1:A:98:ASN:N	2.28	0.42
1:A:228:PRO:HB3	2:W:15:TYR:HE1	1.84	0.42
1:C:244:PRO:HA	1:C:275:TYR:CE2	2.53	0.42
1:C:422:LEU:CD2	1:C:423:LEU:N	2.80	0.42
1:D:69:VAL:HG22	1:D:559:VAL:HB	2.00	0.42
1:D:223:THR:CG2	1:D:225:LEU:HB2	2.49	0.42
1:E:87:ASP:OD1	1:E:89:SER:HB3	2.19	0.42
1:E:179:MET:HE3	1:E:485:ARG:NH2	2.34	0.42
1:E:192:TYR:CD1	1:E:196:GLY:HA3	2.54	0.42
1:E:277:ASP:O	1:E:279:GLU:N	2.46	0.42
2:V:15:TYR:CD2	2:V:15:TYR:C	2.92	0.42
1:A:132:PRO:CD	1:A:551:TYR:CE2	3.02	0.42
1:C:223:THR:CG2	1:C:225:LEU:HB2	2.49	0.42
1:E:228:PRO:CB	2:V:15:TYR:HE1	2.33	0.42
2:T:10:THR:O	2:T:10:THR:CG2	2.60	0.42
1:A:126:ILE:HG12	1:A:521:LEU:CD2	2.49	0.42
1:A:479:VAL:O	1:A:479:VAL:CG1	2.66	0.42
1:B:177:GLU:HG3	1:B:178:THR:H	1.82	0.42
1:B:564:LEU:O	1:B:565:SER:HB3	2.19	0.42
1:C:87:ASP:OD1	1:C:89:SER:HB3	2.19	0.42
1:C:177:GLU:HG3	1:C:178:THR:H	1.82	0.42
1:D:69:VAL:HG23	1:D:69:VAL:O	2.18	0.42
1:D:506:PRO:HA	1:D:507:PRO:HD3	1.81	0.42
1:E:542:THR:HG23	1:E:547:ARG:N	2.34	0.42
1:E:549:CYS:HA	1:E:550:PRO:HD3	1.89	0.42
1:A:243:LEU:HD23	1:A:244:PRO:HD3	2.01	0.42
1:A:428:VAL:HG13	1:A:513:THR:HB	2.00	0.42
1:B:87:ASP:OD1	1:B:89:SER:HB3	2.19	0.42
1:B:129:THR:HB	1:B:130:ASN:H	1.63	0.42
1:B:428:VAL:HG13	1:B:513:THR:HB	2.00	0.42
1:C:282:ASN:HA	1:C:402:ARG:HA	2.02	0.42
1:D:181:ILE:O	1:D:184:MET:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:PRO:HB3	2:U:15:TYR:HE1	1.83	0.42
1:E:69:VAL:O	1:E:69:VAL:HG23	2.18	0.42
1:E:83:ASN:CA	1:E:86:ASN:HD22	2.21	0.42
1:E:282:ASN:HA	1:E:402:ARG:HA	2.02	0.42
1:A:58:SER:OG	1:A:59:GLU:N	2.52	0.42
1:B:75:LYS:HE2	1:B:75:LYS:HB3	1.88	0.42
1:B:132:PRO:CD	1:B:551:TYR:CE2	3.02	0.42
1:B:542:THR:HG21	1:B:546:ARG:HD2	2.01	0.42
1:D:95:VAL:O	1:D:95:VAL:HG12	2.19	0.42
2:W:15:TYR:CD2	2:W:15:TYR:C	2.92	0.42
1:A:422:LEU:CD2	1:A:423:LEU:N	2.80	0.42
1:A:458:PHE:O	1:A:546:ARG:NH2	2.50	0.42
1:B:137:PHE:HE1	1:B:547:ARG:NE	2.18	0.42
1:C:207:GLY:O	1:C:208:VAL:CB	2.64	0.42
1:E:132:PRO:CD	1:E:551:TYR:CE2	3.02	0.42
1:E:181:ILE:O	1:E:184:MET:HB2	2.19	0.42
1:E:564:LEU:O	1:E:565:SER:HB3	2.19	0.42
1:A:137:PHE:HE1	1:A:547:ARG:NE	2.18	0.42
1:A:450:ARG:HH12	1:E:100:ASP:CG	2.23	0.42
1:B:117:SER:HA	1:B:566:SER:HA	2.02	0.42
1:E:95:VAL:O	1:E:95:VAL:HG12	2.19	0.42
2:T:15:TYR:CD2	2:T:15:TYR:C	2.92	0.42
1:A:95:VAL:O	1:A:95:VAL:HG12	2.19	0.42
1:A:228:PRO:HG3	2:W:15:TYR:CD1	2.54	0.42
1:B:88:HIS:HD2	1:C:267:PHE:CZ	2.38	0.42
1:C:126:ILE:HG12	1:C:521:LEU:CD2	2.49	0.42
1:C:277:ASP:O	1:C:279:GLU:N	2.46	0.42
1:D:282:ASN:HA	1:D:402:ARG:HA	2.02	0.42
1:D:542:THR:HG21	1:D:546:ARG:HD2	2.02	0.42
2:S:10:THR:O	2:S:10:THR:CG2	2.60	0.42
1:A:69:VAL:HG23	1:A:69:VAL:O	2.18	0.42
1:A:87:ASP:O	1:A:89:SER:N	2.46	0.42
1:B:426:PRO:O	1:B:427:ASP:CB	2.67	0.42
1:B:479:VAL:O	1:B:479:VAL:CG1	2.66	0.42
1:C:132:PRO:CD	1:C:551:TYR:CE2	3.02	0.42
1:D:117:SER:HA	1:D:566:SER:HA	2.02	0.42
1:E:243:LEU:HD23	1:E:243:LEU:HA	1.82	0.42
1:A:150:SER:OG	1:A:162:LYS:HB2	2.20	0.41
1:A:207:GLY:O	1:A:208:VAL:CB	2.64	0.41
1:A:243:LEU:HD23	1:A:243:LEU:HA	1.82	0.41
1:B:73:ASP:OD1	1:B:73:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:VAL:HG13	1:C:267:PHE:CD2	2.54	0.41
1:B:83:ASN:CA	1:B:86:ASN:HD22	2.21	0.41
1:D:542:THR:HG23	1:D:547:ARG:N	2.34	0.41
1:E:58:SER:OG	1:E:59:GLU:N	2.52	0.41
1:E:117:SER:HA	1:E:566:SER:HA	2.02	0.41
1:E:137:PHE:HE1	1:E:547:ARG:NE	2.18	0.41
1:A:181:ILE:O	1:A:184:MET:HB2	2.19	0.41
1:B:224:GLY:O	1:B:397:THR:HB	2.21	0.41
1:B:243:LEU:CG	1:B:401:TYR:CE2	3.03	0.41
1:B:422:LEU:CD2	1:B:423:LEU:N	2.80	0.41
1:C:137:PHE:HE1	1:C:547:ARG:NE	2.18	0.41
1:C:542:THR:HG21	1:C:546:ARG:HD2	2.02	0.41
1:D:87:ASP:OD1	1:D:89:SER:HB3	2.19	0.41
1:D:126:ILE:HG12	1:D:521:LEU:CD2	2.49	0.41
1:D:132:PRO:CD	1:D:551:TYR:CE2	3.02	0.41
1:D:207:GLY:O	1:D:208:VAL:CB	2.64	0.41
1:A:542:THR:HG23	1:A:547:ARG:N	2.34	0.41
1:C:117:SER:HA	1:C:566:SER:HA	2.02	0.41
1:C:224:GLY:O	1:C:397:THR:HB	2.20	0.41
1:C:442:MET:HE2	1:C:443:MET:SD	2.60	0.41
1:D:224:GLY:O	1:D:397:THR:HB	2.21	0.41
1:A:117:SER:HA	1:A:566:SER:HA	2.01	0.41
1:A:442:MET:HE2	1:A:443:MET:SD	2.60	0.41
1:A:474:TYR:HH	1:A:476:ASP:CG	2.24	0.41
1:D:73:ASP:OD1	1:D:73:ASP:N	2.53	0.41
1:A:183:LEU:HD21	1:B:236:PHE:CE2	2.47	0.41
1:A:217:LEU:HD23	1:A:217:LEU:HA	1.74	0.41
1:A:224:GLY:O	1:A:397:THR:HB	2.20	0.41
1:A:491:THR:HG21	1:A:493:VAL:HG22	2.03	0.41
1:A:549:CYS:HA	1:A:550:PRO:HD3	1.89	0.41
1:B:217:LEU:HD23	1:B:217:LEU:HA	1.74	0.41
1:B:417:ILE:HD12	1:B:417:ILE:HA	1.80	0.41
1:C:171:PRO:O	1:C:172:GLU:C	2.59	0.41
1:C:228:PRO:HG3	2:T:15:TYR:CD1	2.55	0.41
1:C:439:LEU:O	1:C:441:ASP:N	2.54	0.41
1:C:479:VAL:O	1:C:479:VAL:CG1	2.66	0.41
1:A:401:TYR:CE1	1:A:502:ILE:HG12	2.56	0.41
1:B:491:THR:HG21	1:B:493:VAL:HG22	2.02	0.41
1:C:64:PHE:CD1	1:D:118:HIS:NE2	2.88	0.41
1:C:150:SER:OG	1:C:162:LYS:HB2	2.21	0.41
1:C:243:LEU:CG	1:C:401:TYR:CE2	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:PHE:HE1	1:D:547:ARG:NE	2.18	0.41
1:D:154:THR:CG2	1:D:155:LYS:H	2.34	0.41
1:D:243:LEU:HD23	1:D:244:PRO:HD3	2.01	0.41
1:D:392:ILE:HD11	1:D:396:SER:CB	2.51	0.41
1:D:422:LEU:CD2	1:D:423:LEU:N	2.80	0.41
1:E:179:MET:HE2	1:E:485:ARG:NH2	2.35	0.41
1:E:217:LEU:HD23	1:E:217:LEU:HA	1.74	0.41
1:E:563:VAL:CG1	1:E:564:LEU:N	2.84	0.41
1:A:196:GLY:O	1:A:201:VAL:HG12	2.21	0.41
1:B:114:ASP:OD2	1:B:116:ARG:NH1	2.54	0.41
1:B:282:ASN:HA	1:B:402:ARG:HA	2.02	0.41
1:B:442:MET:HE2	1:B:443:MET:SD	2.60	0.41
1:C:405:TYR:O	1:C:409:ASN:OD1	2.39	0.41
1:C:441:ASP:HB2	1:C:537:GLN:OE1	2.21	0.41
1:C:481:SER:O	1:C:482:GLN:C	2.59	0.41
1:C:563:VAL:CG1	1:C:564:LEU:N	2.84	0.41
1:E:385:LYS:HZ2	2:W:16:PRO:HB3	1.85	0.41
1:A:282:ASN:HA	1:A:402:ARG:HA	2.02	0.41
1:A:542:THR:HG21	1:A:546:ARG:HD2	2.02	0.41
1:A:563:VAL:CG1	1:A:564:LEU:N	2.84	0.41
1:C:114:ASP:OD2	1:C:116:ARG:NH1	2.54	0.41
1:C:434:GLN:NE2	1:C:436:TYR:CE2	2.81	0.41
1:D:150:SER:OG	1:D:162:LYS:HB2	2.21	0.41
1:E:231:TYR:OH	1:E:284:PRO:O	2.34	0.41
1:E:405:TYR:O	1:E:409:ASN:OD1	2.39	0.41
1:A:73:ASP:OD1	1:A:73:ASP:N	2.53	0.41
1:A:114:ASP:OD2	1:A:116:ARG:NH1	2.54	0.41
1:A:154:THR:CG2	1:A:155:LYS:H	2.34	0.41
1:A:267:PHE:HD2	1:E:79:VAL:HG13	1.86	0.41
1:A:551:TYR:CZ	1:B:422:LEU:HD21	2.55	0.41
1:B:196:GLY:O	1:B:201:VAL:HG12	2.21	0.41
1:B:563:VAL:CG1	1:B:564:LEU:N	2.84	0.41
1:C:75:LYS:HB3	1:C:75:LYS:HE2	1.88	0.41
1:C:491:THR:HG21	1:C:493:VAL:HG22	2.03	0.41
1:D:58:SER:OG	1:D:59:GLU:N	2.52	0.41
1:D:83:ASN:OD1	1:D:92:LEU:N	2.38	0.41
1:D:114:ASP:OD2	1:D:116:ARG:NH1	2.54	0.41
1:D:439:LEU:O	1:D:441:ASP:N	2.54	0.41
1:D:479:VAL:CG1	1:D:479:VAL:O	2.66	0.41
1:E:224:GLY:O	1:E:397:THR:HB	2.20	0.41
1:E:434:GLN:NE2	1:E:436:TYR:CE2	2.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:18:ASP:O	2:V:19:THR:HB	2.21	0.41
1:A:441:ASP:HB2	1:A:537:GLN:OE1	2.21	0.41
1:B:441:ASP:HB2	1:B:537:GLN:OE1	2.21	0.41
1:C:96:ILE:HD13	1:C:96:ILE:HA	1.82	0.41
1:C:154:THR:CG2	1:C:155:LYS:H	2.34	0.41
1:C:439:LEU:N	1:C:440:PRO:CD	2.79	0.41
1:D:88:HIS:CD2	1:E:267:PHE:CZ	3.09	0.41
1:D:417:ILE:HA	1:D:417:ILE:HD12	1.79	0.41
1:D:491:THR:HG21	1:D:493:VAL:HG22	2.03	0.41
1:E:114:ASP:OD2	1:E:116:ARG:NH1	2.54	0.41
1:E:150:SER:OG	1:E:162:LYS:HB2	2.21	0.41
1:E:491:THR:HG21	1:E:493:VAL:HG22	2.03	0.41
1:E:542:THR:HG21	1:E:546:ARG:HD2	2.02	0.41
1:A:135:ASN:N	1:A:140:THR:OG1	2.54	0.40
1:A:267:PHE:CD2	1:E:79:VAL:HG13	2.56	0.40
1:A:439:LEU:O	1:A:441:ASP:N	2.54	0.40
1:B:149:VAL:HG13	1:B:195:VAL:HG11	2.04	0.40
1:C:53:ASN:ND2	1:C:53:ASN:O	2.54	0.40
1:D:441:ASP:HB2	1:D:537:GLN:OE1	2.21	0.40
1:E:225:LEU:HD23	1:E:397:THR:HB	2.03	0.40
1:E:243:LEU:CG	1:E:401:TYR:CE2	3.03	0.40
2:S:18:ASP:O	2:S:19:THR:HB	2.21	0.40
1:A:481:SER:O	1:A:482:GLN:C	2.59	0.40
1:B:53:ASN:ND2	1:B:53:ASN:O	2.54	0.40
1:B:373:LYS:O	1:B:374:LYS:CG	2.69	0.40
1:C:225:LEU:HD23	1:C:397:THR:HB	2.04	0.40
1:C:373:LYS:O	1:C:374:LYS:CG	2.70	0.40
1:D:88:HIS:HD2	1:E:267:PHE:CZ	2.39	0.40
1:D:401:TYR:CE1	1:D:502:ILE:HG12	2.56	0.40
1:E:171:PRO:O	1:E:172:GLU:C	2.59	0.40
1:E:441:ASP:HB2	1:E:537:GLN:OE1	2.21	0.40
1:B:150:SER:OG	1:B:162:LYS:HB2	2.21	0.40
1:C:149:VAL:HG13	1:C:195:VAL:HG11	2.03	0.40
1:C:208:VAL:HG22	1:C:242:LEU:HD22	2.03	0.40
1:D:75:LYS:HB3	1:D:75:LYS:HE2	1.88	0.40
1:A:243:LEU:O	1:A:244:PRO:C	2.59	0.40
1:B:405:TYR:O	1:B:409:ASN:OD1	2.39	0.40
1:C:220:ASP:HB3	1:C:223:THR:HB	2.04	0.40
1:D:177:GLU:HG3	1:D:178:THR:H	1.82	0.40
1:D:436:TYR:HD1	1:D:460:VAL:HG21	1.86	0.40
1:E:196:GLY:O	1:E:201:VAL:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:373:LYS:O	1:E:374:LYS:CG	2.70	0.40
1:A:179:MET:CE	1:A:485:ARG:HH22	2.34	0.40
1:A:220:ASP:HB3	1:A:223:THR:HB	2.04	0.40
1:A:373:LYS:O	1:A:374:LYS:CG	2.70	0.40
1:A:409:ASN:HD22	1:E:171:PRO:CA	2.35	0.40
1:B:179:MET:HE2	1:B:485:ARG:NH2	2.36	0.40
1:B:392:ILE:HD11	1:B:396:SER:CB	2.51	0.40
1:B:401:TYR:CE1	1:B:502:ILE:HG12	2.56	0.40
1:C:179:MET:CE	1:C:485:ARG:HH22	2.34	0.40
1:C:392:ILE:HD11	1:C:396:SER:CB	2.51	0.40
1:C:436:TYR:HD1	1:C:460:VAL:HG21	1.86	0.40
1:D:225:LEU:HD23	1:D:397:THR:HB	2.03	0.40
1:D:243:LEU:O	1:D:244:PRO:C	2.59	0.40
1:D:405:TYR:O	1:D:409:ASN:OD1	2.39	0.40
1:D:481:SER:O	1:D:482:GLN:C	2.59	0.40
1:E:53:ASN:O	1:E:53:ASN:ND2	2.54	0.40
1:E:434:GLN:HE21	1:E:436:TYR:HE2	1.69	0.40
1:E:439:LEU:O	1:E:441:ASP:N	2.54	0.40
1:E:536:VAL:O	1:E:536:VAL:CG2	2.69	0.40
2:U:18:ASP:O	2:U:19:THR:HB	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	436/523 (83%)	321 (74%)	69 (16%)	46 (11%)	0 8
1	B	436/523 (83%)	320 (73%)	70 (16%)	46 (11%)	0 8
1	C	436/523 (83%)	321 (74%)	69 (16%)	46 (11%)	0 8
1	D	436/523 (83%)	321 (74%)	69 (16%)	46 (11%)	0 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	436/523 (83%)	321 (74%)	69 (16%)	46 (11%)	0	8
2	S	8/19 (42%)	5 (62%)	3 (38%)	0	100	100
2	T	8/19 (42%)	5 (62%)	3 (38%)	0	100	100
2	U	8/19 (42%)	5 (62%)	3 (38%)	0	100	100
2	V	8/19 (42%)	5 (62%)	3 (38%)	0	100	100
2	W	8/19 (42%)	5 (62%)	3 (38%)	0	100	100
All	All	2220/2710 (82%)	1629 (73%)	361 (16%)	230 (10%)	1	8

All (230) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	LEU
1	A	130	ASN
1	A	172	GLU
1	A	174	ASN
1	A	201	VAL
1	A	216	ARG
1	A	280	GLY
1	A	376	VAL
1	A	447	VAL
1	A	455	ILE
1	A	467	PRO
1	A	479	VAL
1	A	496	ARG
1	B	82	LEU
1	B	130	ASN
1	B	172	GLU
1	B	174	ASN
1	B	201	VAL
1	B	216	ARG
1	B	280	GLY
1	B	376	VAL
1	B	447	VAL
1	B	467	PRO
1	B	479	VAL
1	B	496	ARG
1	C	82	LEU
1	C	130	ASN
1	C	172	GLU
1	C	174	ASN

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Mol	Chain	Res	Type
1	C	201	VAL
1	C	216	ARG
1	C	280	GLY
1	C	376	VAL
1	C	447	VAL
1	C	455	ILE
1	C	467	PRO
1	C	479	VAL
1	C	496	ARG
1	D	82	LEU
1	D	130	ASN
1	D	172	GLU
1	D	174	ASN
1	D	201	VAL
1	D	216	ARG
1	D	280	GLY
1	D	376	VAL
1	D	447	VAL
1	D	455	ILE
1	D	467	PRO
1	D	479	VAL
1	D	496	ARG
1	E	82	LEU
1	E	130	ASN
1	E	172	GLU
1	E	174	ASN
1	E	201	VAL
1	E	216	ARG
1	E	280	GLY
1	E	376	VAL
1	E	447	VAL
1	E	455	ILE
1	E	467	PRO
1	E	479	VAL
1	E	496	ARG
1	A	58	SER
1	A	84	TYR
1	A	175	TYR
1	A	196	GLY
1	A	215	PHE
1	A	219	PHE
1	A	251	THR

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Mol	Chain	Res	Type
1	A	279	GLU
1	A	377	ILE
1	A	385	LYS
1	A	386	LYS
1	A	426	PRO
1	A	440	PRO
1	A	503	LEU
1	B	58	SER
1	B	84	TYR
1	B	175	TYR
1	B	196	GLY
1	B	215	PHE
1	B	219	PHE
1	B	251	THR
1	B	279	GLU
1	B	377	ILE
1	B	385	LYS
1	B	386	LYS
1	B	426	PRO
1	B	440	PRO
1	B	455	ILE
1	B	503	LEU
1	C	58	SER
1	C	84	TYR
1	C	175	TYR
1	C	196	GLY
1	C	215	PHE
1	C	219	PHE
1	C	251	THR
1	C	279	GLU
1	C	377	ILE
1	C	385	LYS
1	C	386	LYS
1	C	426	PRO
1	C	440	PRO
1	C	503	LEU
1	D	58	SER
1	D	84	TYR
1	D	175	TYR
1	D	196	GLY
1	D	215	PHE
1	D	219	PHE

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Mol	Chain	Res	Type
1	D	251	THR
1	D	279	GLU
1	D	377	ILE
1	D	385	LYS
1	D	386	LYS
1	D	426	PRO
1	D	440	PRO
1	D	503	LEU
1	E	58	SER
1	E	84	TYR
1	E	175	TYR
1	E	196	GLY
1	E	215	PHE
1	E	219	PHE
1	E	251	THR
1	E	279	GLU
1	E	377	ILE
1	E	385	LYS
1	E	386	LYS
1	E	426	PRO
1	E	440	PRO
1	E	503	LEU
1	A	75	LYS
1	A	81	SER
1	A	88	HIS
1	A	89	SER
1	A	101	TYR
1	A	114	ASP
1	A	176	SER
1	A	199	ASN
1	A	233	ASN
1	A	270	GLY
1	A	498	PRO
1	A	511	ILE
1	B	75	LYS
1	B	81	SER
1	B	88	HIS
1	B	89	SER
1	B	101	TYR
1	B	114	ASP
1	B	176	SER
1	B	199	ASN

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Mol	Chain	Res	Type
1	B	233	ASN
1	B	270	GLY
1	B	498	PRO
1	B	511	ILE
1	C	75	LYS
1	C	81	SER
1	C	88	HIS
1	C	89	SER
1	C	101	TYR
1	C	114	ASP
1	C	176	SER
1	C	199	ASN
1	C	233	ASN
1	C	270	GLY
1	C	498	PRO
1	C	511	ILE
1	D	75	LYS
1	D	81	SER
1	D	88	HIS
1	D	89	SER
1	D	101	TYR
1	D	114	ASP
1	D	176	SER
1	D	199	ASN
1	D	233	ASN
1	D	270	GLY
1	D	498	PRO
1	D	511	ILE
1	E	75	LYS
1	E	81	SER
1	E	88	HIS
1	E	89	SER
1	E	101	TYR
1	E	114	ASP
1	E	176	SER
1	E	199	ASN
1	E	233	ASN
1	E	270	GLY
1	E	498	PRO
1	E	511	ILE
1	A	55	ILE
1	A	67	THR

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Mol	Chain	Res	Type
1	A	208	VAL
1	A	380	LEU
1	B	55	ILE
1	B	67	THR
1	B	208	VAL
1	B	380	LEU
1	C	55	ILE
1	C	67	THR
1	C	208	VAL
1	C	380	LEU
1	D	55	ILE
1	D	67	THR
1	D	208	VAL
1	D	380	LEU
1	E	55	ILE
1	E	67	THR
1	E	208	VAL
1	E	380	LEU
1	A	390	ASN
1	B	390	ASN
1	C	390	ASN
1	D	390	ASN
1	E	390	ASN
1	D	416	GLY
1	A	379	PRO
1	A	416	GLY
1	B	379	PRO
1	B	416	GLY
1	C	379	PRO
1	C	416	GLY
1	D	379	PRO
1	E	379	PRO
1	E	416	GLY

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	399/451 (88%)	369 (92%)	30 (8%)	13	38
1	B	399/451 (88%)	370 (93%)	29 (7%)	14	39
1	C	399/451 (88%)	369 (92%)	30 (8%)	13	38
1	D	399/451 (88%)	369 (92%)	30 (8%)	13	38
1	E	399/451 (88%)	369 (92%)	30 (8%)	13	38
2	S	10/17 (59%)	9 (90%)	1 (10%)	7	26
2	T	10/17 (59%)	9 (90%)	1 (10%)	7	26
2	U	10/17 (59%)	9 (90%)	1 (10%)	7	26
2	V	10/17 (59%)	9 (90%)	1 (10%)	7	26
2	W	10/17 (59%)	9 (90%)	1 (10%)	7	26
All	All	2045/2340 (87%)	1891 (92%)	154 (8%)	17	38

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	98	ASN
1	A	107	SER
1	A	124	LYS
1	A	130	ASN
1	A	133	ASN
1	A	168	PHE
1	A	199	ASN
1	A	202	LEU
1	A	214	ASN
1	A	249	ASP
1	A	256	SER
1	A	271	PHE
1	A	276	ASP
1	A	279	GLU
1	A	399	THR
1	A	402	ARG
1	A	409	ASN
1	A	417	ILE
1	A	422	LEU
1	A	427	ASP
1	A	434	GLN
1	A	438	SER
1	A	448	THR

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Mol	Chain	Res	Type
1	A	457	ASN
1	A	476	ASP
1	A	482	GLN
1	A	510	THR
1	A	543	ASP
1	A	560	SER
1	B	83	ASN
1	B	98	ASN
1	B	107	SER
1	B	124	LYS
1	B	130	ASN
1	B	133	ASN
1	B	168	PHE
1	B	199	ASN
1	B	202	LEU
1	B	214	ASN
1	B	249	ASP
1	B	256	SER
1	B	271	PHE
1	B	276	ASP
1	B	399	THR
1	B	402	ARG
1	B	409	ASN
1	B	417	ILE
1	B	422	LEU
1	B	427	ASP
1	B	434	GLN
1	B	438	SER
1	B	448	THR
1	B	457	ASN
1	B	476	ASP
1	B	482	GLN
1	B	510	THR
1	B	543	ASP
1	B	560	SER
1	C	83	ASN
1	C	98	ASN
1	C	107	SER
1	C	124	LYS
1	C	130	ASN
1	C	133	ASN
1	C	168	PHE

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Mol	Chain	Res	Type
1	C	199	ASN
1	C	202	LEU
1	C	214	ASN
1	C	249	ASP
1	C	256	SER
1	C	271	PHE
1	C	276	ASP
1	C	279	GLU
1	C	399	THR
1	C	402	ARG
1	C	409	ASN
1	C	417	ILE
1	C	422	LEU
1	C	427	ASP
1	C	434	GLN
1	C	438	SER
1	C	448	THR
1	C	457	ASN
1	C	476	ASP
1	C	482	GLN
1	C	510	THR
1	C	543	ASP
1	C	560	SER
1	D	83	ASN
1	D	98	ASN
1	D	107	SER
1	D	124	LYS
1	D	130	ASN
1	D	133	ASN
1	D	168	PHE
1	D	199	ASN
1	D	202	LEU
1	D	214	ASN
1	D	249	ASP
1	D	256	SER
1	D	271	PHE
1	D	276	ASP
1	D	279	GLU
1	D	399	THR
1	D	402	ARG
1	D	409	ASN
1	D	417	ILE

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Mol	Chain	Res	Type
1	D	422	LEU
1	D	427	ASP
1	D	434	GLN
1	D	438	SER
1	D	448	THR
1	D	457	ASN
1	D	476	ASP
1	D	482	GLN
1	D	510	THR
1	D	543	ASP
1	D	560	SER
1	E	83	ASN
1	E	98	ASN
1	E	107	SER
1	E	124	LYS
1	E	130	ASN
1	E	133	ASN
1	E	168	PHE
1	E	199	ASN
1	E	202	LEU
1	E	214	ASN
1	E	249	ASP
1	E	256	SER
1	E	271	PHE
1	E	276	ASP
1	E	279	GLU
1	E	399	THR
1	E	402	ARG
1	E	409	ASN
1	E	417	ILE
1	E	422	LEU
1	E	427	ASP
1	E	434	GLN
1	E	438	SER
1	E	448	THR
1	E	457	ASN
1	E	476	ASP
1	E	482	GLN
1	E	510	THR
1	E	543	ASP
1	E	560	SER
2	S	15	TYR

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Mol	Chain	Res	Type
2	T	15	TYR
2	U	15	TYR
2	V	15	TYR
2	W	15	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	86	ASN
1	A	98	ASN
1	A	109	GLN
1	A	130	ASN
1	A	174	ASN
1	A	198	GLN
1	A	199	ASN
1	A	214	ASN
1	A	237	HIS
1	A	400	GLN
1	A	434	GLN
1	A	457	ASN
1	A	469	HIS
1	A	495	ASN
1	A	501	GLN
1	B	53	ASN
1	B	86	ASN
1	B	98	ASN
1	B	109	GLN
1	B	130	ASN
1	B	174	ASN
1	B	198	GLN
1	B	199	ASN
1	B	214	ASN
1	B	237	HIS
1	B	400	GLN
1	B	434	GLN
1	B	457	ASN
1	B	469	HIS
1	B	495	ASN
1	B	501	GLN
1	C	53	ASN
1	C	86	ASN

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Mol	Chain	Res	Type
1	C	98	ASN
1	C	109	GLN
1	C	130	ASN
1	C	174	ASN
1	C	198	GLN
1	C	199	ASN
1	C	214	ASN
1	C	237	HIS
1	C	400	GLN
1	C	434	GLN
1	C	457	ASN
1	C	469	HIS
1	C	495	ASN
1	C	501	GLN
1	D	53	ASN
1	D	86	ASN
1	D	98	ASN
1	D	109	GLN
1	D	130	ASN
1	D	174	ASN
1	D	198	GLN
1	D	199	ASN
1	D	214	ASN
1	D	237	HIS
1	D	400	GLN
1	D	434	GLN
1	D	457	ASN
1	D	469	HIS
1	D	495	ASN
1	D	501	GLN
1	E	53	ASN
1	E	86	ASN
1	E	98	ASN
1	E	109	GLN
1	E	130	ASN
1	E	174	ASN
1	E	198	GLN
1	E	199	ASN
1	E	214	ASN
1	E	237	HIS
1	E	400	GLN
1	E	457	ASN

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Mol	Chain	Res	Type
1	E	469	HIS
1	E	495	ASN
1	E	501	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

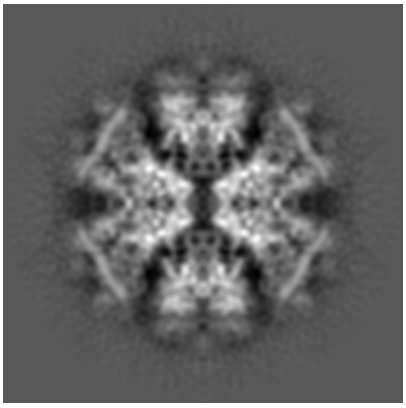
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-1178. These allow visual inspection of the internal detail of the map and identification of artifacts.

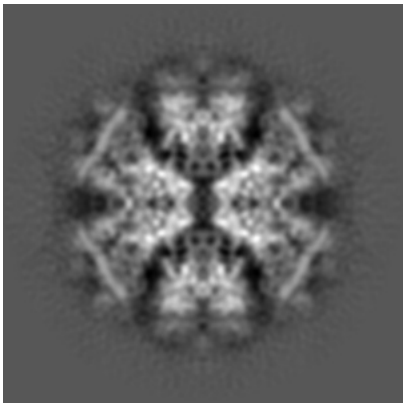
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

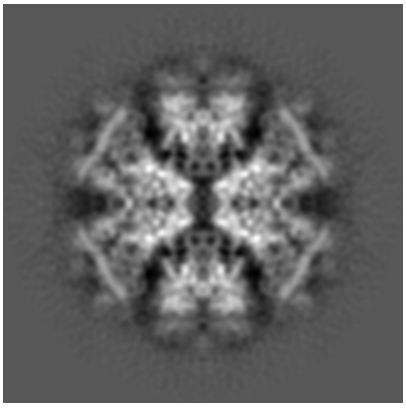
6.1.1 Primary map



X



Y

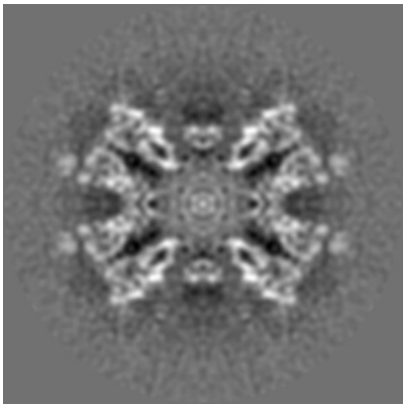


Z

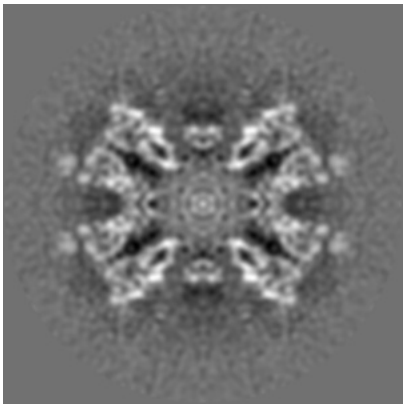
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

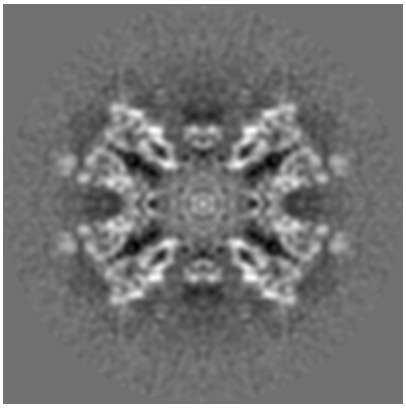
6.2.1 Primary map



X Index: 139



Y Index: 139

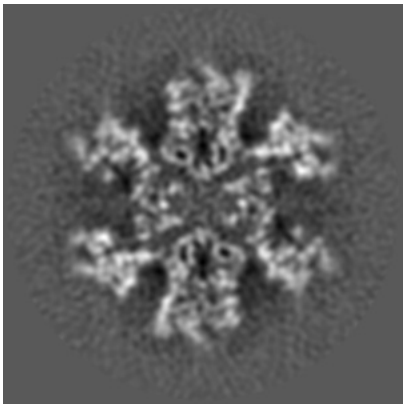


Z Index: 139

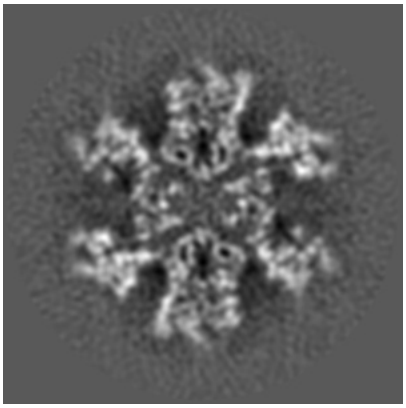
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

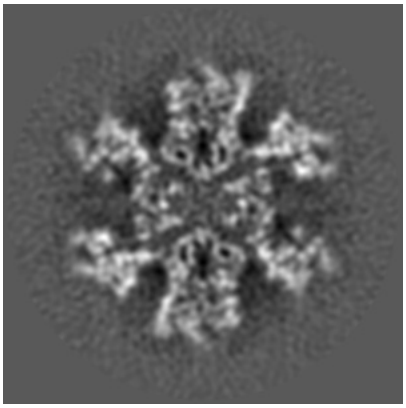
6.3.1 Primary map



X Index: 164



Y Index: 164

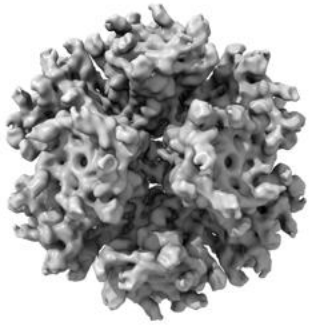


Z Index: 164

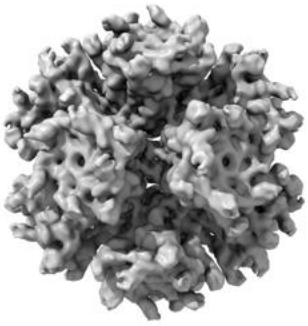
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

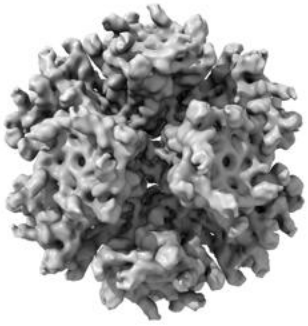
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 91.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

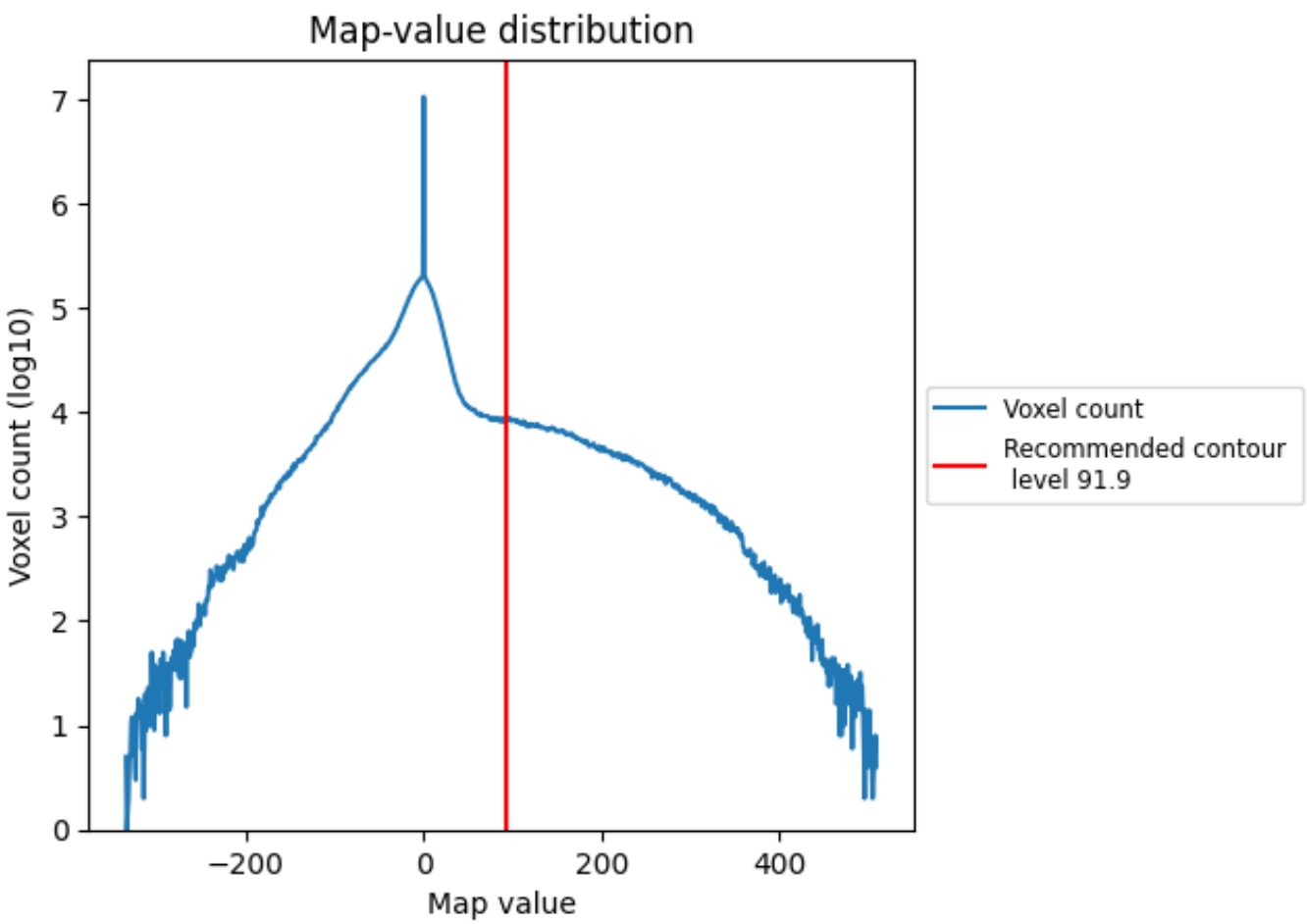
6.5 Mask visualisation (i)

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

7 Map analysis (i)

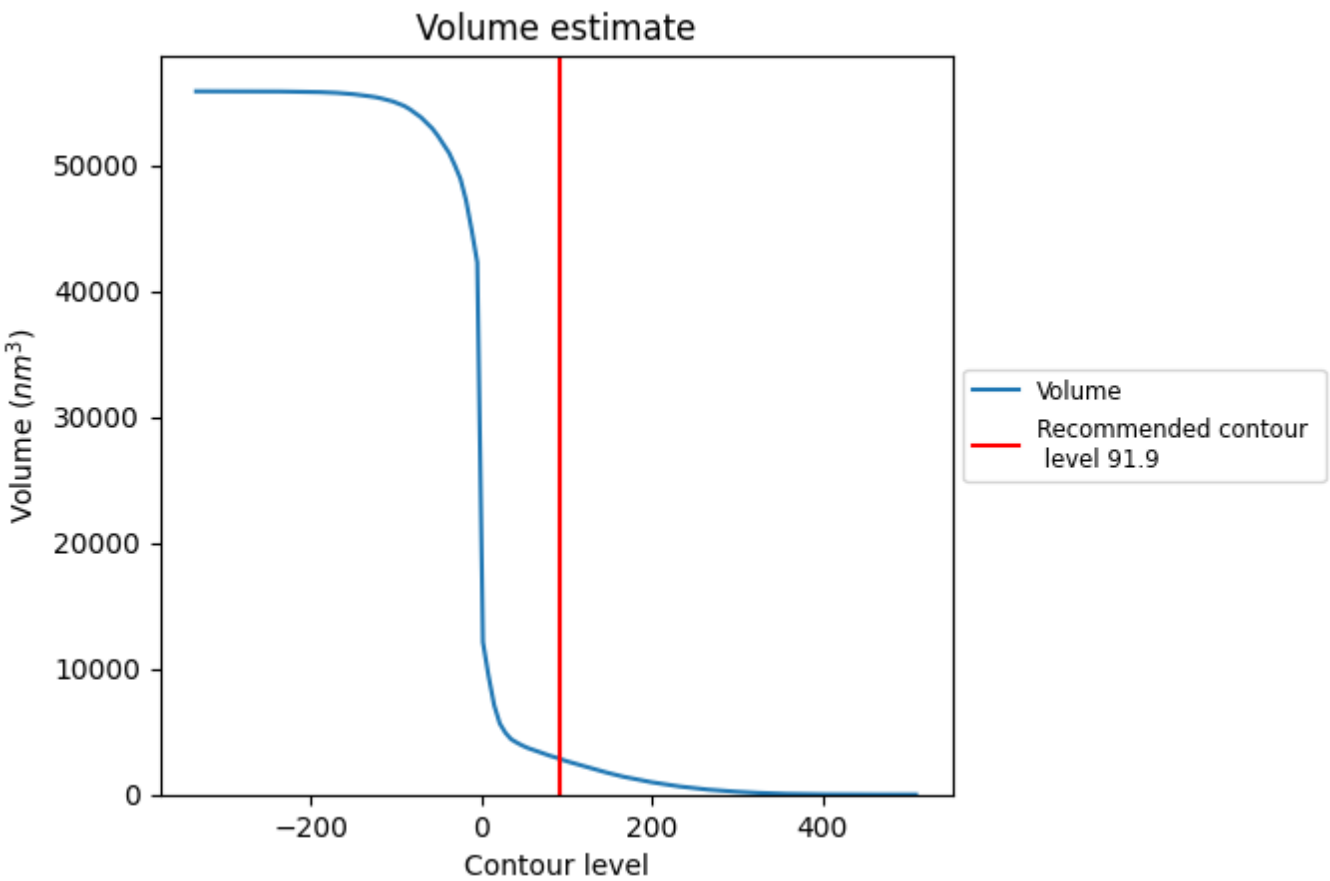
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

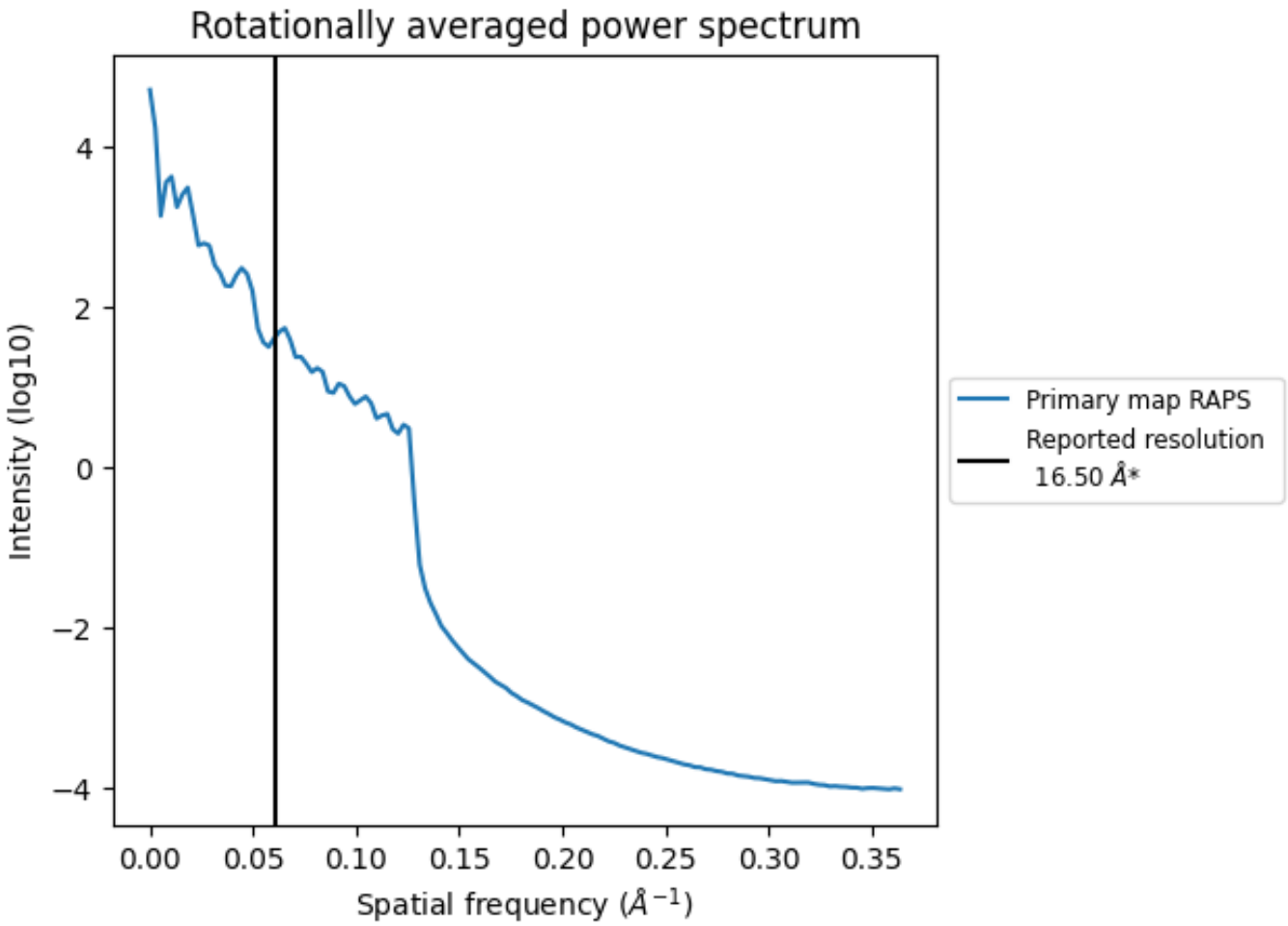
7.2 Volume estimate (i)



The volume at the recommended contour level is 2826 nm^3; this corresponds to an approximate mass of 2552 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 0.061 Å^{-1}

8 Fourier-Shell correlation (i)

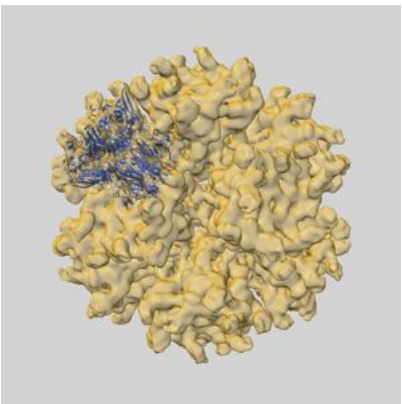
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

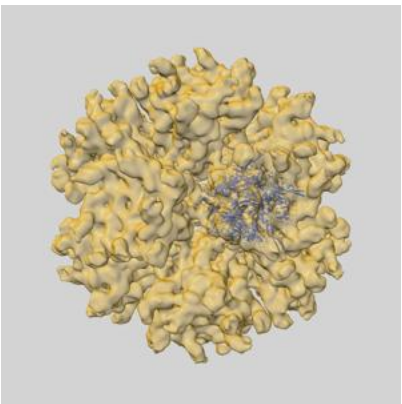
This section contains information regarding the fit between EMDB map EMD-1178 and PDB model 2C9F. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

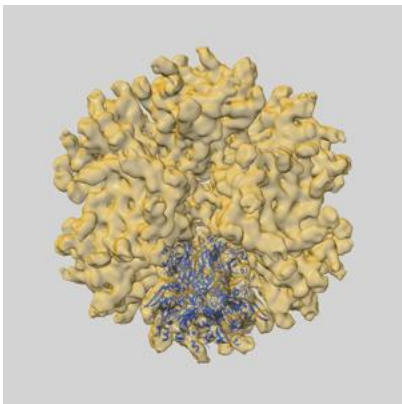
9.1.1 Map-model overlay (i)



X

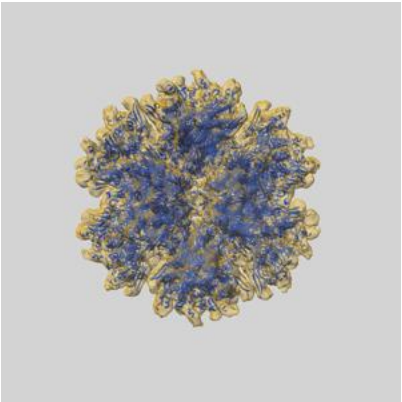


Y

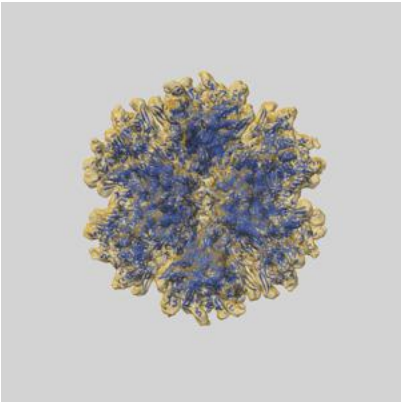


Z

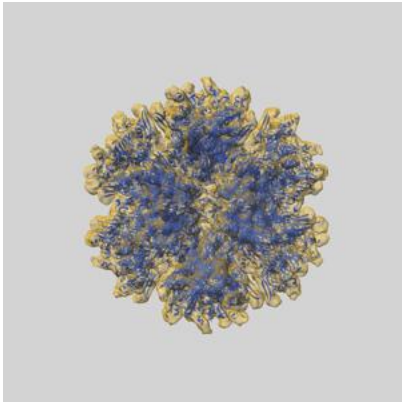
9.1.2 Map-model assembly overlay (i)



X



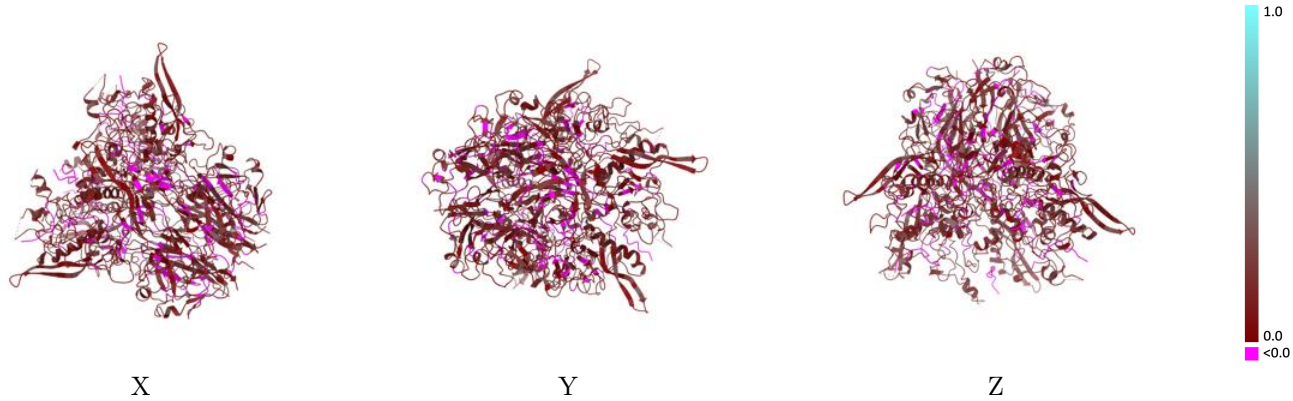
Y



Z

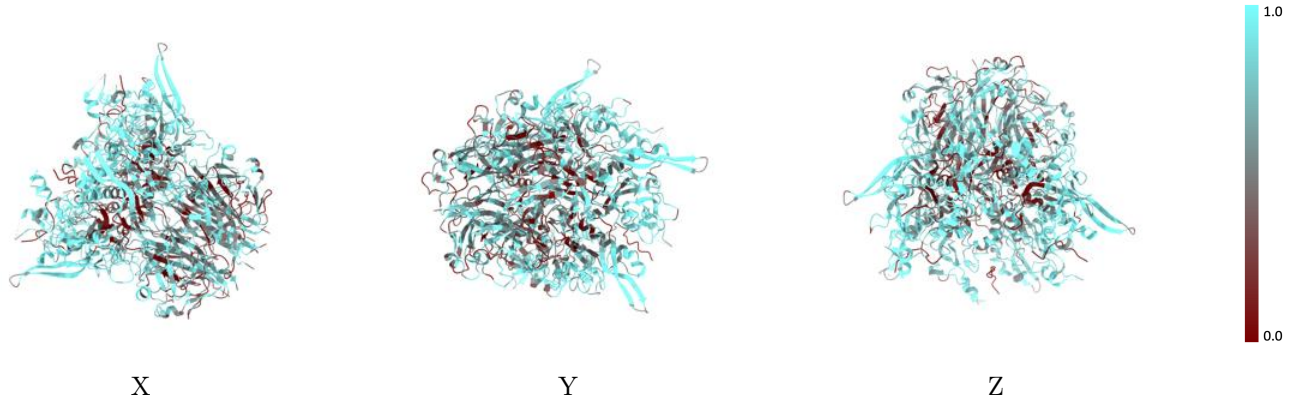
The images above show the 3D surface view of the map at the recommended contour level 91.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



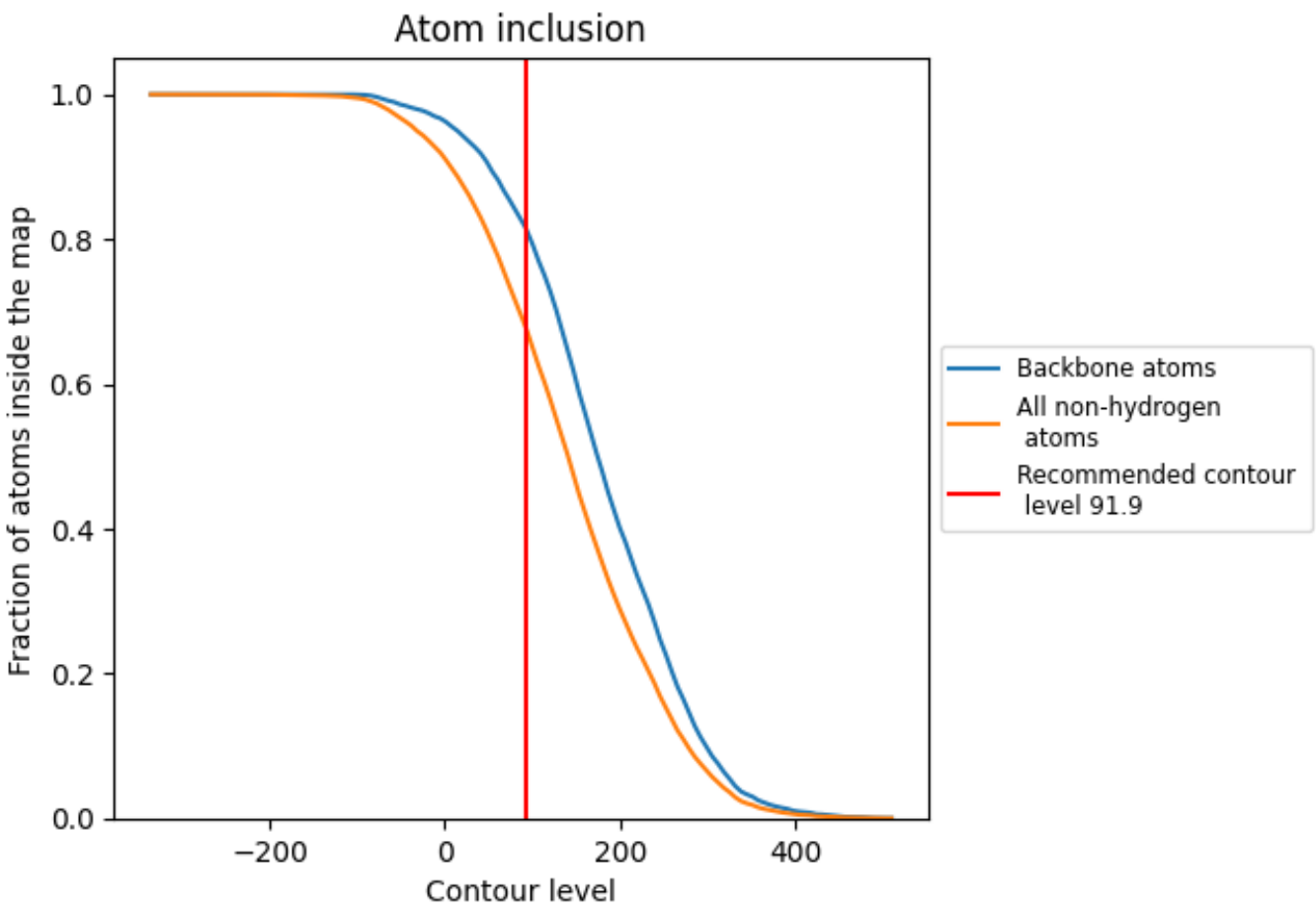
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (91.9).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (91.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6793	0.1090
A	0.6930	0.1140
B	0.6962	0.1170
C	0.6959	0.1160
D	0.6962	0.1170
E	0.6951	0.1140
S	0.0357	-0.1530
T	0.0238	-0.1540
U	0.0238	-0.1490
V	0.0238	-0.1550
W	0.0238	-0.1590