



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 04:37 PM UTC

PDB ID : 3J2P / pdb_00003j2p
EMDB ID : EMD-5499
Title : CryoEM structure of Dengue virus envelope protein heterotetramer
Authors : Zhang, X.; Ge, P.; Yu, X.; Brannan, J.M.; Bi, G.; Zhang, Q.; Schein, S.; Zhou, Z.H.
Deposited on : 2012-11-30
Resolution : 3.60 Å(reported)

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We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

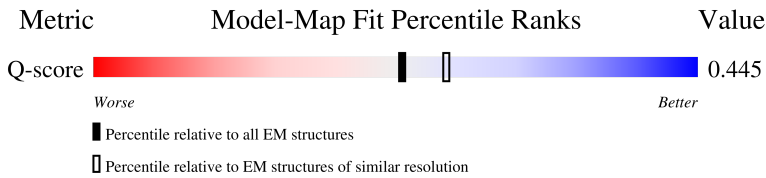
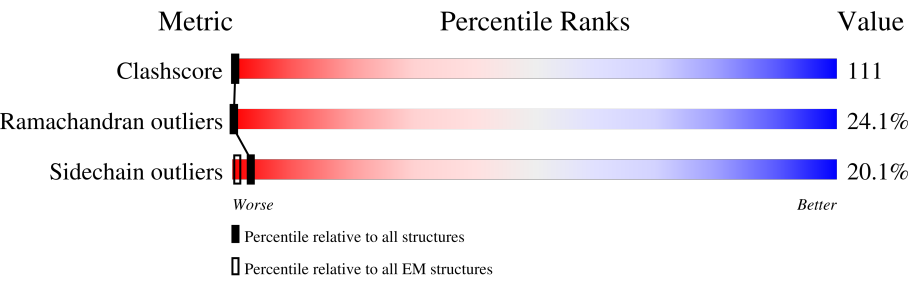
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	495	11% 11% 49% 34% 5%
1	C	495	11% 11% 50% 34% 5%
2	B	75	11% 11% 55% 28% . .
2	D	75	9% 9% 56% 28% . .

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Mol	Chain	Length	Quality of chain
3	E	2	50% 100%
3	F	2	50% 100%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9890 atoms, of which 1086 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 Envelope protein E.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	495	Total	C	H	N	O	S	0	0
			4276	2410	475	648	711	32		
1	C	495	Total	C	H	N	O	S	0	0
			4276	2410	475	648	711	32		

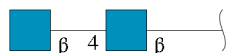
- Molecule 2 is a protein called Small envelope protein M.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	72	Total	C	H	N	O	S	0	0
			627	366	68	95	95	3		
2	D	72	Total	C	H	N	O	S	0	0
			627	366	68	95	95	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	15	ALA	ARG	SEE REMARK 999	UNP P14340
D	15	ALA	ARG	SEE REMARK 999	UNP P14340

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C₈H₁₅NO₆).

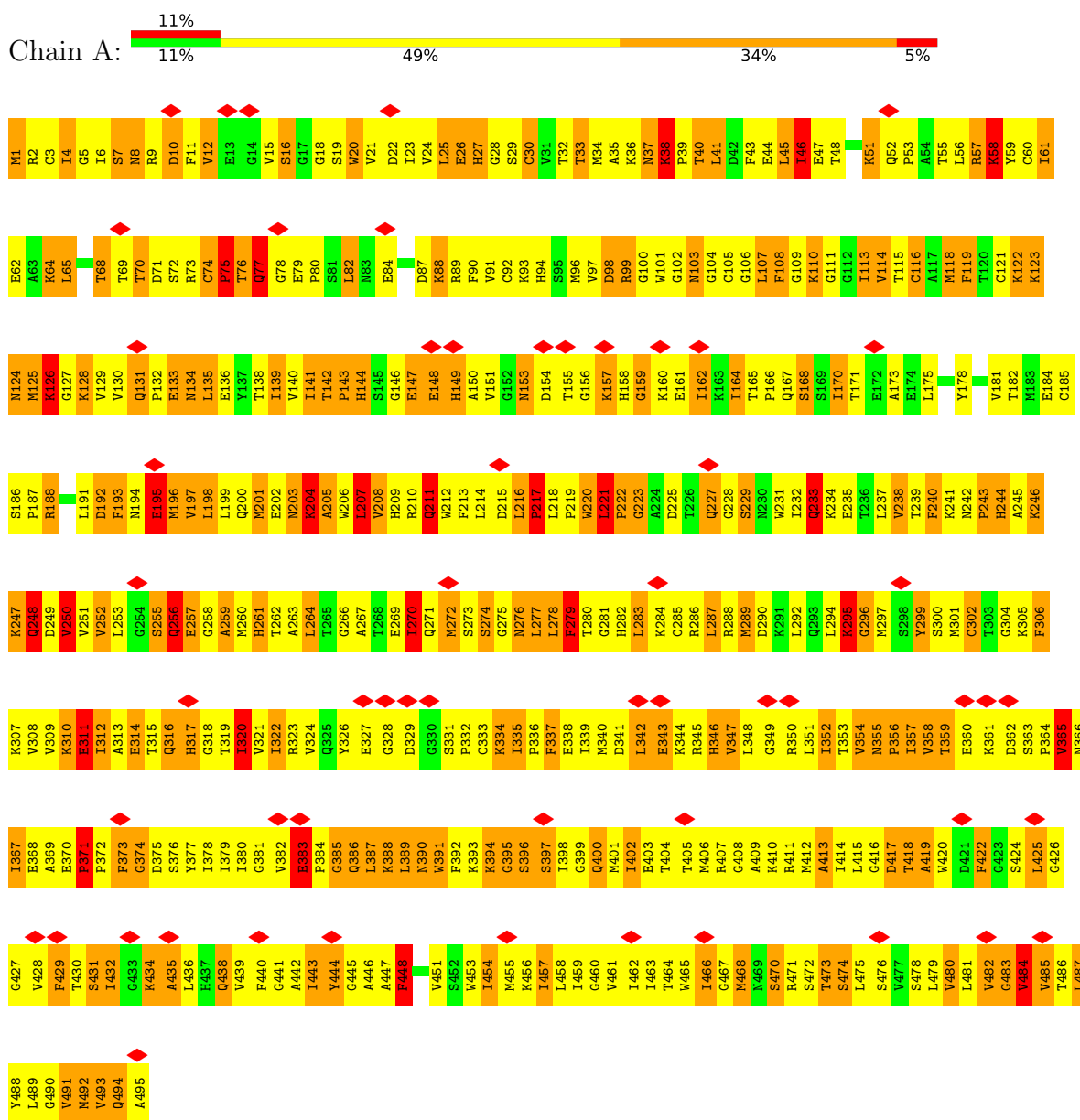


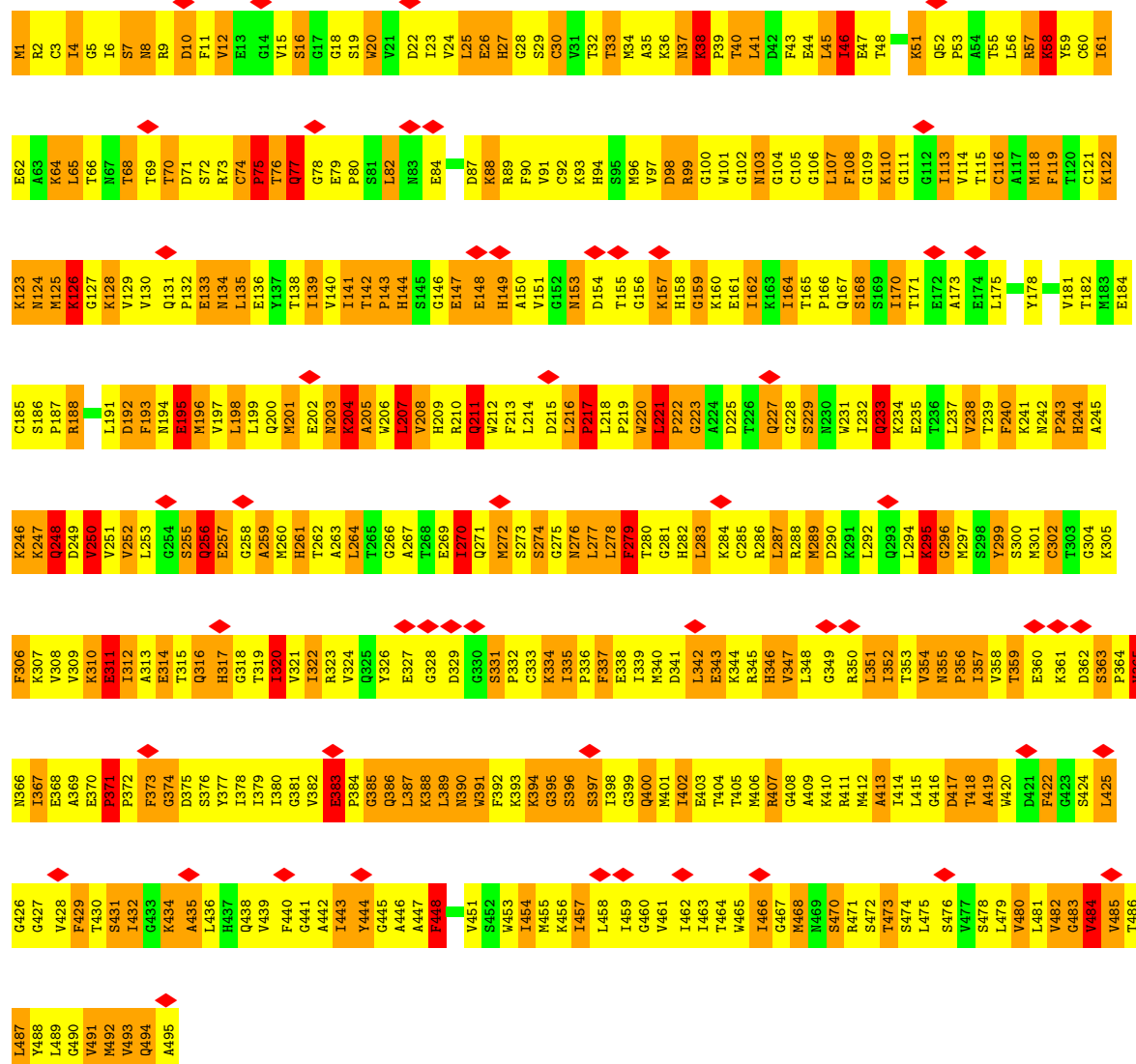
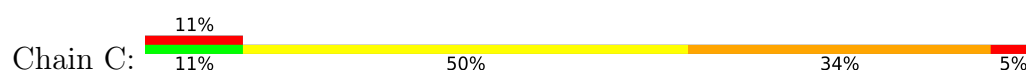
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots

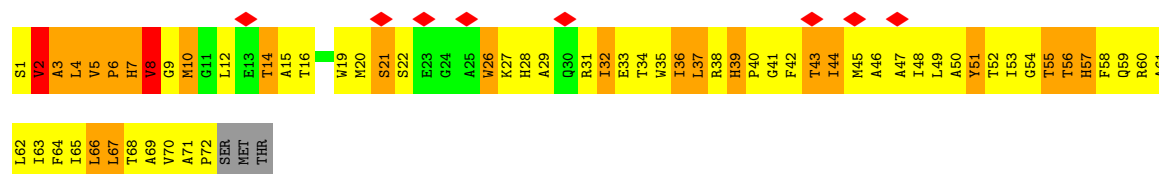
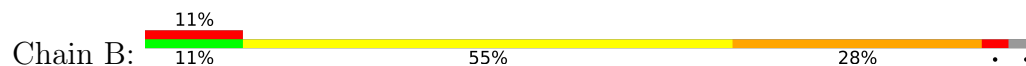
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Envelope protein E

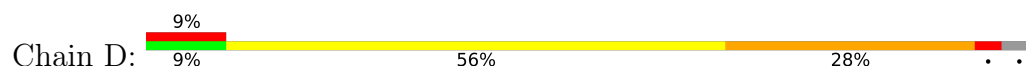


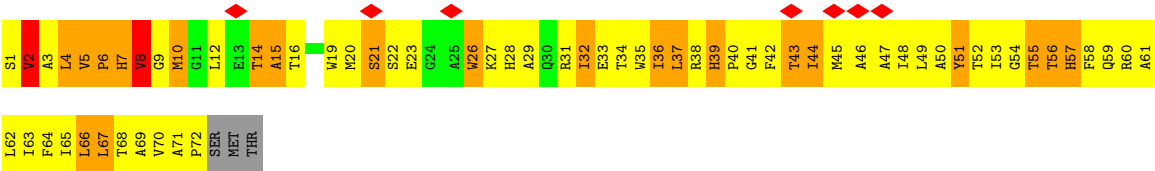


• Molecule 2: Small envelope protein M



• Molecule 2: Small envelope protein M





● Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



● Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	9288	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	EMAN, per particle, with astigmatism compensation	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	57518	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	24.021	Depositor
Minimum map value	-17.318	Depositor
Average map value	0.100	Depositor
Map value standard deviation	2.332	Depositor
Recommended contour level	4	Depositor
Map size ($\text{\AA}$)	132.48, 176.64, 132.48	wwPDB
Map dimensions	120, 160, 120	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.104, 1.104, 1.104	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.56	0/3876	1.20	48/5237 (0.9%)
1	C	0.56	0/3876	1.20	48/5237 (0.9%)
2	B	0.63	0/575	1.09	7/786 (0.9%)
2	D	0.64	0/575	1.09	6/786 (0.8%)
All	All	0.57	0/8902	1.19	109/12046 (0.9%)

There are no bond length outliers.

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	221	LEU	CA-C-N	-7.90	109.97	119.84
1	C	221	LEU	C-N-CA	-7.90	109.97	119.84
1	A	221	LEU	CA-C-N	-7.89	109.98	119.84
1	A	221	LEU	C-N-CA	-7.89	109.98	119.84
1	C	79	GLU	CA-C-N	7.55	129.28	119.84
1	C	79	GLU	C-N-CA	7.55	129.28	119.84
1	C	142	THR	CA-C-N	7.52	129.24	119.84
1	C	142	THR	C-N-CA	7.52	129.24	119.84
1	A	142	THR	CA-C-N	7.45	129.15	119.84
1	A	142	THR	C-N-CA	7.45	129.15	119.84
1	A	79	GLU	CA-C-N	7.44	129.14	119.84
1	A	79	GLU	C-N-CA	7.44	129.14	119.84
1	A	383	GLU	CA-C-N	-7.21	110.83	119.84
1	A	383	GLU	C-N-CA	-7.21	110.83	119.84
2	D	43	THR	N-CA-C	-7.19	102.48	111.11
1	C	383	GLU	CA-C-N	-7.18	110.86	119.84
1	C	383	GLU	C-N-CA	-7.18	110.86	119.84
2	B	43	THR	N-CA-C	-7.17	102.50	111.11
1	C	295	LYS	N-CA-C	7.02	118.82	111.03
1	A	295	LYS	N-CA-C	7.01	118.81	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	26	GLU	N-CA-C	6.98	120.00	108.49
1	C	252	VAL	N-CA-C	6.92	117.06	110.42
1	A	252	VAL	N-CA-C	6.89	117.03	110.42
1	A	124	ASN	N-CA-C	-6.88	99.14	109.94
1	A	148	GLU	N-CA-C	-6.88	103.84	111.82
1	A	26	GLU	N-CA-C	6.84	119.78	108.49
1	C	124	ASN	N-CA-C	-6.84	99.20	109.94
1	A	207	LEU	N-CA-C	-6.77	98.99	109.76
1	C	207	LEU	N-CA-C	-6.75	99.03	109.76
1	C	322	ILE	N-CA-C	6.74	117.61	108.17
1	C	142	THR	N-CA-C	6.72	114.27	108.22
1	A	322	ILE	N-CA-C	6.67	117.51	108.17
1	A	142	THR	N-CA-C	6.66	114.21	108.22
1	C	148	GLU	N-CA-C	-6.64	103.86	112.23
2	D	32	ILE	N-CA-C	-6.64	103.39	110.36
1	A	149	HIS	N-CA-C	-6.63	104.06	111.28
2	B	32	ILE	N-CA-C	-6.61	103.42	110.36
1	C	149	HIS	N-CA-C	-6.58	104.11	111.28
1	C	153	ASN	N-CA-C	-6.49	104.63	112.54
1	A	153	ASN	N-CA-C	-6.47	104.64	112.54
1	A	41	LEU	N-CA-C	6.40	119.96	109.72
1	A	159	GLY	N-CA-C	-6.34	107.15	114.69
1	C	159	GLY	N-CA-C	-6.33	107.15	114.69
1	C	41	LEU	N-CA-C	6.31	119.82	109.72
1	C	8	ASN	N-CA-C	-6.30	101.52	110.35
1	A	8	ASN	N-CA-C	-6.28	101.55	110.35
1	A	208	VAL	N-CA-C	6.25	116.83	108.27
1	A	118	MET	N-CA-C	-6.24	99.84	109.76
1	C	208	VAL	N-CA-C	6.17	116.73	108.27
1	C	118	MET	N-CA-C	-6.16	99.97	109.76
1	A	195	GLU	N-CA-C	-6.14	97.71	110.80
1	C	195	GLU	N-CA-C	-6.14	97.72	110.80
1	A	133	GLU	N-CA-C	-6.10	100.37	109.15
1	C	133	GLU	N-CA-C	-6.09	100.39	109.15
1	A	287	LEU	N-CA-C	-6.02	99.39	108.96
1	C	287	LEU	N-CA-C	-5.99	99.44	108.96
1	C	419	ALA	N-CA-C	-5.98	104.67	111.07
2	D	10	MET	N-CA-C	-5.98	104.67	111.07
1	A	448	PHE	N-CA-C	-5.96	103.16	110.61
1	C	448	PHE	N-CA-C	-5.95	103.17	110.61
1	A	250	VAL	N-CA-C	5.93	118.30	109.17
1	A	304	GLY	N-CA-C	5.92	118.56	110.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	10	MET	N-CA-C	-5.90	104.75	111.07
1	C	304	GLY	N-CA-C	5.89	118.52	110.69
1	A	33	THR	N-CA-C	5.86	118.44	108.90
1	C	250	VAL	N-CA-C	5.84	118.17	109.17
1	C	33	THR	N-CA-C	5.84	118.41	108.90
2	D	5	VAL	CA-C-N	5.70	126.96	119.84
2	D	5	VAL	C-N-CA	5.70	126.96	119.84
1	A	216	LEU	CA-C-N	5.68	126.94	119.84
1	A	216	LEU	C-N-CA	5.68	126.94	119.84
2	B	5	VAL	CA-C-N	5.65	126.90	119.84
2	B	5	VAL	C-N-CA	5.65	126.90	119.84
1	C	216	LEU	CA-C-N	5.64	126.89	119.84
1	C	216	LEU	C-N-CA	5.64	126.89	119.84
2	D	32	ILE	N-CA-CB	5.56	116.68	110.51
1	C	373	PHE	N-CA-C	5.55	117.19	111.03
1	C	278	LEU	N-CA-C	5.50	122.52	110.80
1	A	278	LEU	N-CA-C	5.50	122.51	110.80
1	A	79	GLU	N-CA-C	-5.49	97.67	109.81
2	B	32	ILE	N-CA-CB	5.49	116.60	110.51
1	A	373	PHE	N-CA-C	5.46	117.09	111.03
1	C	79	GLU	N-CA-C	-5.45	97.76	109.81
1	A	419	ALA	N-CA-C	-5.34	104.70	111.11
1	A	119	PHE	N-CA-C	5.33	118.13	107.62
1	C	119	PHE	N-CA-C	5.33	118.11	107.62
1	C	387	LEU	N-CA-C	5.32	118.05	108.48
1	C	205	ALA	N-CA-C	5.30	116.85	108.96
1	A	205	ALA	N-CA-C	5.28	116.83	108.96
1	C	252	VAL	CB-CA-C	-5.28	105.21	111.97
1	A	168	SER	N-CA-C	-5.28	99.56	110.80
1	A	114	VAL	CB-CA-C	-5.27	103.65	111.19
1	A	387	LEU	N-CA-C	5.27	117.97	108.48
1	A	259	ALA	N-CA-C	-5.26	104.60	111.02
1	C	385	GLY	N-CA-C	-5.25	106.78	114.61
1	C	259	ALA	N-CA-C	-5.24	104.62	111.02
1	C	168	SER	N-CA-C	-5.24	99.64	110.80
1	A	385	GLY	N-CA-C	-5.24	106.81	114.61
1	A	252	VAL	CB-CA-C	-5.22	105.29	111.97
1	C	391	TRP	N-CA-C	5.19	121.86	110.80
1	C	204	LYS	N-CA-C	-5.17	99.80	110.80
1	A	391	TRP	N-CA-C	5.14	121.74	110.80
1	A	337	PHE	N-CA-C	5.13	117.44	108.76
1	A	204	LYS	N-CA-C	-5.12	99.89	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	337	PHE	N-CA-C	5.09	117.37	108.76
1	A	197	VAL	CB-CA-C	-5.09	105.44	111.09
2	B	3	ALA	N-CA-C	-5.02	106.50	113.18
1	C	371	PRO	CA-C-N	5.00	126.10	119.84
1	C	371	PRO	C-N-CA	5.00	126.10	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3801	475	3844	869	0
1	C	3801	475	3844	853	0
2	B	559	68	569	128	0
2	D	559	68	569	128	0
3	E	28	0	25	3	0
3	F	28	0	25	3	0
4	A	14	0	13	0	0
4	C	14	0	13	0	0
All	All	8804	1086	8902	1914	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 111.

All (1914) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:51:TYR:HA	2:D:60:ARG:HD3	1.18	1.17
2:B:51:TYR:HA	2:B:60:ARG:HD3	1.17	1.14
2:B:55:THR:HA	2:B:60:ARG:HH11	1.01	1.14
1:C:125:MET:HE3	1:C:260:MET:HE1	1.16	1.13
2:B:55:THR:HA	2:B:60:ARG:NH1	1.65	1.10
1:A:125:MET:HE3	1:A:260:MET:HE1	1.17	1.08
2:D:55:THR:HA	2:D:60:ARG:HH11	1.01	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:55:THR:HA	2:D:60:ARG:NH1	1.66	1.08
1:C:464:THR:HB	1:C:482:VAL:HG11	1.33	1.07
1:A:464:THR:HB	1:A:482:VAL:HG11	1.33	1.04
1:C:463:ILE:HG23	1:C:482:VAL:HG22	1.39	1.03
2:B:56:THR:OG1	2:B:59:GLN:HB2	1.61	1.01
1:C:270:ILE:CD1	1:C:278:LEU:HA	1.90	1.01
1:A:270:ILE:CD1	1:A:278:LEU:HA	1.90	1.00
2:B:47:ALA:O	2:B:50:ALA:HB3	1.63	0.99
1:A:463:ILE:HG23	1:A:482:VAL:HG22	1.39	0.99
2:D:56:THR:OG1	2:D:59:GLN:HB2	1.60	0.99
1:A:62:GLU:HB3	1:A:122:LYS:O	1.63	0.98
1:A:89:ARG:HD3	1:A:118:MET:HE2	1.44	0.98
1:A:99:ARG:HH11	1:A:105:CYS:HB3	1.28	0.98
1:C:99:ARG:HH11	1:C:105:CYS:HB3	1.29	0.98
1:C:101:TRP:H	1:C:108:PHE:HB3	1.28	0.98
2:D:47:ALA:O	2:D:50:ALA:HB3	1.63	0.97
1:A:166:PRO:HB3	1:A:187:PRO:HG2	1.47	0.97
1:C:1:MET:HE2	1:C:151:VAL:HG22	1.46	0.97
1:A:173:ALA:HB3	1:A:181:VAL:HG12	1.44	0.96
1:C:173:ALA:HB3	1:C:181:VAL:HG12	1.44	0.96
1:C:62:GLU:HB3	1:C:122:LYS:O	1.64	0.96
1:A:306:PHE:HB3	1:A:326:TYR:HA	1.46	0.96
1:A:101:TRP:H	1:A:108:PHE:HB3	1.28	0.96
1:A:270:ILE:HD11	1:A:278:LEU:HA	1.47	0.95
1:C:464:THR:HA	1:C:482:VAL:HG21	1.47	0.95
1:C:89:ARG:HD3	1:C:118:MET:HE2	1.44	0.95
1:A:65:LEU:HD21	1:A:252:VAL:HA	1.48	0.95
1:A:1:MET:HE2	1:A:151:VAL:HG22	1.47	0.95
1:C:166:PRO:HB3	1:C:187:PRO:HG2	1.48	0.95
1:C:101:TRP:HB2	1:C:108:PHE:HD2	1.32	0.94
1:C:270:ILE:HD11	1:C:278:LEU:HA	1.46	0.94
1:C:306:PHE:HB3	1:C:326:TYR:HA	1.46	0.94
1:A:101:TRP:HB2	1:A:108:PHE:HD2	1.32	0.94
1:A:464:THR:HA	1:A:482:VAL:HG21	1.47	0.94
1:C:65:LEU:HD21	1:C:252:VAL:HA	1.48	0.94
1:A:460:GLY:O	1:A:463:ILE:HG22	1.69	0.93
1:C:206:TRP:CG	1:C:264:LEU:HD21	2.03	0.93
1:A:206:TRP:CG	1:A:264:LEU:HD21	2.02	0.93
1:A:178:TYR:HE2	1:A:295:LYS:HZ2	0.99	0.93
2:B:4:LEU:HB3	2:D:31:ARG:HH22	1.31	0.93
2:B:31:ARG:HH22	2:D:4:LEU:HB3	1.31	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:460:GLY:O	1:C:463:ILE:HG22	1.69	0.93
1:C:191:LEU:HD21	1:C:281:GLY:HA2	1.50	0.92
1:A:60:CYS:HA	1:A:124:ASN:HA	1.51	0.92
1:A:309:VAL:O	1:A:310:LYS:HB2	1.69	0.92
1:C:60:CYS:HA	1:C:124:ASN:HA	1.51	0.92
1:A:185:CYS:HA	1:A:285:CYS:HB3	1.50	0.92
1:A:256:GLN:HA	1:A:256:GLN:HE21	1.35	0.91
1:C:256:GLN:HE21	1:C:256:GLN:HA	1.35	0.91
1:A:191:LEU:HD21	1:A:281:GLY:HA2	1.50	0.91
1:A:311:GLU:HG2	1:A:312:ILE:H	1.33	0.91
1:C:309:VAL:O	1:C:310:LYS:HB2	1.69	0.91
1:C:311:GLU:HG2	1:C:312:ILE:H	1.33	0.91
1:C:320:ILE:H	1:C:320:ILE:HD12	1.35	0.91
1:A:492:MET:HE2	1:A:492:MET:HA	1.50	0.91
1:C:185:CYS:HA	1:C:285:CYS:HB3	1.50	0.90
1:C:61:ILE:HB	1:C:256:GLN:HB2	1.53	0.90
1:A:61:ILE:HB	1:A:256:GLN:HB2	1.53	0.90
1:A:139:ILE:HG22	1:A:162:ILE:HG23	1.54	0.90
1:C:492:MET:HE2	1:C:492:MET:HA	1.50	0.90
1:A:320:ILE:H	1:A:320:ILE:HD12	1.34	0.90
1:C:139:ILE:HG22	1:C:162:ILE:HG23	1.54	0.90
1:C:178:TYR:HE2	1:C:295:LYS:HZ2	0.99	0.89
1:A:92:CYS:SG	1:A:116:CYS:HB3	2.12	0.89
1:A:484:VAL:HA	1:A:488:TYR:HB2	1.55	0.89
2:B:52:THR:HG21	1:C:466:ILE:HD11	1.53	0.89
1:C:484:VAL:HA	1:C:488:TYR:HB2	1.55	0.89
1:A:466:ILE:HD11	2:D:52:THR:HG21	1.53	0.89
1:C:92:CYS:SG	1:C:116:CYS:HB3	2.12	0.89
1:C:73:ARG:O	1:C:74:CYS:HB3	1.72	0.88
1:A:101:TRP:HE1	1:C:310:LYS:NZ	1.71	0.88
1:C:296:GLY:HA2	1:C:299:TYR:HE1	1.39	0.88
1:A:310:LYS:NZ	1:C:101:TRP:HE1	1.71	0.87
1:C:410:LYS:O	1:C:414:ILE:HD13	1.74	0.87
1:A:164:ILE:O	1:A:164:ILE:HD13	1.74	0.87
1:A:53:PRO:HB3	1:A:130:VAL:HG12	1.57	0.87
1:A:56:LEU:O	1:A:57:ARG:HB2	1.74	0.87
1:C:58:LYS:HD2	1:C:221:LEU:HD23	1.57	0.87
1:A:170:ILE:HG22	1:A:184:GLU:HG3	1.55	0.87
1:A:296:GLY:HA2	1:A:299:TYR:HE1	1.38	0.87
1:C:170:ILE:HG22	1:C:184:GLU:HG3	1.55	0.87
1:C:164:ILE:HD13	1:C:164:ILE:O	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ILE:CG2	1:A:349:GLY:HA3	2.04	0.86
1:C:4:ILE:HB	1:C:151:VAL:CG1	2.06	0.86
1:A:410:LYS:O	1:A:414:ILE:HD13	1.75	0.86
1:C:339:ILE:CG2	1:C:349:GLY:HA3	2.04	0.86
1:C:53:PRO:HB3	1:C:130:VAL:HG12	1.57	0.86
1:C:282:HIS:CG	1:C:282:HIS:O	2.29	0.86
1:C:94:HIS:HA	1:C:114:VAL:HG12	1.57	0.86
1:A:282:HIS:CG	1:A:282:HIS:O	2.29	0.86
1:A:310:LYS:HZ3	1:C:101:TRP:HE1	1.24	0.85
1:C:56:LEU:O	1:C:57:ARG:HB2	1.73	0.85
1:A:390:ASN:HD22	1:A:391:TRP:N	1.73	0.85
1:A:4:ILE:HB	1:A:151:VAL:CG1	2.06	0.85
1:A:73:ARG:O	1:A:74:CYS:HB3	1.73	0.85
1:C:390:ASN:HD22	1:C:391:TRP:N	1.73	0.85
1:A:320:ILE:HD13	1:A:371:PRO:HD2	1.57	0.85
1:C:305:LYS:HD2	1:C:327:GLU:HB3	1.58	0.85
1:A:94:HIS:HA	1:A:114:VAL:HG12	1.56	0.85
2:D:55:THR:CA	2:D:60:ARG:HH11	1.88	0.85
1:A:58:LYS:HD2	1:A:221:LEU:HD23	1.57	0.85
1:A:259:ALA:O	1:A:262:THR:HG22	1.77	0.85
2:B:44:ILE:O	2:B:48:ILE:HG13	1.77	0.85
1:C:339:ILE:CD1	1:C:378:ILE:HG22	2.07	0.85
1:A:90:PHE:HE2	1:A:118:MET:HE3	1.40	0.85
1:A:306:PHE:HZ	1:A:381:GLY:HA3	1.40	0.85
2:B:1:SER:C	2:B:3:ALA:H	1.82	0.84
1:C:125:MET:HE3	1:C:260:MET:CE	2.05	0.84
1:C:233:GLN:HE21	1:C:233:GLN:HA	1.41	0.84
2:D:1:SER:C	2:D:3:ALA:H	1.82	0.84
1:C:90:PHE:HE2	1:C:118:MET:HE3	1.40	0.84
2:D:44:ILE:O	2:D:48:ILE:HG13	1.76	0.84
1:A:125:MET:HE3	1:A:260:MET:CE	2.06	0.84
1:C:306:PHE:HZ	1:C:381:GLY:HA3	1.39	0.84
1:A:200:GLN:HB2	1:A:272:MET:HE3	1.60	0.84
2:B:55:THR:CA	2:B:60:ARG:HH11	1.88	0.84
1:C:259:ALA:O	1:C:262:THR:HG22	1.77	0.84
1:C:270:ILE:HD12	1:C:271:GLN:N	1.93	0.83
1:A:270:ILE:HD12	1:A:271:GLN:N	1.94	0.83
1:C:320:ILE:HD13	1:C:371:PRO:HD2	1.58	0.83
1:A:233:GLN:HA	1:A:233:GLN:HE21	1.41	0.83
1:A:305:LYS:HD2	1:A:327:GLU:HB3	1.59	0.83
2:B:31:ARG:HH22	2:D:4:LEU:CB	1.91	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:63:ILE:HD12	2:D:64:PHE:N	1.93	0.83
1:C:200:GLN:HB2	1:C:272:MET:HE3	1.60	0.83
1:A:339:ILE:CD1	1:A:378:ILE:HG22	2.08	0.83
1:C:336:PRO:HG2	1:C:381:GLY:HA2	1.60	0.83
2:B:66:LEU:HD23	2:D:66:LEU:HB3	1.61	0.83
2:B:63:ILE:HD12	2:B:64:PHE:N	1.94	0.82
1:A:156:GLY:C	1:A:157:LYS:HE2	2.05	0.82
2:B:4:LEU:CB	2:D:31:ARG:HH22	1.91	0.82
1:A:220:TRP:HD1	1:A:221:LEU:O	1.63	0.82
1:A:336:PRO:HG2	1:A:381:GLY:HA2	1.60	0.82
1:A:101:TRP:HE1	1:C:310:LYS:HZ3	1.24	0.81
1:C:156:GLY:C	1:C:157:LYS:HE2	2.05	0.81
1:C:220:TRP:CD1	1:C:221:LEU:O	2.33	0.81
1:A:25:LEU:HB2	1:A:45:LEU:HD12	1.61	0.81
1:A:220:TRP:CD1	1:A:221:LEU:O	2.33	0.81
1:C:25:LEU:HB2	1:C:45:LEU:HD12	1.61	0.81
1:A:23:ILE:HD13	1:A:25:LEU:HD21	1.62	0.81
1:C:23:ILE:HD13	1:C:25:LEU:HD21	1.61	0.81
1:C:220:TRP:HD1	1:C:221:LEU:O	1.63	0.81
1:A:240:PHE:HA	1:A:250:VAL:HA	1.62	0.80
1:C:311:GLU:O	1:C:312:ILE:HG23	1.82	0.80
1:C:196:MET:HE2	1:C:196:MET:HA	1.64	0.80
1:A:320:ILE:H	1:A:320:ILE:CD1	1.94	0.80
1:C:320:ILE:H	1:C:320:ILE:CD1	1.94	0.80
1:A:61:ILE:HD13	1:A:123:LYS:O	1.81	0.80
1:A:196:MET:HE2	1:A:196:MET:HA	1.63	0.80
2:B:66:LEU:HB3	2:D:66:LEU:HD23	1.62	0.80
1:C:240:PHE:HA	1:C:250:VAL:HA	1.61	0.80
1:A:320:ILE:HD12	1:A:320:ILE:N	1.96	0.80
1:C:197:VAL:CG2	1:C:210:ARG:HA	2.13	0.79
1:A:466:ILE:O	1:A:466:ILE:HD13	1.82	0.79
1:C:320:ILE:HD12	1:C:320:ILE:N	1.97	0.79
1:A:6:ILE:HG22	1:A:6:ILE:O	1.80	0.79
1:C:247:LYS:HA	1:C:247:LYS:NZ	1.97	0.79
1:A:233:GLN:HA	1:A:233:GLN:NE2	1.97	0.79
1:A:270:ILE:HD12	1:A:270:ILE:C	2.07	0.79
1:C:61:ILE:HD13	1:C:123:LYS:O	1.82	0.79
1:A:247:LYS:HA	1:A:247:LYS:NZ	1.97	0.79
2:B:26:TRP:HA	2:B:26:TRP:CE3	2.14	0.79
2:D:26:TRP:HA	2:D:26:TRP:CE3	2.15	0.79
1:A:311:GLU:O	1:A:312:ILE:HG23	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:ASN:C	1:C:38:LYS:HD2	2.08	0.79
1:C:339:ILE:HB	1:C:349:GLY:HA3	1.65	0.79
1:C:270:ILE:HD12	1:C:270:ILE:C	2.07	0.79
1:A:74:CYS:SG	1:A:75:PRO:HD2	2.23	0.79
1:C:466:ILE:O	1:C:466:ILE:HD13	1.81	0.79
1:C:367:ILE:HG22	1:C:368:GLU:H	1.48	0.78
1:A:99:ARG:HH11	1:A:105:CYS:CB	1.96	0.78
2:D:37:LEU:HD23	2:D:38:ARG:N	1.99	0.78
1:A:380:ILE:HG13	1:A:380:ILE:O	1.83	0.78
1:A:197:VAL:CG2	1:A:210:ARG:HA	2.13	0.78
1:A:37:ASN:C	1:A:38:LYS:HD2	2.08	0.78
1:C:6:ILE:O	1:C:6:ILE:HG22	1.80	0.78
1:C:443:ILE:HG13	1:C:444:TYR:H	1.48	0.78
1:C:53:PRO:HG2	1:C:128:LYS:HZ2	1.49	0.78
1:C:99:ARG:HH11	1:C:105:CYS:CB	1.97	0.78
1:A:367:ILE:HG22	1:A:368:GLU:H	1.48	0.77
1:C:122:LYS:HG3	1:C:123:LYS:HD3	1.66	0.77
1:C:74:CYS:SG	1:C:75:PRO:HD2	2.24	0.77
1:C:51:LYS:HZ2	1:C:136:GLU:HB2	1.50	0.77
1:A:135:LEU:HD21	1:A:193:PHE:HE1	1.49	0.77
1:A:270:ILE:CG1	1:A:271:GLN:H	1.97	0.77
1:A:339:ILE:HB	1:A:349:GLY:HA3	1.65	0.77
1:A:488:TYR:O	1:A:489:LEU:C	2.28	0.77
1:C:270:ILE:CG1	1:C:271:GLN:H	1.97	0.77
1:C:185:CYS:HA	1:C:285:CYS:CB	2.14	0.77
1:C:454:ILE:HD13	1:C:455:MET:N	2.00	0.77
1:A:122:LYS:HG3	1:A:123:LYS:HD3	1.67	0.76
2:B:37:LEU:HD23	2:B:38:ARG:N	1.99	0.76
1:C:463:ILE:HG23	1:C:482:VAL:CG2	2.15	0.76
1:A:30:CYS:HA	1:A:43:PHE:O	1.86	0.76
1:A:185:CYS:HA	1:A:285:CYS:CB	2.15	0.76
1:A:383:GLU:HB3	1:A:384:PRO:CD	2.16	0.76
2:D:51:TYR:HA	2:D:60:ARG:CD	2.09	0.76
1:A:443:ILE:HG13	1:A:444:TYR:H	1.49	0.76
1:A:488:TYR:HA	1:A:491:VAL:HG22	1.67	0.76
2:B:51:TYR:HA	2:B:60:ARG:CD	2.09	0.76
1:C:1:MET:HG3	1:C:151:VAL:HA	1.67	0.76
1:C:203:ASN:C	1:C:204:LYS:HG2	2.11	0.76
1:C:135:LEU:HD21	1:C:193:PHE:HE1	1.49	0.76
1:C:339:ILE:HD13	1:C:378:ILE:HG22	1.68	0.75
1:A:413:ALA:C	1:A:414:ILE:HD12	2.11	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ILE:HD12	1:C:23:ILE:O	1.86	0.75
1:C:30:CYS:HA	1:C:43:PHE:O	1.86	0.75
1:C:380:ILE:HG13	1:C:380:ILE:O	1.83	0.75
1:A:203:ASN:C	1:A:204:LYS:HG2	2.11	0.75
1:C:413:ALA:C	1:C:414:ILE:HD12	2.11	0.75
1:A:201:MET:HB3	1:A:206:TRP:HZ3	1.50	0.75
2:D:55:THR:O	2:D:56:THR:HG23	1.86	0.75
1:A:1:MET:HG3	1:A:151:VAL:HA	1.67	0.75
1:A:47:GLU:O	1:A:138:THR:HG22	1.87	0.75
1:C:233:GLN:HA	1:C:233:GLN:NE2	1.98	0.75
1:A:454:ILE:HG23	1:A:455:MET:H	1.50	0.75
1:C:454:ILE:HG23	1:C:455:MET:H	1.50	0.75
1:C:488:TYR:HA	1:C:491:VAL:HG22	1.67	0.75
1:A:385:GLY:O	1:A:387:LEU:N	2.20	0.75
1:A:35:ALA:HB3	1:A:37:ASN:O	1.87	0.74
1:A:463:ILE:HG23	1:A:482:VAL:CG2	2.15	0.74
1:C:35:ALA:HB3	1:C:37:ASN:O	1.87	0.74
1:C:327:GLU:HG2	1:C:328:GLY:H	1.52	0.74
1:A:206:TRP:CD2	1:A:264:LEU:HD21	2.22	0.74
1:A:454:ILE:HD13	1:A:455:MET:N	2.01	0.74
1:C:146:GLY:O	1:C:147:GLU:HG3	1.88	0.74
1:A:101:TRP:N	1:A:108:PHE:HB3	2.00	0.74
1:A:327:GLU:HG2	1:A:328:GLY:H	1.51	0.74
2:B:55:THR:O	2:B:56:THR:HG23	1.86	0.74
1:C:470:SER:HB3	1:C:475:LEU:HB3	1.70	0.74
1:A:470:SER:HB3	1:A:475:LEU:HB3	1.70	0.74
1:C:385:GLY:O	1:C:387:LEU:N	2.20	0.74
1:A:339:ILE:CB	1:A:349:GLY:HA3	2.17	0.74
1:C:47:GLU:O	1:C:138:THR:HG22	1.87	0.74
1:C:239:THR:O	1:C:251:VAL:HG22	1.87	0.74
1:C:383:GLU:HB3	1:C:384:PRO:CD	2.16	0.74
1:C:206:TRP:CD2	1:C:264:LEU:HD21	2.22	0.74
1:A:239:THR:O	1:A:251:VAL:HG22	1.88	0.74
1:C:20:TRP:HZ3	1:C:288:ARG:HE	1.35	0.74
1:C:488:TYR:O	1:C:489:LEU:C	2.28	0.74
1:C:101:TRP:N	1:C:108:PHE:HB3	2.01	0.74
1:C:375:ASP:HA	1:C:392:PHE:HA	1.70	0.74
1:C:4:ILE:HB	1:C:151:VAL:HG11	1.68	0.74
1:A:146:GLY:O	1:A:147:GLU:HG3	1.88	0.74
1:C:201:MET:HB3	1:C:206:TRP:HZ3	1.50	0.74
1:C:263:ALA:HB2	2:D:2:VAL:C	2.13	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:ILE:CB	1:C:349:GLY:HA3	2.17	0.74
1:A:4:ILE:HB	1:A:151:VAL:HG11	1.69	0.73
1:C:387:LEU:HD22	1:C:388:LYS:H	1.54	0.73
1:A:20:TRP:HA	1:A:20:TRP:CE3	2.23	0.73
1:A:9:ARG:HG3	1:A:10:ASP:N	2.03	0.73
1:A:23:ILE:HD12	1:A:23:ILE:O	1.89	0.73
1:A:339:ILE:HD13	1:A:378:ILE:HG22	1.69	0.73
1:A:367:ILE:HD12	1:A:367:ILE:N	2.04	0.73
1:A:387:LEU:HD22	1:A:388:LYS:H	1.53	0.73
1:A:270:ILE:HG13	1:A:271:GLN:H	1.54	0.73
1:C:20:TRP:HA	1:C:20:TRP:CE3	2.23	0.72
1:C:170:ILE:H	1:C:170:ILE:HD13	1.54	0.72
1:A:20:TRP:HZ3	1:A:288:ARG:HE	1.36	0.72
1:A:247:LYS:HA	1:A:247:LYS:HZ2	1.52	0.72
1:C:39:PRO:HD3	1:C:294:LEU:HA	1.72	0.72
1:C:193:PHE:O	1:C:195:GLU:HG2	1.90	0.72
1:A:37:ASN:O	1:A:38:LYS:HD2	1.90	0.72
1:A:193:PHE:O	1:A:195:GLU:HG2	1.89	0.72
1:A:263:ALA:HB2	2:B:2:VAL:C	2.14	0.72
1:A:384:PRO:HG2	1:A:386:GLN:HE21	1.55	0.72
1:C:44:GLU:O	1:C:140:VAL:HG22	1.88	0.72
1:C:4:ILE:HB	1:C:151:VAL:HG13	1.71	0.72
1:C:9:ARG:HG3	1:C:10:ASP:N	2.03	0.72
1:C:338:GLU:HB2	1:C:379:ILE:HG23	1.72	0.72
1:C:367:ILE:N	1:C:367:ILE:HD12	2.05	0.72
1:C:464:THR:CB	1:C:482:VAL:HG11	2.17	0.72
2:D:56:THR:O	2:D:58:PHE:N	2.23	0.71
1:A:39:PRO:HD3	1:A:294:LEU:HA	1.72	0.71
1:A:44:GLU:O	1:A:140:VAL:HG22	1.89	0.71
1:A:219:PRO:HA	1:A:233:GLN:HB2	1.72	0.71
2:B:14:THR:O	2:B:16:THR:N	2.23	0.71
1:A:338:GLU:HB2	1:A:379:ILE:HG23	1.72	0.71
2:D:3:ALA:HB3	2:D:4:LEU:HD22	1.73	0.71
2:B:3:ALA:HB3	2:B:4:LEU:HD22	1.73	0.71
2:B:31:ARG:HD2	2:B:32:ILE:N	2.06	0.71
1:C:302:CYS:SG	1:C:333:CYS:HB2	2.31	0.71
1:A:5:GLY:HA2	1:A:315:THR:HG21	1.73	0.71
1:A:170:ILE:HD13	1:A:170:ILE:H	1.54	0.71
2:B:56:THR:O	2:B:58:PHE:N	2.23	0.71
1:C:37:ASN:O	1:C:38:LYS:HD2	1.90	0.71
1:C:270:ILE:HG13	1:C:271:GLN:H	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:14:THR:O	2:D:16:THR:N	2.24	0.71
1:A:365:VAL:HG23	1:A:366:ASN:N	2.04	0.71
1:A:51:LYS:HZ2	1:A:136:GLU:HB2	1.55	0.71
1:A:375:ASP:HA	1:A:392:PHE:HA	1.71	0.71
1:A:424:SER:O	1:A:425:LEU:HB2	1.90	0.71
1:C:272:MET:HA	1:C:276:ASN:HB3	1.73	0.71
1:A:414:ILE:HG22	1:A:415:LEU:HD23	1.72	0.71
1:C:461:VAL:O	1:C:464:THR:HG22	1.91	0.71
1:A:4:ILE:HB	1:A:151:VAL:HG13	1.71	0.70
1:A:302:CYS:SG	1:A:333:CYS:HB2	2.31	0.70
1:C:197:VAL:HG23	1:C:210:ARG:HA	1.73	0.70
1:C:397:SER:O	1:C:400:GLN:HB2	1.91	0.70
1:A:221:LEU:HG	1:A:222:PRO:HD2	1.72	0.70
1:A:397:SER:O	1:A:400:GLN:HB2	1.91	0.70
1:C:5:GLY:HA2	1:C:315:THR:HG21	1.73	0.70
1:C:269:GLU:HG2	1:C:270:ILE:H	1.55	0.70
1:C:365:VAL:HG23	1:C:366:ASN:N	2.05	0.70
1:C:414:ILE:HG22	1:C:415:LEU:HD23	1.72	0.70
1:C:283:LEU:C	1:C:283:LEU:HD12	2.16	0.70
1:C:424:SER:O	1:C:425:LEU:HB2	1.90	0.70
1:A:58:LYS:HB2	1:A:58:LYS:NZ	2.06	0.70
2:B:4:LEU:HD22	2:B:4:LEU:N	2.06	0.70
1:A:35:ALA:C	1:A:37:ASN:H	1.99	0.70
1:A:283:LEU:C	1:A:283:LEU:HD12	2.16	0.70
1:C:384:PRO:HG2	1:C:386:GLN:HE21	1.56	0.70
2:D:4:LEU:HD22	2:D:4:LEU:N	2.07	0.70
1:A:272:MET:HA	1:A:276:ASN:HB3	1.72	0.70
1:A:367:ILE:HG22	1:A:368:GLU:N	2.07	0.70
1:A:464:THR:CB	1:A:482:VAL:HG11	2.17	0.70
1:C:277:LEU:HD23	1:C:277:LEU:H	1.55	0.70
1:C:296:GLY:HA2	1:C:299:TYR:CE1	2.25	0.70
1:C:339:ILE:HG21	1:C:349:GLY:HA3	1.72	0.70
1:A:64:LYS:NZ	1:A:64:LYS:HB3	2.07	0.70
1:A:277:LEU:HD23	1:A:277:LEU:H	1.55	0.70
1:A:339:ILE:HG21	1:A:349:GLY:HA3	1.72	0.70
1:A:269:GLU:HG2	1:A:270:ILE:H	1.55	0.70
1:C:64:LYS:NZ	1:C:64:LYS:HB3	2.07	0.70
1:C:122:LYS:HB2	1:C:122:LYS:HZ3	1.57	0.69
1:C:221:LEU:HG	1:C:222:PRO:CD	2.22	0.69
2:D:62:LEU:C	2:D:62:LEU:HD13	2.17	0.69
1:A:387:LEU:HD22	1:A:388:LYS:N	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:GLY:O	1:A:128:LYS:HB2	1.91	0.69
1:A:221:LEU:HG	1:A:222:PRO:CD	2.22	0.69
1:A:492:MET:HA	1:A:492:MET:CE	2.22	0.69
1:C:34:MET:HA	1:C:40:THR:HG22	1.73	0.69
1:C:100:GLY:O	1:C:103:ASN:HB3	1.92	0.69
1:A:20:TRP:CD1	1:A:286:ARG:HH12	2.11	0.69
1:A:101:TRP:NE1	1:C:310:LYS:NZ	2.39	0.69
1:A:109:GLY:HA2	1:C:315:THR:HB	1.72	0.69
1:C:221:LEU:HG	1:C:222:PRO:HD2	1.72	0.69
1:C:457:ILE:C	1:C:457:ILE:HD12	2.16	0.69
2:D:31:ARG:HD2	2:D:32:ILE:N	2.06	0.69
1:A:457:ILE:C	1:A:457:ILE:HD12	2.16	0.69
1:C:57:ARG:NH2	1:C:214:LEU:HD22	2.08	0.69
1:C:387:LEU:HD22	1:C:388:LYS:N	2.08	0.69
1:A:57:ARG:NH2	1:A:214:LEU:HD22	2.08	0.69
1:A:315:THR:HB	1:C:109:GLY:HA2	1.73	0.69
2:B:62:LEU:HD13	2:B:62:LEU:C	2.17	0.69
1:A:100:GLY:O	1:A:103:ASN:HB3	1.92	0.69
1:A:310:LYS:NZ	1:C:101:TRP:NE1	2.39	0.69
1:A:34:MET:HA	1:A:40:THR:HG22	1.73	0.69
1:A:197:VAL:HG23	1:A:210:ARG:HA	1.74	0.69
1:A:307:LYS:HG2	1:A:308:VAL:H	1.58	0.69
1:A:461:VAL:O	1:A:464:THR:HG22	1.91	0.69
1:C:58:LYS:HB2	1:C:58:LYS:NZ	2.07	0.69
1:C:127:GLY:O	1:C:128:LYS:HB2	1.92	0.69
1:C:219:PRO:HA	1:C:233:GLN:HB2	1.73	0.69
1:C:9:ARG:HG3	1:C:10:ASP:H	1.58	0.68
1:A:320:ILE:CD1	1:A:371:PRO:HD2	2.23	0.68
1:C:367:ILE:HG22	1:C:368:GLU:N	2.06	0.68
1:A:205:ALA:C	1:A:206:TRP:CE3	2.72	0.68
1:C:35:ALA:C	1:C:37:ASN:H	1.99	0.68
1:A:53:PRO:HG2	1:A:128:LYS:HZ2	1.58	0.68
1:C:202:GLU:HG3	1:C:257:GLU:OE2	1.93	0.68
1:A:296:GLY:HA2	1:A:299:TYR:CE1	2.25	0.68
1:A:478:SER:O	1:A:482:VAL:HG23	1.94	0.68
1:C:45:LEU:C	1:C:45:LEU:HD22	2.19	0.68
1:C:205:ALA:C	1:C:206:TRP:CE3	2.72	0.68
1:C:307:LYS:HG2	1:C:308:VAL:H	1.58	0.68
1:A:9:ARG:HG3	1:A:10:ASP:H	1.58	0.68
1:C:448:PHE:HZ	1:C:456:LYS:HD3	1.59	0.68
1:C:162:ILE:HD11	1:C:171:THR:HB	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:GLU:C	1:A:312:ILE:HD13	2.19	0.68
1:C:20:TRP:CD1	1:C:286:ARG:HH12	2.11	0.67
1:C:27:HIS:CE1	1:C:279:PHE:HA	2.29	0.67
1:C:320:ILE:CD1	1:C:371:PRO:HD2	2.23	0.67
1:A:122:LYS:HZ3	1:A:122:LYS:HB2	1.59	0.67
1:A:27:HIS:CE1	1:A:279:PHE:HA	2.29	0.67
1:A:53:PRO:HG2	1:A:128:LYS:NZ	2.09	0.67
1:A:202:GLU:HG3	1:A:257:GLU:OE2	1.93	0.67
2:B:26:TRP:HA	2:B:26:TRP:HE3	1.59	0.67
1:C:443:ILE:HG13	1:C:444:TYR:N	2.10	0.67
1:A:178:TYR:HE2	1:A:295:LYS:NZ	1.86	0.67
1:A:443:ILE:HG13	1:A:444:TYR:N	2.10	0.67
1:A:448:PHE:HZ	1:A:456:LYS:HD3	1.58	0.67
2:B:63:ILE:HD12	2:B:63:ILE:C	2.20	0.67
1:C:87:ASP:O	1:C:89:ARG:N	2.27	0.67
1:C:311:GLU:C	1:C:312:ILE:HD13	2.19	0.67
1:C:270:ILE:CG1	1:C:271:GLN:N	2.57	0.67
1:C:340:MET:SD	1:C:345:ARG:HD2	2.35	0.67
1:C:393:LYS:HZ2	1:C:395:GLY:CA	2.07	0.67
1:C:478:SER:O	1:C:482:VAL:HG23	1.94	0.67
1:A:45:LEU:C	1:A:45:LEU:HD22	2.20	0.67
1:A:233:GLN:C	1:A:235:GLU:H	2.03	0.67
1:A:383:GLU:HB3	1:A:384:PRO:HD2	1.77	0.67
1:A:453:TRP:O	1:A:456:LYS:HB3	1.95	0.67
1:A:463:ILE:HA	1:A:466:ILE:HG22	1.77	0.67
1:C:398:ILE:O	1:C:402:ILE:HG22	1.95	0.67
1:C:463:ILE:HA	1:C:466:ILE:HG22	1.77	0.67
1:A:416:GLY:O	1:A:417:ASP:C	2.37	0.67
1:A:3:CYS:HB2	1:A:30:CYS:SG	2.35	0.66
1:A:149:HIS:O	3:E:1:NAG:H83	1.94	0.66
1:C:383:GLU:HB3	1:C:384:PRO:HD2	1.77	0.66
1:A:33:THR:O	1:A:40:THR:HB	1.94	0.66
1:C:53:PRO:HG2	1:C:128:LYS:NZ	2.09	0.66
1:C:73:ARG:O	1:C:74:CYS:CB	2.42	0.66
1:C:416:GLY:O	1:C:417:ASP:C	2.37	0.66
2:D:63:ILE:HD12	2:D:63:ILE:C	2.20	0.66
2:B:66:LEU:O	2:B:67:LEU:C	2.37	0.66
1:C:453:TRP:O	1:C:456:LYS:HB3	1.95	0.66
1:A:162:ILE:HD11	1:A:171:THR:HB	1.76	0.66
1:A:257:GLU:O	1:A:260:MET:HB3	1.96	0.66
1:A:270:ILE:CG1	1:A:271:GLN:N	2.57	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:TRP:O	1:A:392:PHE:HB3	1.95	0.66
1:A:398:ILE:O	1:A:402:ILE:HG22	1.95	0.66
1:C:33:THR:O	1:C:40:THR:HB	1.94	0.66
1:C:233:GLN:C	1:C:235:GLU:H	2.03	0.66
1:A:87:ASP:O	1:A:89:ARG:N	2.27	0.66
1:C:133:GLU:O	1:C:134:ASN:HB2	1.96	0.66
1:C:173:ALA:HB3	1:C:181:VAL:CG1	2.24	0.66
1:A:166:PRO:C	1:A:168:SER:H	2.04	0.66
1:A:294:LEU:HD23	1:A:295:LYS:N	2.11	0.66
1:C:93:LYS:O	1:C:114:VAL:HA	1.96	0.66
1:C:149:HIS:O	3:F:1:NAG:H83	1.94	0.66
1:C:220:TRP:CD1	1:C:220:TRP:C	2.74	0.66
1:A:20:TRP:HA	1:A:20:TRP:HE3	1.61	0.65
1:A:51:LYS:NZ	1:A:136:GLU:HB2	2.11	0.65
1:A:220:TRP:CD1	1:A:220:TRP:C	2.75	0.65
1:A:240:PHE:HB3	1:A:250:VAL:HG13	1.77	0.65
1:C:3:CYS:HB2	1:C:30:CYS:SG	2.35	0.65
1:C:87:ASP:C	1:C:89:ARG:H	2.04	0.65
1:C:200:GLN:CG	1:C:272:MET:HG2	2.26	0.65
2:D:26:TRP:HA	2:D:26:TRP:HE3	1.60	0.65
1:A:318:GLY:N	1:A:393:LYS:HE2	2.12	0.65
1:C:357:ILE:HG23	1:C:357:ILE:O	1.96	0.65
1:A:200:GLN:CG	1:A:272:MET:HG2	2.26	0.65
1:C:166:PRO:C	1:C:168:SER:H	2.04	0.65
1:A:357:ILE:O	1:A:357:ILE:HG23	1.96	0.65
1:C:240:PHE:HB3	1:C:250:VAL:HG13	1.77	0.65
1:A:57:ARG:HH21	1:A:57:ARG:HG3	1.62	0.65
1:A:101:TRP:NE1	1:C:310:LYS:HZ3	1.95	0.65
1:A:434:LYS:O	1:A:436:LEU:N	2.28	0.65
1:C:57:ARG:HG3	1:C:57:ARG:HH21	1.62	0.65
1:A:173:ALA:HB3	1:A:181:VAL:CG1	2.24	0.65
1:A:340:MET:SD	1:A:345:ARG:HD2	2.36	0.65
1:A:427:GLY:O	1:A:428:VAL:HB	1.97	0.65
1:C:434:LYS:O	1:C:436:LEU:N	2.29	0.65
1:A:26:GLU:HB3	1:A:282:HIS:HB2	1.78	0.65
1:A:393:LYS:HZ2	1:A:395:GLY:CA	2.09	0.65
1:C:270:ILE:CD1	1:C:271:GLN:N	2.60	0.65
1:C:352:ILE:HG22	1:C:368:GLU:HB2	1.79	0.65
1:A:182:THR:OG1	1:A:288:ARG:HB3	1.97	0.65
1:A:352:ILE:HG22	1:A:368:GLU:HB2	1.79	0.65
1:C:26:GLU:HB3	1:C:282:HIS:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:PHE:O	1:A:448:PHE:CD1	2.50	0.65
1:A:133:GLU:O	1:A:134:ASN:HB2	1.95	0.64
1:A:270:ILE:CD1	1:A:271:GLN:N	2.60	0.64
1:C:170:ILE:CG2	1:C:184:GLU:HG3	2.27	0.64
1:C:463:ILE:O	1:C:466:ILE:HG22	1.97	0.64
2:D:66:LEU:O	2:D:67:LEU:C	2.38	0.64
1:A:93:LYS:O	1:A:114:VAL:HA	1.96	0.64
1:A:319:THR:H	1:A:320:ILE:HD12	1.61	0.64
1:C:294:LEU:HD23	1:C:295:LYS:N	2.11	0.64
1:C:448:PHE:CD1	1:C:448:PHE:O	2.50	0.64
1:A:141:ILE:O	1:A:159:GLY:HA3	1.98	0.64
1:A:233:GLN:HE21	1:A:233:GLN:CA	2.10	0.64
1:C:305:LYS:C	1:C:305:LYS:HD3	2.22	0.64
1:C:484:VAL:O	1:C:486:THR:N	2.30	0.64
1:A:73:ARG:O	1:A:74:CYS:CB	2.43	0.64
1:A:428:VAL:O	1:A:432:ILE:HB	1.97	0.64
1:C:390:ASN:HD22	1:C:391:TRP:H	1.44	0.64
1:A:463:ILE:O	1:A:466:ILE:HG22	1.96	0.64
1:C:188:ARG:HH21	1:C:188:ARG:HG3	1.62	0.64
1:C:428:VAL:O	1:C:429:PHE:O	2.16	0.64
1:A:9:ARG:O	1:A:10:ASP:HB3	1.97	0.64
1:A:390:ASN:HD22	1:A:391:TRP:H	1.43	0.64
1:A:428:VAL:O	1:A:429:PHE:O	2.15	0.64
1:C:257:GLU:O	1:C:260:MET:HB3	1.96	0.64
1:C:269:GLU:HG2	1:C:270:ILE:N	2.13	0.64
1:C:390:ASN:ND2	1:C:391:TRP:N	2.45	0.64
2:D:40:PRO:O	2:D:44:ILE:HG12	1.97	0.64
1:A:153:ASN:O	1:A:155:THR:N	2.31	0.64
1:A:188:ARG:HH21	1:A:188:ARG:HG3	1.62	0.64
1:A:390:ASN:ND2	1:A:391:TRP:N	2.45	0.64
2:D:1:SER:C	2:D:3:ALA:N	2.52	0.64
1:A:305:LYS:HD3	1:A:305:LYS:C	2.23	0.64
1:C:318:GLY:N	1:C:393:LYS:HE2	2.12	0.64
1:C:427:GLY:O	1:C:428:VAL:HB	1.97	0.64
1:C:448:PHE:CZ	1:C:456:LYS:HD3	2.33	0.64
1:C:391:TRP:O	1:C:392:PHE:HB3	1.96	0.64
1:C:479:LEU:O	1:C:480:VAL:C	2.40	0.64
1:A:484:VAL:O	1:A:486:THR:N	2.30	0.64
1:C:232:ILE:O	1:C:233:GLN:HG2	1.98	0.64
1:C:319:THR:H	1:C:320:ILE:HD12	1.61	0.64
2:D:3:ALA:O	2:D:4:LEU:HD13	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:THR:O	1:A:475:LEU:HD23	1.98	0.63
2:B:40:PRO:O	2:B:44:ILE:HG12	1.97	0.63
1:C:9:ARG:O	1:C:10:ASP:HB3	1.97	0.63
1:C:178:TYR:HE2	1:C:295:LYS:NZ	1.86	0.63
1:A:232:ILE:O	1:A:233:GLN:HG2	1.98	0.63
1:A:448:PHE:CZ	1:A:456:LYS:HD3	2.33	0.63
1:C:233:GLN:HE21	1:C:233:GLN:CA	2.11	0.63
1:C:336:PRO:CG	1:C:381:GLY:HA2	2.29	0.63
1:C:473:THR:O	1:C:475:LEU:HD23	1.98	0.63
1:A:87:ASP:C	1:A:89:ARG:H	2.05	0.63
1:A:393:LYS:O	1:A:394:LYS:HB2	1.98	0.63
1:C:74:CYS:C	1:C:77:GLN:HE22	2.06	0.63
1:C:182:THR:OG1	1:C:288:ARG:HB3	1.96	0.63
1:C:153:ASN:O	1:C:155:THR:N	2.31	0.63
1:A:269:GLU:HG2	1:A:270:ILE:N	2.13	0.63
1:C:141:ILE:O	1:C:159:GLY:HA3	1.98	0.63
1:C:320:ILE:HG12	1:C:371:PRO:HG2	1.81	0.63
1:C:428:VAL:O	1:C:432:ILE:HB	1.98	0.63
1:A:3:CYS:HA	1:A:6:ILE:HG13	1.79	0.63
1:A:320:ILE:HG12	1:A:371:PRO:HG2	1.81	0.63
1:A:240:PHE:HA	1:A:249:ASP:O	1.99	0.63
1:A:413:ALA:O	1:A:414:ILE:HD12	1.99	0.63
1:C:441:GLY:O	1:C:446:ALA:HB3	1.99	0.63
1:A:74:CYS:C	1:A:77:GLN:HE22	2.06	0.63
1:A:209:HIS:ND1	2:B:10:MET:HB3	2.14	0.63
2:B:54:GLY:HA2	2:D:59:GLN:OE1	1.99	0.63
1:C:3:CYS:HA	1:C:6:ILE:HG13	1.79	0.63
2:B:3:ALA:O	2:B:4:LEU:HD13	1.98	0.62
1:C:459:ILE:HA	1:C:462:ILE:HG22	1.80	0.62
1:C:240:PHE:HA	1:C:249:ASP:O	1.99	0.62
1:A:56:LEU:O	1:A:56:LEU:HG	1.98	0.62
1:A:65:LEU:HD21	1:A:252:VAL:CA	2.27	0.62
1:A:442:ALA:O	1:A:446:ALA:O	2.18	0.62
1:C:12:VAL:HG23	1:C:33:THR:OG1	1.99	0.62
1:A:479:LEU:O	1:A:480:VAL:C	2.40	0.62
1:A:53:PRO:HB3	1:A:130:VAL:CG1	2.29	0.62
1:A:305:LYS:CD	1:A:327:GLU:HB3	2.30	0.62
2:B:33:GLU:O	2:B:34:THR:C	2.41	0.62
1:C:413:ALA:O	1:C:414:ILE:HD12	1.99	0.62
1:C:51:LYS:NZ	1:C:136:GLU:HB2	2.12	0.62
1:C:200:GLN:HG3	1:C:272:MET:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:LYS:O	1:C:394:LYS:HB2	1.98	0.62
1:C:101:TRP:HB2	1:C:108:PHE:CD2	2.24	0.62
2:B:59:GLN:OE1	2:D:54:GLY:HA2	1.99	0.62
1:C:20:TRP:CG	1:C:286:ARG:NH1	2.68	0.62
1:C:53:PRO:HB3	1:C:130:VAL:CG1	2.29	0.62
1:C:209:HIS:ND1	2:D:10:MET:HB3	2.14	0.62
1:A:20:TRP:HB3	1:A:425:LEU:HD21	1.82	0.62
1:A:361:LYS:HD3	1:A:361:LYS:N	2.15	0.62
1:A:441:GLY:O	1:A:446:ALA:HB3	1.99	0.62
1:C:277:LEU:HD23	1:C:277:LEU:N	2.15	0.62
1:C:316:GLN:O	1:C:317:HIS:C	2.43	0.62
1:C:442:ALA:O	1:C:446:ALA:O	2.17	0.62
1:A:20:TRP:CG	1:A:286:ARG:NH1	2.68	0.61
1:A:490:GLY:C	1:A:492:MET:H	2.08	0.61
1:C:20:TRP:HB3	1:C:425:LEU:HD21	1.82	0.61
1:A:19:SER:HB3	1:A:289:MET:N	2.15	0.61
1:A:459:ILE:HA	1:A:462:ILE:HG22	1.80	0.61
1:C:19:SER:HB3	1:C:289:MET:N	2.15	0.61
1:C:20:TRP:HA	1:C:20:TRP:HE3	1.61	0.61
1:C:361:LYS:HD3	1:C:361:LYS:N	2.15	0.61
1:C:443:ILE:O	1:C:446:ALA:C	2.43	0.61
1:A:58:LYS:O	1:A:58:LYS:HG2	2.00	0.61
1:A:99:ARG:NH1	1:A:105:CYS:HB3	2.10	0.61
1:A:200:GLN:HG3	1:A:272:MET:HG2	1.81	0.61
1:A:336:PRO:CG	1:A:381:GLY:HA2	2.29	0.61
1:C:205:ALA:HA	1:C:206:TRP:CE3	2.36	0.61
1:A:125:MET:O	1:A:126:LYS:HB3	2.01	0.61
1:A:277:LEU:HD23	1:A:277:LEU:N	2.15	0.61
1:A:306:PHE:CB	1:A:326:TYR:HA	2.27	0.61
1:A:486:THR:O	1:A:487:LEU:C	2.43	0.61
1:C:56:LEU:O	1:C:56:LEU:HG	1.99	0.61
1:C:58:LYS:O	1:C:58:LYS:HG2	2.00	0.61
1:C:443:ILE:HG23	1:C:444:TYR:N	2.15	0.61
2:D:3:ALA:C	2:D:4:LEU:HD22	2.26	0.61
1:A:170:ILE:CG2	1:A:184:GLU:HG3	2.27	0.61
1:A:178:TYR:CE2	1:A:295:LYS:NZ	2.66	0.61
1:C:343:GLU:O	1:C:345:ARG:HD2	2.01	0.61
1:A:153:ASN:ND2	3:E:1:NAG:C7	2.64	0.61
1:A:205:ALA:HA	1:A:206:TRP:CE3	2.35	0.61
1:A:233:GLN:O	1:A:234:LYS:HB2	2.01	0.61
1:A:443:ILE:O	1:A:446:ALA:C	2.44	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:ALA:C	2:B:4:LEU:HD22	2.25	0.61
1:C:309:VAL:HB	1:C:323:ARG:HG2	1.82	0.61
1:A:99:ARG:NE	1:A:105:CYS:SG	2.74	0.61
1:A:312:ILE:HD13	1:A:312:ILE:N	2.16	0.61
1:A:378:ILE:CG1	1:A:389:LEU:HB3	2.31	0.61
1:C:378:ILE:CG1	1:C:389:LEU:HB3	2.31	0.61
1:C:312:ILE:HD13	1:C:312:ILE:N	2.16	0.61
2:D:48:ILE:C	2:D:50:ALA:N	2.57	0.61
1:A:443:ILE:HG23	1:A:444:TYR:N	2.15	0.61
1:A:12:VAL:HG23	1:A:33:THR:OG1	2.00	0.60
1:C:99:ARG:NH1	1:C:105:CYS:HB3	2.11	0.60
1:C:233:GLN:O	1:C:234:LYS:HB2	2.01	0.60
1:A:101:TRP:HB2	1:A:108:PHE:CD2	2.24	0.60
1:A:309:VAL:HB	1:A:323:ARG:HG2	1.82	0.60
1:A:483:GLY:O	1:A:484:VAL:C	2.44	0.60
1:C:197:VAL:HG21	1:C:210:ARG:HA	1.83	0.60
1:A:7:SER:O	1:A:8:ASN:C	2.43	0.60
1:A:316:GLN:O	1:A:317:HIS:C	2.43	0.60
1:C:463:ILE:CG2	1:C:482:VAL:HG22	2.24	0.60
1:C:342:LEU:H	1:C:342:LEU:HD12	1.66	0.60
1:C:486:THR:O	1:C:487:LEU:C	2.43	0.60
1:A:23:ILE:HD11	1:A:285:CYS:SG	2.42	0.60
2:B:28:HIS:O	2:B:31:ARG:HG3	2.01	0.60
1:C:490:GLY:C	1:C:492:MET:H	2.08	0.60
1:A:193:PHE:CZ	1:A:278:LEU:HD11	2.37	0.60
1:A:259:ALA:HB2	1:C:259:ALA:HB2	1.83	0.60
1:A:310:LYS:HZ3	1:C:101:TRP:NE1	1.95	0.60
1:C:153:ASN:ND2	3:F:1:NAG:C7	2.64	0.60
2:D:28:HIS:O	2:D:31:ARG:HG3	2.02	0.60
1:A:92:CYS:HA	1:A:115:THR:O	2.02	0.60
1:A:197:VAL:HG21	1:A:210:ARG:HA	1.83	0.60
2:B:48:ILE:C	2:B:50:ALA:N	2.56	0.60
2:D:33:GLU:O	2:D:34:THR:C	2.42	0.60
1:A:58:LYS:CD	1:A:221:LEU:HD23	2.32	0.60
1:A:312:ILE:HG13	1:A:391:TRP:CD1	2.37	0.60
1:A:463:ILE:CG2	1:A:482:VAL:HG22	2.24	0.60
2:B:5:VAL:N	2:B:6:PRO:HD3	2.17	0.60
1:C:23:ILE:HD11	1:C:285:CYS:SG	2.42	0.60
1:C:58:LYS:HB2	1:C:58:LYS:HZ3	1.66	0.60
1:C:99:ARG:NE	1:C:105:CYS:SG	2.74	0.60
1:A:193:PHE:O	1:A:194:ASN:C	2.45	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LEU:HD23	1:A:294:LEU:C	2.27	0.60
1:A:315:THR:HG22	1:C:108:PHE:CE1	2.37	0.60
1:C:360:GLU:O	1:C:360:GLU:HG2	2.02	0.60
1:A:270:ILE:HD13	1:A:278:LEU:HA	1.79	0.59
1:A:487:LEU:C	1:A:487:LEU:HD13	2.26	0.59
1:C:94:HIS:CA	1:C:114:VAL:HG12	2.32	0.59
1:C:125:MET:O	1:C:126:LYS:HB3	2.00	0.59
1:C:193:PHE:CZ	1:C:278:LEU:HD11	2.37	0.59
2:D:36:ILE:HD13	2:D:37:LEU:N	2.17	0.59
1:A:337:PHE:CD1	1:A:337:PHE:C	2.80	0.59
1:A:343:GLU:O	1:A:345:ARG:HD2	2.01	0.59
1:A:352:ILE:HB	1:A:368:GLU:O	2.02	0.59
1:C:92:CYS:HA	1:C:115:THR:O	2.02	0.59
1:A:108:PHE:CE1	1:C:315:THR:HG22	2.37	0.59
1:A:222:PRO:HG2	1:A:223:GLY:H	1.67	0.59
1:C:193:PHE:O	1:C:194:ASN:C	2.45	0.59
1:C:222:PRO:HG2	1:C:223:GLY:H	1.67	0.59
2:B:36:ILE:HD13	2:B:37:LEU:N	2.17	0.59
1:C:270:ILE:HD13	1:C:278:LEU:HA	1.80	0.59
1:C:337:PHE:CD1	1:C:337:PHE:C	2.80	0.59
2:D:5:VAL:N	2:D:6:PRO:HD3	2.17	0.59
1:A:12:VAL:HG23	1:A:33:THR:CB	2.32	0.59
1:A:141:ILE:H	1:A:141:ILE:HD13	1.68	0.59
1:A:200:GLN:HG2	1:A:201:MET:H	1.68	0.59
1:A:383:GLU:CB	1:A:384:PRO:CD	2.80	0.59
1:C:12:VAL:HG23	1:C:33:THR:CB	2.31	0.59
1:C:93:LYS:HB2	1:C:240:PHE:CZ	2.38	0.59
1:C:270:ILE:HD11	1:C:278:LEU:CA	2.27	0.59
1:C:305:LYS:CD	1:C:327:GLU:HB3	2.29	0.59
1:C:312:ILE:HG13	1:C:391:TRP:CD1	2.37	0.59
1:C:352:ILE:HB	1:C:368:GLU:O	2.02	0.59
1:C:457:ILE:HG22	1:C:490:GLY:HA3	1.83	0.59
1:A:101:TRP:CZ2	1:C:310:LYS:HG2	2.38	0.59
1:C:7:SER:O	1:C:8:ASN:C	2.43	0.59
1:C:60:CYS:SG	1:C:219:PRO:HG2	2.42	0.59
1:C:208:VAL:HG21	1:C:212:TRP:HZ3	1.68	0.59
1:C:312:ILE:HG13	1:C:391:TRP:NE1	2.18	0.59
1:C:448:PHE:CD1	1:C:448:PHE:C	2.80	0.59
1:C:200:GLN:HG2	1:C:201:MET:H	1.67	0.59
1:C:404:THR:HA	1:C:407:ARG:NH1	2.18	0.59
1:C:487:LEU:C	1:C:487:LEU:HD13	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:LEU:HD23	1:A:278:LEU:H	1.68	0.59
1:A:404:THR:HA	1:A:407:ARG:NH1	2.18	0.59
1:A:457:ILE:HG22	1:A:490:GLY:HA3	1.83	0.59
1:C:20:TRP:HZ3	1:C:288:ARG:NE	2.01	0.59
1:C:20:TRP:CZ3	1:C:288:ARG:NE	2.70	0.59
1:C:260:MET:HA	2:D:2:VAL:HB	1.84	0.59
1:C:383:GLU:CB	1:C:384:PRO:CD	2.80	0.59
1:C:492:MET:HA	1:C:492:MET:CE	2.22	0.59
1:A:87:ASP:C	1:A:89:ARG:N	2.61	0.59
1:A:93:LYS:HB2	1:A:240:PHE:CZ	2.38	0.59
1:A:121:CYS:HG	1:A:231:TRP:HZ2	1.50	0.59
1:A:133:GLU:O	1:A:134:ASN:CB	2.51	0.58
1:A:260:MET:HA	2:B:2:VAL:HB	1.84	0.58
1:A:310:LYS:HG2	1:C:101:TRP:CZ2	2.37	0.58
1:A:312:ILE:HG13	1:A:391:TRP:NE1	2.18	0.58
1:A:327:GLU:HG2	1:A:328:GLY:N	2.18	0.58
1:C:3:CYS:O	1:C:6:ILE:HG12	2.03	0.58
1:C:393:LYS:HZ2	1:C:395:GLY:HA2	1.67	0.58
1:A:20:TRP:CZ3	1:A:288:ARG:NE	2.70	0.58
1:C:479:LEU:O	1:C:482:VAL:N	2.35	0.58
1:C:483:GLY:O	1:C:484:VAL:C	2.44	0.58
2:D:41:GLY:O	2:D:44:ILE:HB	2.03	0.58
1:A:360:GLU:O	1:A:360:GLU:HG2	2.02	0.58
1:C:1:MET:HA	1:C:1:MET:HE3	1.85	0.58
1:A:279:PHE:N	1:A:279:PHE:CD2	2.72	0.58
1:A:436:LEU:C	1:A:436:LEU:HD13	2.29	0.58
2:B:3:ALA:CB	2:B:4:LEU:HD22	2.33	0.58
2:B:32:ILE:HD12	2:B:33:GLU:N	2.19	0.58
1:C:133:GLU:O	1:C:134:ASN:CB	2.51	0.58
1:C:191:LEU:O	1:C:192:ASP:HB2	2.03	0.58
1:C:247:LYS:HA	1:C:247:LYS:HZ2	1.66	0.58
1:C:327:GLU:HG2	1:C:328:GLY:N	2.18	0.58
1:A:20:TRP:HZ3	1:A:288:ARG:NE	2.01	0.58
1:A:60:CYS:SG	1:A:219:PRO:HG2	2.44	0.58
1:A:62:GLU:HG3	1:A:122:LYS:HB3	1.85	0.58
1:A:393:LYS:HG2	1:A:394:LYS:N	2.18	0.58
1:C:34:MET:HG2	1:C:40:THR:HG21	1.84	0.58
1:C:294:LEU:HD23	1:C:294:LEU:C	2.27	0.58
1:A:270:ILE:CD1	1:A:270:ILE:C	2.77	0.58
1:C:59:TYR:HD2	1:C:218:LEU:HB2	1.68	0.58
1:C:211:GLN:O	1:C:212:TRP:C	2.47	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:THR:O	1:C:316:GLN:HB2	2.04	0.58
1:A:34:MET:HG2	1:A:40:THR:HG21	1.85	0.58
1:A:273:SER:O	1:A:274:SER:CB	2.52	0.58
1:A:448:PHE:CD1	1:A:448:PHE:C	2.81	0.58
1:C:102:GLY:C	1:C:104:GLY:N	2.60	0.58
2:B:32:ILE:HG13	2:B:33:GLU:H	1.68	0.58
1:C:273:SER:O	1:C:274:SER:CB	2.52	0.58
1:C:393:LYS:HG2	1:C:394:LYS:N	2.18	0.58
1:C:406:MET:O	1:C:409:ALA:N	2.36	0.58
2:D:3:ALA:CB	2:D:4:LEU:HD22	2.33	0.58
1:A:255:SER:O	1:A:256:GLN:HG2	2.04	0.58
1:C:141:ILE:HD13	1:C:141:ILE:H	1.68	0.58
2:D:32:ILE:HD12	2:D:33:GLU:N	2.19	0.58
2:D:32:ILE:HG13	2:D:33:GLU:H	1.68	0.58
2:D:50:ALA:CB	2:D:63:ILE:HD11	2.34	0.58
2:D:50:ALA:HA	2:D:63:ILE:HD11	1.85	0.58
1:A:6:ILE:O	1:A:6:ILE:CG2	2.52	0.58
1:A:314:GLU:HA	1:A:319:THR:HB	1.85	0.58
2:B:38:ARG:HA	2:B:38:ARG:HE	1.69	0.58
2:B:38:ARG:HA	2:B:38:ARG:NE	2.18	0.58
1:C:211:GLN:O	1:C:214:LEU:N	2.33	0.58
1:C:229:SER:HA	1:C:231:TRP:NE1	2.19	0.58
1:C:278:LEU:HD23	1:C:278:LEU:H	1.68	0.58
1:C:436:LEU:C	1:C:436:LEU:HD13	2.28	0.58
1:A:208:VAL:HG12	1:A:267:ALA:HB2	1.85	0.57
1:A:211:GLN:O	1:A:212:TRP:C	2.46	0.57
1:A:342:LEU:H	1:A:342:LEU:HD12	1.67	0.57
1:A:406:MET:O	1:A:409:ALA:N	2.37	0.57
1:C:178:TYR:CE2	1:C:295:LYS:NZ	2.66	0.57
1:C:448:PHE:O	1:C:448:PHE:CG	2.57	0.57
1:A:140:VAL:HG23	1:A:140:VAL:O	2.03	0.57
1:A:208:VAL:HG21	1:A:212:TRP:HZ3	1.69	0.57
1:A:309:VAL:O	1:A:310:LYS:CB	2.50	0.57
1:A:314:GLU:O	1:A:315:THR:C	2.47	0.57
1:A:409:ALA:O	1:A:412:MET:HB3	2.04	0.57
1:C:62:GLU:HG3	1:C:122:LYS:HB3	1.85	0.57
1:C:314:GLU:HA	1:C:319:THR:HB	1.85	0.57
1:C:490:GLY:O	1:C:492:MET:N	2.37	0.57
2:D:38:ARG:HA	2:D:38:ARG:HE	1.69	0.57
1:A:1:MET:HE3	1:A:1:MET:HA	1.86	0.57
1:A:383:GLU:HG2	1:A:384:PRO:HD3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:LEU:O	1:A:482:VAL:N	2.35	0.57
2:B:41:GLY:O	2:B:44:ILE:HB	2.04	0.57
1:C:87:ASP:C	1:C:89:ARG:N	2.61	0.57
1:C:166:PRO:HB3	1:C:187:PRO:O	2.05	0.57
2:D:44:ILE:HG22	2:D:48:ILE:HD11	1.86	0.57
1:A:102:GLY:C	1:A:104:GLY:N	2.60	0.57
1:A:270:ILE:HD11	1:A:278:LEU:CA	2.28	0.57
1:C:409:ALA:O	1:C:412:MET:HB3	2.04	0.57
2:D:38:ARG:HA	2:D:38:ARG:NE	2.18	0.57
1:A:166:PRO:HB3	1:A:187:PRO:O	2.04	0.57
1:A:199:LEU:HG	1:A:199:LEU:O	2.03	0.57
1:A:244:HIS:HD2	2:D:16:THR:HG21	1.70	0.57
2:B:50:ALA:HA	2:B:63:ILE:HD11	1.85	0.57
1:C:199:LEU:O	1:C:199:LEU:HG	2.04	0.57
1:C:407:ARG:HB3	1:C:407:ARG:CZ	2.35	0.57
1:A:3:CYS:O	1:A:6:ILE:HG12	2.04	0.57
1:A:229:SER:HA	1:A:231:TRP:NE1	2.19	0.57
1:A:315:THR:O	1:A:316:GLN:HB2	2.04	0.57
2:B:16:THR:HG21	1:C:244:HIS:HD2	1.70	0.57
1:C:140:VAL:O	1:C:140:VAL:HG23	2.03	0.57
1:C:273:SER:O	1:C:274:SER:HB3	2.03	0.57
1:A:59:TYR:HD2	1:A:218:LEU:HB2	1.68	0.57
1:A:84:GLU:HB3	1:A:90:PHE:CE1	2.40	0.57
1:C:122:LYS:O	1:C:123:LYS:HB2	2.04	0.57
1:C:255:SER:O	1:C:256:GLN:HG2	2.05	0.57
1:C:319:THR:O	1:C:321:VAL:HG22	2.05	0.57
1:C:383:GLU:HG2	1:C:384:PRO:HD3	1.86	0.57
1:A:126:LYS:HG2	1:A:127:GLY:O	2.05	0.57
1:A:490:GLY:C	1:A:492:MET:N	2.63	0.57
2:B:44:ILE:HG22	2:B:48:ILE:HD11	1.86	0.57
1:C:340:MET:SD	1:C:345:ARG:CD	2.93	0.57
1:C:473:THR:C	1:C:475:LEU:HD23	2.30	0.57
1:A:299:TYR:N	1:A:299:TYR:CD1	2.71	0.57
1:A:406:MET:O	1:A:407:ARG:C	2.48	0.57
1:C:202:GLU:O	1:C:203:ASN:CB	2.53	0.57
1:A:90:PHE:CE2	1:A:118:MET:HE3	2.32	0.57
1:A:191:LEU:O	1:A:192:ASP:HB2	2.04	0.57
1:A:211:GLN:O	1:A:214:LEU:N	2.33	0.57
1:A:215:ASP:O	1:A:216:LEU:C	2.48	0.57
1:C:58:LYS:CD	1:C:221:LEU:HD23	2.32	0.57
1:C:65:LEU:HD21	1:C:252:VAL:CA	2.27	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLY:HA3	1:A:366:ASN:OD1	2.05	0.56
1:A:339:ILE:O	1:A:339:ILE:HG22	2.04	0.56
1:A:340:MET:SD	1:A:345:ARG:CD	2.93	0.56
1:A:390:ASN:HD22	1:A:390:ASN:C	2.12	0.56
1:A:475:LEU:O	1:A:478:SER:N	2.38	0.56
1:C:165:THR:C	1:C:167:GLN:H	2.12	0.56
1:C:200:GLN:CB	1:C:272:MET:HE3	2.35	0.56
1:C:270:ILE:CD1	1:C:270:ILE:C	2.77	0.56
1:C:340:MET:HG2	1:C:341:ASP:N	2.19	0.56
1:A:56:LEU:O	1:A:57:ARG:CB	2.50	0.56
1:A:201:MET:HB3	1:A:206:TRP:CZ3	2.37	0.56
1:A:448:PHE:O	1:A:448:PHE:CG	2.57	0.56
2:B:1:SER:C	2:B:3:ALA:N	2.52	0.56
1:C:279:PHE:CD2	1:C:279:PHE:N	2.72	0.56
1:C:309:VAL:O	1:C:310:LYS:CB	2.50	0.56
1:A:192:ASP:O	1:A:195:GLU:HB2	2.05	0.56
1:A:273:SER:O	1:A:274:SER:HB3	2.03	0.56
1:A:475:LEU:HG	1:A:476:SER:N	2.21	0.56
1:C:126:LYS:HG2	1:C:127:GLY:O	2.04	0.56
1:C:208:VAL:HG12	1:C:267:ALA:HB2	1.86	0.56
1:C:465:TRP:C	1:C:467:GLY:N	2.59	0.56
1:C:490:GLY:C	1:C:492:MET:N	2.62	0.56
1:A:72:SER:HA	1:A:113:ILE:HA	1.87	0.56
1:A:340:MET:HG2	1:A:341:ASP:N	2.19	0.56
1:A:378:ILE:O	1:A:378:ILE:HG13	2.04	0.56
1:C:203:ASN:O	1:C:204:LYS:HG2	2.06	0.56
1:C:299:TYR:N	1:C:299:TYR:CD1	2.71	0.56
1:C:339:ILE:HG22	1:C:339:ILE:O	2.04	0.56
1:C:378:ILE:HD11	1:C:389:LEU:HB3	1.88	0.56
1:C:378:ILE:HG13	1:C:378:ILE:O	2.05	0.56
1:A:122:LYS:O	1:A:123:LYS:HB2	2.04	0.56
1:C:406:MET:O	1:C:407:ARG:C	2.48	0.56
1:C:475:LEU:O	1:C:478:SER:N	2.38	0.56
1:A:240:PHE:HB3	1:A:250:VAL:CG1	2.36	0.56
1:C:80:PRO:HG3	1:C:113:ILE:N	2.20	0.56
1:C:84:GLU:HB3	1:C:90:PHE:CE1	2.41	0.56
1:C:215:ASP:O	1:C:216:LEU:C	2.48	0.56
1:C:443:ILE:HG23	1:C:444:TYR:H	1.71	0.56
1:A:178:TYR:CD2	1:A:178:TYR:N	2.73	0.56
1:A:200:GLN:CB	1:A:272:MET:HE3	2.35	0.56
1:A:473:THR:C	1:A:475:LEU:HD23	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:GLY:O	1:A:492:MET:N	2.38	0.56
2:B:50:ALA:CB	2:B:63:ILE:HD11	2.35	0.56
1:C:60:CYS:SG	1:C:219:PRO:CG	2.94	0.56
1:C:121:CYS:HG	1:C:231:TRP:HZ2	1.51	0.56
1:C:475:LEU:HG	1:C:476:SER:N	2.20	0.56
1:A:39:PRO:HD3	1:A:294:LEU:CA	2.35	0.56
1:A:58:LYS:HB2	1:A:58:LYS:HZ3	1.71	0.56
1:A:80:PRO:HG3	1:A:113:ILE:N	2.20	0.56
1:A:122:LYS:HA	1:A:122:LYS:HZ2	1.71	0.56
1:A:319:THR:O	1:A:321:VAL:HG22	2.06	0.56
1:A:465:TRP:C	1:A:467:GLY:N	2.59	0.56
1:C:72:SER:HA	1:C:113:ILE:HA	1.87	0.56
1:C:394:LYS:C	1:C:396:SER:H	2.13	0.56
2:D:60:ARG:O	2:D:61:ALA:C	2.49	0.56
1:A:407:ARG:HB3	1:A:407:ARG:CZ	2.35	0.56
2:D:66:LEU:C	2:D:70:VAL:HG23	2.31	0.56
1:C:74:CYS:SG	1:C:75:PRO:CD	2.95	0.55
1:C:367:ILE:HD12	1:C:367:ILE:H	1.70	0.55
1:C:400:GLN:HE21	1:C:400:GLN:HA	1.71	0.55
2:D:62:LEU:HD13	2:D:66:LEU:HD13	1.87	0.55
1:A:24:VAL:C	1:A:25:LEU:HD23	2.31	0.55
1:A:378:ILE:HD11	1:A:389:LEU:HB3	1.87	0.55
1:C:39:PRO:HD3	1:C:294:LEU:CA	2.35	0.55
1:C:340:MET:HA	1:C:347:VAL:HA	1.88	0.55
1:A:74:CYS:SG	1:A:75:PRO:CD	2.93	0.55
1:A:165:THR:C	1:A:167:GLN:H	2.12	0.55
1:A:203:ASN:O	1:A:204:LYS:HG2	2.06	0.55
1:A:394:LYS:C	1:A:396:SER:H	2.13	0.55
1:A:443:ILE:HG23	1:A:444:TYR:H	1.71	0.55
2:B:62:LEU:HD13	2:B:66:LEU:HD13	1.87	0.55
1:A:94:HIS:CA	1:A:114:VAL:HG12	2.32	0.55
2:B:49:LEU:CD1	1:C:459:ILE:HD12	2.37	0.55
1:C:192:ASP:O	1:C:195:GLU:HB2	2.05	0.55
1:C:260:MET:HA	2:D:2:VAL:CG1	2.37	0.55
1:C:350:ARG:HB2	1:C:350:ARG:CZ	2.37	0.55
2:D:32:ILE:O	2:D:36:ILE:HG22	2.07	0.55
1:A:202:GLU:O	1:A:203:ASN:CB	2.53	0.55
2:B:51:TYR:CA	2:B:60:ARG:HD3	2.12	0.55
1:C:135:LEU:HD21	1:C:193:PHE:CE1	2.36	0.55
1:C:178:TYR:CD2	1:C:178:TYR:N	2.73	0.55
1:C:233:GLN:O	1:C:234:LYS:CB	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:LEU:O	1:A:238:VAL:C	2.50	0.55
1:A:383:GLU:CG	1:A:384:PRO:HD3	2.37	0.55
1:C:24:VAL:C	1:C:25:LEU:HD23	2.32	0.55
1:A:37:ASN:O	1:A:38:LYS:HB2	2.07	0.55
1:A:350:ARG:CZ	1:A:350:ARG:HB2	2.37	0.55
1:C:306:PHE:CZ	1:C:381:GLY:HA3	2.31	0.55
1:A:264:LEU:C	1:A:264:LEU:HD12	2.31	0.55
1:A:400:GLN:HA	1:A:400:GLN:HE21	1.71	0.55
1:A:459:ILE:HD12	2:D:49:LEU:CD1	2.37	0.55
1:C:212:TRP:CD2	2:D:7:HIS:HB2	2.42	0.55
1:A:212:TRP:CD2	2:B:7:HIS:HB2	2.42	0.55
1:A:367:ILE:HD12	1:A:367:ILE:H	1.68	0.55
1:A:470:SER:CB	1:A:475:LEU:HB3	2.37	0.55
2:B:66:LEU:C	2:B:70:VAL:HG23	2.31	0.55
1:C:240:PHE:HB3	1:C:250:VAL:CG1	2.36	0.55
1:A:260:MET:HA	2:B:2:VAL:CG1	2.37	0.54
1:A:475:LEU:O	1:A:476:SER:C	2.49	0.54
1:C:37:ASN:O	1:C:38:LYS:HB2	2.07	0.54
1:C:74:CYS:O	1:C:77:GLN:NE2	2.40	0.54
1:C:146:GLY:HA3	1:C:366:ASN:OD1	2.06	0.54
1:C:264:LEU:C	1:C:264:LEU:HD12	2.32	0.54
1:A:232:ILE:O	1:A:233:GLN:CB	2.55	0.54
1:A:340:MET:HA	1:A:347:VAL:HA	1.88	0.54
1:A:453:TRP:CG	1:A:454:ILE:N	2.76	0.54
2:B:60:ARG:O	2:B:61:ALA:C	2.49	0.54
1:C:20:TRP:CB	1:C:425:LEU:HD21	2.37	0.54
1:C:237:LEU:O	1:C:238:VAL:C	2.50	0.54
1:C:301:MET:HA	1:C:334:LYS:HB2	1.89	0.54
1:A:311:GLU:HG2	1:A:312:ILE:N	2.14	0.54
1:C:232:ILE:O	1:C:233:GLN:CB	2.54	0.54
1:C:464:THR:CA	1:C:482:VAL:HG21	2.30	0.54
1:A:74:CYS:O	1:A:77:GLN:NE2	2.40	0.54
1:A:80:PRO:HG2	1:A:114:VAL:HG13	1.89	0.54
1:A:301:MET:HA	1:A:334:LYS:HB2	1.89	0.54
1:A:311:GLU:HB2	1:A:312:ILE:HD13	1.90	0.54
2:B:32:ILE:O	2:B:36:ILE:HG22	2.07	0.54
1:C:97:VAL:HG23	1:C:113:ILE:HG21	1.89	0.54
1:C:165:THR:C	1:C:167:GLN:N	2.64	0.54
1:C:247:LYS:HA	1:C:247:LYS:HZ3	1.71	0.54
1:A:60:CYS:SG	1:A:219:PRO:CG	2.96	0.54
1:A:373:PHE:CD1	1:A:374:GLY:N	2.76	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:LEU:O	1:C:57:ARG:CB	2.49	0.54
1:C:475:LEU:O	1:C:476:SER:C	2.49	0.54
1:A:233:GLN:O	1:A:234:LYS:CB	2.55	0.54
1:A:306:PHE:CZ	1:A:381:GLY:HA3	2.32	0.54
1:A:484:VAL:O	1:A:485:VAL:C	2.51	0.54
1:A:20:TRP:CB	1:A:425:LEU:HD21	2.37	0.54
1:A:34:MET:HA	1:A:40:THR:CG2	2.38	0.54
1:C:314:GLU:O	1:C:315:THR:C	2.47	0.54
1:C:373:PHE:CD1	1:C:374:GLY:N	2.76	0.54
1:A:75:PRO:HA	1:A:110:LYS:O	2.08	0.54
1:A:108:PHE:HE2	1:C:321:VAL:HG21	1.73	0.54
1:A:143:PRO:HB3	1:A:178:TYR:HE1	1.73	0.54
2:B:4:LEU:HB3	2:D:31:ARG:NH2	2.13	0.54
1:C:20:TRP:CD1	1:C:286:ARG:NH1	2.76	0.54
1:C:75:PRO:HA	1:C:110:LYS:O	2.08	0.54
1:C:306:PHE:CB	1:C:326:TYR:HA	2.27	0.54
1:A:97:VAL:HG23	1:A:113:ILE:HG21	1.89	0.54
1:A:135:LEU:HD21	1:A:193:PHE:CE1	2.36	0.54
1:C:80:PRO:HG2	1:C:114:VAL:HG13	1.90	0.54
1:C:201:MET:HB3	1:C:206:TRP:CZ3	2.37	0.54
1:C:206:TRP:CD1	1:C:264:LEU:HD11	2.43	0.54
1:C:229:SER:O	1:C:231:TRP:HD1	1.91	0.54
1:C:340:MET:CE	1:C:345:ARG:HG3	2.38	0.54
1:C:383:GLU:CG	1:C:384:PRO:HD3	2.37	0.54
1:A:229:SER:O	1:A:231:TRP:HD1	1.91	0.54
1:C:122:LYS:HA	1:C:122:LYS:HZ2	1.73	0.54
1:C:279:PHE:N	1:C:279:PHE:HD2	2.06	0.54
1:C:341:ASP:O	1:C:342:LEU:C	2.51	0.54
1:C:484:VAL:HA	1:C:488:TYR:CB	2.35	0.54
1:A:311:GLU:CG	1:A:312:ILE:H	2.10	0.53
1:C:90:PHE:CE2	1:C:118:MET:HE3	2.32	0.53
1:C:454:ILE:HD13	1:C:454:ILE:C	2.34	0.53
2:D:5:VAL:N	2:D:6:PRO:CD	2.71	0.53
1:A:62:GLU:O	1:A:122:LYS:HB3	2.09	0.53
1:A:283:LEU:C	1:A:283:LEU:CD1	2.81	0.53
1:A:484:VAL:HA	1:A:488:TYR:CB	2.35	0.53
1:C:311:GLU:HB2	1:C:312:ILE:HD13	1.90	0.53
1:C:453:TRP:CG	1:C:454:ILE:N	2.76	0.53
1:A:20:TRP:CD1	1:A:286:ARG:NH1	2.76	0.53
1:A:393:LYS:HZ2	1:A:395:GLY:HA2	1.71	0.53
1:C:216:LEU:O	1:C:217:PRO:O	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:ILE:O	2:B:50:ALA:N	2.42	0.53
1:C:51:LYS:HZ2	1:C:136:GLU:CB	2.19	0.53
1:C:62:GLU:O	1:C:122:LYS:HB3	2.09	0.53
1:C:234:LYS:O	1:C:238:VAL:HG12	2.08	0.53
1:A:165:THR:C	1:A:167:GLN:N	2.64	0.53
1:A:327:GLU:CG	1:A:328:GLY:H	2.21	0.53
1:A:383:GLU:C	1:A:385:GLY:H	2.16	0.53
1:A:454:ILE:HD13	1:A:454:ILE:C	2.34	0.53
1:C:208:VAL:HG12	1:C:267:ALA:CB	2.39	0.53
1:C:284:LYS:O	1:C:285:CYS:HB3	2.07	0.53
1:C:335:ILE:HB	1:C:356:PRO:CG	2.39	0.53
2:D:32:ILE:CG1	2:D:33:GLU:N	2.72	0.53
1:A:27:HIS:H	1:A:45:LEU:HD11	1.74	0.53
1:A:340:MET:CE	1:A:345:ARG:HG3	2.39	0.53
1:A:482:VAL:O	1:A:483:GLY:O	2.27	0.53
1:C:283:LEU:C	1:C:283:LEU:CD1	2.81	0.53
1:A:108:PHE:CE2	1:C:313:ALA:HB3	2.44	0.53
1:A:206:TRP:CD1	1:A:264:LEU:HD11	2.43	0.53
1:A:390:ASN:ND2	1:A:390:ASN:C	2.66	0.53
2:B:5:VAL:N	2:B:6:PRO:CD	2.71	0.53
2:B:48:ILE:O	2:B:49:LEU:C	2.52	0.53
1:C:153:ASN:HA	3:F:1:NAG:O7	2.09	0.53
1:A:45:LEU:HD22	1:A:45:LEU:O	2.09	0.53
1:A:205:ALA:C	1:A:206:TRP:CD2	2.87	0.53
1:A:205:ALA:HB3	1:A:270:ILE:HG23	1.91	0.53
1:A:335:ILE:HB	1:A:356:PRO:CG	2.39	0.53
1:A:341:ASP:O	1:A:342:LEU:C	2.51	0.53
1:C:143:PRO:HB3	1:C:178:TYR:HE1	1.73	0.53
1:C:200:GLN:HG2	1:C:201:MET:N	2.24	0.53
1:C:390:ASN:ND2	1:C:390:ASN:C	2.66	0.53
1:C:482:VAL:O	1:C:483:GLY:O	2.27	0.53
2:D:48:ILE:O	2:D:50:ALA:N	2.42	0.53
1:A:208:VAL:HG12	1:A:267:ALA:CB	2.39	0.52
2:B:6:PRO:O	2:B:7:HIS:C	2.52	0.52
1:C:91:VAL:O	1:C:116:CYS:HA	2.09	0.52
1:C:205:ALA:C	1:C:206:TRP:CD2	2.87	0.52
1:C:484:VAL:O	1:C:485:VAL:C	2.51	0.52
2:D:6:PRO:O	2:D:7:HIS:C	2.52	0.52
1:A:20:TRP:CE3	1:A:20:TRP:CA	2.92	0.52
1:A:91:VAL:O	1:A:116:CYS:HA	2.09	0.52
1:A:234:LYS:O	1:A:238:VAL:HG12	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:LYS:O	1:A:285:CYS:HB3	2.08	0.52
1:C:20:TRP:CE3	1:C:20:TRP:CA	2.92	0.52
1:C:97:VAL:HG13	1:C:246:LYS:HA	1.91	0.52
1:C:240:PHE:CA	1:C:249:ASP:O	2.58	0.52
1:C:417:ASP:O	1:C:419:ALA:N	2.42	0.52
1:C:427:GLY:N	1:C:431:SER:OG	2.42	0.52
1:C:432:ILE:HD13	1:C:435:ALA:HB3	1.91	0.52
1:A:313:ALA:HB3	1:C:108:PHE:CE2	2.43	0.52
1:A:432:ILE:HD13	1:A:435:ALA:HB3	1.92	0.52
1:C:241:LYS:HD2	1:C:241:LYS:O	2.09	0.52
1:A:128:LYS:HB3	1:A:198:LEU:HB3	1.92	0.52
1:A:153:ASN:HA	3:E:1:NAG:O7	2.10	0.52
1:A:221:LEU:HD22	1:A:231:TRP:CZ2	2.45	0.52
2:B:31:ARG:NH2	2:D:4:LEU:HB3	2.13	0.52
1:C:43:PHE:CE2	1:C:141:ILE:HG21	2.45	0.52
1:C:205:ALA:HB3	1:C:270:ILE:HG23	1.91	0.52
1:A:242:ASN:HB2	1:A:248:GLN:HG2	1.90	0.52
1:A:257:GLU:OE1	1:A:257:GLU:HA	2.10	0.52
1:A:417:ASP:O	1:A:419:ALA:N	2.42	0.52
1:C:307:LYS:HG2	1:C:308:VAL:N	2.24	0.52
1:C:383:GLU:C	1:C:385:GLY:H	2.16	0.52
1:A:270:ILE:HG23	1:A:271:GLN:N	2.24	0.52
1:A:335:ILE:HB	1:A:356:PRO:HG2	1.92	0.52
1:A:427:GLY:N	1:A:431:SER:OG	2.42	0.52
1:A:478:SER:O	1:A:481:LEU:HB3	2.10	0.52
1:C:128:LYS:HB3	1:C:198:LEU:HB3	1.92	0.52
1:A:9:ARG:CG	1:A:10:ASP:N	2.73	0.52
1:A:43:PHE:CE2	1:A:141:ILE:HG21	2.44	0.52
1:A:279:PHE:N	1:A:279:PHE:HD2	2.06	0.52
1:C:141:ILE:O	1:C:141:ILE:HD13	2.09	0.52
1:C:221:LEU:HD22	1:C:231:TRP:CZ2	2.45	0.52
1:C:327:GLU:CG	1:C:328:GLY:H	2.20	0.52
1:C:360:GLU:C	1:C:362:ASP:N	2.68	0.52
1:C:242:ASN:HB2	1:C:248:GLN:HG2	1.90	0.52
2:D:31:ARG:O	2:D:32:ILE:C	2.50	0.52
1:A:20:TRP:HD1	1:A:425:LEU:HD11	1.75	0.52
1:A:240:PHE:CA	1:A:249:ASP:O	2.58	0.52
2:B:1:SER:OG	2:B:2:VAL:N	2.43	0.52
1:C:19:SER:HB3	1:C:289:MET:H	1.75	0.52
1:C:237:LEU:O	1:C:238:VAL:O	2.28	0.52
1:C:270:ILE:HG23	1:C:271:GLN:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ILE:O	1:A:141:ILE:HD13	2.10	0.52
1:A:193:PHE:C	1:A:195:GLU:N	2.66	0.52
1:A:216:LEU:O	1:A:217:PRO:O	2.27	0.52
1:A:241:LYS:HD2	1:A:241:LYS:O	2.10	0.52
1:A:321:VAL:HG21	1:C:108:PHE:HE2	1.74	0.52
1:C:27:HIS:H	1:C:45:LEU:HD11	1.74	0.52
1:C:45:LEU:HD22	1:C:45:LEU:O	2.09	0.52
1:C:260:MET:O	1:C:261:HIS:C	2.53	0.52
2:D:48:ILE:O	2:D:49:LEU:C	2.52	0.52
1:A:19:SER:HB3	1:A:289:MET:H	1.74	0.51
1:A:97:VAL:HG13	1:A:246:LYS:HA	1.91	0.51
1:A:310:LYS:HZ2	1:C:101:TRP:NE1	2.08	0.51
1:C:257:GLU:HA	1:C:257:GLU:OE1	2.09	0.51
1:C:459:ILE:HA	1:C:462:ILE:CG2	2.40	0.51
1:C:482:VAL:C	1:C:483:GLY:O	2.53	0.51
1:A:457:ILE:C	1:A:457:ILE:CD1	2.82	0.51
2:D:50:ALA:O	2:D:51:TYR:C	2.53	0.51
1:A:434:LYS:O	1:A:435:ALA:C	2.53	0.51
1:A:459:ILE:HA	1:A:462:ILE:CG2	2.39	0.51
1:C:416:GLY:O	1:C:418:THR:N	2.44	0.51
1:C:481:LEU:O	1:C:481:LEU:HD13	2.11	0.51
2:D:32:ILE:HG13	2:D:33:GLU:N	2.26	0.51
1:A:88:LYS:HG2	1:A:88:LYS:O	2.11	0.51
1:A:102:GLY:O	1:A:104:GLY:N	2.43	0.51
1:A:200:GLN:HG2	1:A:201:MET:N	2.24	0.51
1:A:260:MET:O	1:A:261:HIS:C	2.53	0.51
1:A:277:LEU:HD12	1:A:279:PHE:HE2	1.76	0.51
1:A:416:GLY:O	1:A:418:THR:N	2.44	0.51
2:B:32:ILE:CG1	2:B:33:GLU:N	2.72	0.51
1:C:277:LEU:HD12	1:C:279:PHE:HE2	1.75	0.51
1:A:202:GLU:O	1:A:203:ASN:HB3	2.10	0.51
1:A:378:ILE:HG13	1:A:389:LEU:HB3	1.92	0.51
2:B:32:ILE:HG13	2:B:33:GLU:N	2.26	0.51
1:C:20:TRP:HD1	1:C:425:LEU:HD11	1.75	0.51
1:C:302:CYS:SG	1:C:333:CYS:CB	2.99	0.51
1:A:237:LEU:O	1:A:238:VAL:O	2.29	0.51
1:A:340:MET:HG2	1:A:341:ASP:H	1.76	0.51
1:A:484:VAL:HG12	1:A:485:VAL:H	1.75	0.51
2:B:19:TRP:O	2:B:20:MET:SD	2.69	0.51
2:B:29:ALA:O	2:B:32:ILE:HG13	2.11	0.51
2:B:31:ARG:O	2:B:32:ILE:C	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:ARG:CG	1:C:10:ASP:N	2.73	0.51
1:C:102:GLY:O	1:C:104:GLY:N	2.43	0.51
1:C:335:ILE:HB	1:C:356:PRO:HG2	1.92	0.51
1:C:443:ILE:O	1:C:444:TYR:C	2.54	0.51
1:C:479:LEU:HD23	1:C:479:LEU:C	2.35	0.51
1:A:201:MET:SD	1:A:260:MET:HE3	2.51	0.51
1:A:471:ARG:O	1:A:472:SER:HB2	2.11	0.51
1:C:205:ALA:C	1:C:270:ILE:HG22	2.36	0.51
1:C:378:ILE:HG13	1:C:389:LEU:HB3	1.92	0.51
1:C:470:SER:CB	1:C:475:LEU:HB3	2.37	0.51
1:C:484:VAL:HG12	1:C:485:VAL:H	1.75	0.51
1:A:302:CYS:SG	1:A:333:CYS:CB	2.98	0.51
1:A:404:THR:O	1:A:405:THR:C	2.53	0.51
1:A:440:PHE:C	1:A:443:ILE:HG22	2.36	0.51
1:A:464:THR:CA	1:A:482:VAL:HG21	2.30	0.51
1:C:356:PRO:O	1:C:357:ILE:CB	2.59	0.51
1:C:434:LYS:O	1:C:435:ALA:C	2.54	0.51
1:A:238:VAL:O	1:A:238:VAL:HG13	2.11	0.51
1:A:270:ILE:HG12	1:A:278:LEU:HB3	1.93	0.51
1:A:356:PRO:C	1:A:357:ILE:HG22	2.36	0.51
1:C:323:ARG:HD2	1:C:364:PRO:O	2.11	0.51
1:C:352:ILE:CG2	1:C:368:GLU:HB2	2.40	0.51
2:D:7:HIS:C	2:D:7:HIS:CD2	2.88	0.51
1:A:64:LYS:HB3	1:A:64:LYS:HZ2	1.76	0.51
1:A:345:ARG:CD	1:A:345:ARG:H	2.24	0.51
1:C:198:LEU:HD21	1:C:278:LEU:HD13	1.93	0.51
1:C:322:ILE:O	1:C:366:ASN:HA	2.10	0.51
1:C:356:PRO:C	1:C:357:ILE:HG22	2.36	0.51
2:D:29:ALA:O	2:D:32:ILE:HG13	2.11	0.51
1:A:19:SER:HA	1:A:289:MET:HB2	1.93	0.50
1:A:456:LYS:NZ	1:A:493:VAL:HG11	2.27	0.50
1:A:486:THR:O	1:A:488:TYR:N	2.44	0.50
1:C:1:MET:C	1:C:3:CYS:H	2.19	0.50
1:C:34:MET:HA	1:C:40:THR:CG2	2.38	0.50
1:C:193:PHE:C	1:C:195:GLU:N	2.66	0.50
1:C:270:ILE:HG12	1:C:278:LEU:HB3	1.93	0.50
1:C:339:ILE:HB	1:C:349:GLY:CA	2.39	0.50
1:C:345:ARG:CD	1:C:345:ARG:H	2.24	0.50
1:A:1:MET:C	1:A:3:CYS:H	2.19	0.50
1:A:15:VAL:HG13	1:A:35:ALA:CB	2.41	0.50
1:A:84:GLU:HB3	1:A:90:PHE:CD1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:TRP:NE1	1:C:310:LYS:HZ2	2.08	0.50
1:A:479:LEU:HD23	1:A:479:LEU:C	2.35	0.50
1:C:201:MET:SD	1:C:260:MET:HE3	2.51	0.50
1:C:232:ILE:O	1:C:233:GLN:HB2	2.11	0.50
1:C:440:PHE:C	1:C:443:ILE:HG22	2.36	0.50
1:A:76:THR:O	1:A:78:GLY:N	2.44	0.50
1:A:454:ILE:HG23	1:A:455:MET:N	2.23	0.50
1:C:19:SER:HA	1:C:289:MET:HB2	1.93	0.50
1:A:205:ALA:C	1:A:270:ILE:HG22	2.36	0.50
1:A:443:ILE:O	1:A:444:TYR:C	2.53	0.50
1:C:197:VAL:HG11	1:C:213:PHE:CD2	2.46	0.50
1:C:240:PHE:HD1	1:C:250:VAL:CG1	2.24	0.50
1:C:312:ILE:CG2	1:C:322:ILE:HG12	2.42	0.50
1:C:478:SER:O	1:C:481:LEU:HB3	2.10	0.50
2:D:19:TRP:O	2:D:20:MET:SD	2.70	0.50
1:A:232:ILE:O	1:A:233:GLN:HB2	2.12	0.50
1:A:309:VAL:O	1:A:323:ARG:HB3	2.12	0.50
1:A:322:ILE:O	1:A:366:ASN:HA	2.10	0.50
1:A:481:LEU:O	1:A:481:LEU:HD13	2.11	0.50
2:B:50:ALA:O	2:B:51:TYR:C	2.53	0.50
1:C:97:VAL:CG2	1:C:113:ILE:HG21	2.42	0.50
1:C:157:LYS:HE2	1:C:157:LYS:N	2.26	0.50
1:C:202:GLU:O	1:C:203:ASN:HB3	2.10	0.50
1:C:387:LEU:C	1:C:387:LEU:HD13	2.37	0.50
1:C:457:ILE:C	1:C:457:ILE:CD1	2.81	0.50
1:A:68:THR:HA	1:A:116:CYS:O	2.12	0.50
2:B:7:HIS:C	2:B:7:HIS:CD2	2.88	0.50
1:C:9:ARG:CG	1:C:10:ASP:H	2.24	0.50
1:C:146:GLY:O	1:C:147:GLU:CG	2.59	0.50
1:C:319:THR:N	1:C:320:ILE:HD12	2.26	0.50
1:C:340:MET:HE3	1:C:379:ILE:HG21	1.93	0.50
1:A:323:ARG:HD2	1:A:364:PRO:O	2.12	0.50
1:A:342:LEU:HD12	1:A:342:LEU:N	2.27	0.50
1:C:283:LEU:HD12	1:C:283:LEU:O	2.12	0.50
1:C:342:LEU:HD12	1:C:342:LEU:N	2.27	0.50
1:C:486:THR:O	1:C:488:TYR:N	2.44	0.50
1:A:146:GLY:O	1:A:147:GLU:CG	2.59	0.50
1:A:312:ILE:CG2	1:A:322:ILE:HG12	2.42	0.50
2:D:1:SER:OG	2:D:2:VAL:N	2.44	0.50
1:A:29:SER:O	1:A:30:CYS:SG	2.68	0.50
1:A:370:GLU:O	1:A:370:GLU:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:LEU:HD13	1:A:387:LEU:C	2.36	0.50
1:C:465:TRP:C	1:C:467:GLY:H	2.19	0.50
1:A:240:PHE:HD1	1:A:250:VAL:CG1	2.24	0.49
1:A:282:HIS:O	1:A:282:HIS:ND1	2.44	0.49
1:A:315:THR:O	1:A:316:GLN:CB	2.60	0.49
1:A:393:LYS:HG2	1:A:394:LYS:H	1.77	0.49
1:C:88:LYS:O	1:C:88:LYS:HG2	2.11	0.49
1:C:340:MET:HG2	1:C:341:ASP:H	1.75	0.49
1:A:205:ALA:CA	1:A:206:TRP:CE3	2.95	0.49
1:A:264:LEU:CD1	1:A:267:ALA:HB3	2.41	0.49
1:A:339:ILE:HB	1:A:349:GLY:CA	2.39	0.49
1:C:68:THR:HA	1:C:116:CYS:O	2.12	0.49
1:C:76:THR:O	1:C:78:GLY:N	2.44	0.49
1:C:258:GLY:O	1:C:259:ALA:C	2.55	0.49
1:C:311:GLU:HG2	1:C:312:ILE:N	2.15	0.49
1:C:356:PRO:O	1:C:357:ILE:HB	2.13	0.49
1:C:471:ARG:O	1:C:472:SER:HB2	2.11	0.49
1:C:480:VAL:O	1:C:481:LEU:C	2.55	0.49
1:A:9:ARG:CG	1:A:10:ASP:H	2.24	0.49
1:A:283:LEU:HD12	1:A:283:LEU:O	2.12	0.49
1:C:23:ILE:HD12	1:C:23:ILE:C	2.37	0.49
1:C:282:HIS:O	1:C:282:HIS:ND1	2.45	0.49
1:C:315:THR:O	1:C:316:GLN:CB	2.60	0.49
1:C:332:PRO:HB3	1:C:359:THR:HA	1.94	0.49
1:C:370:GLU:O	1:C:370:GLU:HG2	2.12	0.49
1:A:8:ASN:O	1:A:9:ARG:HB2	2.13	0.49
1:A:11:PHE:N	1:A:11:PHE:CD1	2.81	0.49
1:A:26:GLU:HB3	1:A:282:HIS:CB	2.43	0.49
1:A:121:CYS:SG	1:A:231:TRP:CZ2	3.06	0.49
1:A:264:LEU:HD11	1:A:267:ALA:HB3	1.95	0.49
1:C:84:GLU:HB3	1:C:90:PHE:CD1	2.47	0.49
1:C:263:ALA:HB2	2:D:2:VAL:O	2.13	0.49
1:A:258:GLY:O	1:A:259:ALA:C	2.55	0.49
1:A:332:PRO:HB3	1:A:359:THR:HA	1.93	0.49
1:A:352:ILE:CG2	1:A:368:GLU:HB2	2.40	0.49
1:C:11:PHE:N	1:C:11:PHE:CD1	2.80	0.49
1:C:15:VAL:HG13	1:C:35:ALA:CB	2.42	0.49
1:C:205:ALA:CA	1:C:206:TRP:CE3	2.95	0.49
1:C:404:THR:O	1:C:405:THR:C	2.54	0.49
1:A:57:ARG:NH2	1:A:214:LEU:CD2	2.76	0.49
1:A:482:VAL:C	1:A:483:GLY:O	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:SER:O	1:C:30:CYS:SG	2.68	0.49
1:C:144:HIS:HB3	1:C:353:THR:HG23	1.95	0.49
1:C:388:LYS:HB3	1:C:388:LYS:NZ	2.28	0.49
1:C:456:LYS:NZ	1:C:493:VAL:HG11	2.27	0.49
1:A:135:LEU:HD22	1:A:135:LEU:HA	1.62	0.49
1:A:157:LYS:HE2	1:A:157:LYS:N	2.26	0.49
1:A:263:ALA:HB2	2:B:2:VAL:O	2.13	0.49
1:A:340:MET:HE3	1:A:379:ILE:HG21	1.93	0.49
1:A:356:PRO:O	1:A:357:ILE:CB	2.60	0.49
1:A:458:LEU:C	1:A:458:LEU:HD13	2.38	0.49
1:A:465:TRP:C	1:A:467:GLY:H	2.19	0.49
1:C:64:LYS:HB3	1:C:64:LYS:HZ2	1.77	0.49
1:C:100:GLY:HA2	1:C:108:PHE:CB	2.42	0.49
1:C:264:LEU:CD1	1:C:267:ALA:HB3	2.42	0.49
1:A:9:ARG:O	1:A:10:ASP:CB	2.61	0.49
1:A:480:VAL:O	1:A:481:LEU:C	2.54	0.49
1:C:1:MET:HG2	1:C:150:ALA:O	2.13	0.49
1:C:35:ALA:C	1:C:37:ASN:N	2.68	0.49
1:C:58:LYS:O	1:C:59:TYR:C	2.54	0.49
1:C:121:CYS:SG	1:C:231:TRP:CZ2	3.06	0.49
1:C:458:LEU:C	1:C:458:LEU:HD13	2.38	0.49
1:A:197:VAL:HG11	1:A:213:PHE:CD2	2.48	0.49
1:A:388:LYS:NZ	1:A:388:LYS:HB3	2.28	0.49
1:A:489:LEU:C	1:A:493:VAL:HG13	2.38	0.49
1:C:26:GLU:HB3	1:C:282:HIS:CB	2.43	0.49
1:C:164:ILE:HD13	1:C:164:ILE:C	2.38	0.49
1:C:170:ILE:H	1:C:170:ILE:CD1	2.25	0.49
1:C:308:VAL:HA	1:C:324:VAL:HA	1.95	0.49
1:C:309:VAL:O	1:C:323:ARG:HB3	2.12	0.49
1:C:411:ARG:HD2	1:C:422:PHE:CD1	2.48	0.49
1:C:443:ILE:O	1:C:446:ALA:N	2.45	0.49
1:A:57:ARG:O	1:A:58:LYS:HB2	2.13	0.49
2:B:32:ILE:O	2:B:33:GLU:C	2.55	0.49
1:C:57:ARG:O	1:C:58:LYS:HB2	2.13	0.49
1:A:1:MET:HG2	1:A:150:ALA:O	2.12	0.48
1:A:307:LYS:HG2	1:A:308:VAL:N	2.24	0.48
1:A:407:ARG:HH21	1:A:407:ARG:HG2	1.78	0.48
1:C:8:ASN:O	1:C:9:ARG:HB2	2.13	0.48
1:C:74:CYS:HB2	1:C:99:ARG:NH1	2.28	0.48
1:C:125:MET:HB2	1:C:201:MET:SD	2.52	0.48
1:C:191:LEU:HB3	1:C:193:PHE:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:VAL:O	1:C:238:VAL:HG13	2.12	0.48
1:C:270:ILE:HG12	1:C:278:LEU:CB	2.43	0.48
1:C:367:ILE:N	1:C:367:ILE:CD1	2.75	0.48
1:A:411:ARG:HD2	1:A:422:PHE:CD1	2.48	0.48
1:C:160:LYS:HG3	1:C:161:GLU:H	1.78	0.48
1:C:393:LYS:NZ	1:C:395:GLY:HA2	2.28	0.48
1:C:410:LYS:O	1:C:411:ARG:C	2.56	0.48
2:D:32:ILE:O	2:D:33:GLU:C	2.55	0.48
1:A:125:MET:HB2	1:A:201:MET:SD	2.53	0.48
1:A:157:LYS:HG2	1:A:157:LYS:O	2.13	0.48
1:A:356:PRO:O	1:A:357:ILE:HB	2.13	0.48
1:A:443:ILE:O	1:A:446:ALA:N	2.45	0.48
1:C:201:MET:HE3	1:C:202:GLU:N	2.29	0.48
1:C:213:PHE:CG	1:C:213:PHE:O	2.66	0.48
1:C:264:LEU:HD11	1:C:267:ALA:HB3	1.95	0.48
1:A:74:CYS:HB2	1:A:99:ARG:NH1	2.29	0.48
1:A:100:GLY:HA2	1:A:108:PHE:CB	2.42	0.48
1:A:201:MET:HE3	1:A:202:GLU:N	2.29	0.48
1:A:482:VAL:O	1:A:483:GLY:C	2.57	0.48
1:A:160:LYS:HG3	1:A:161:GLU:H	1.78	0.48
1:A:213:PHE:O	1:A:213:PHE:CG	2.67	0.48
1:C:141:ILE:H	1:C:141:ILE:CD1	2.26	0.48
1:C:489:LEU:C	1:C:493:VAL:HG13	2.38	0.48
1:A:45:LEU:H	1:A:45:LEU:HD13	1.79	0.48
1:A:187:PRO:HG2	1:A:187:PRO:O	2.13	0.48
1:A:191:LEU:HB3	1:A:193:PHE:CE2	2.48	0.48
1:A:256:GLN:O	1:A:257:GLU:C	2.56	0.48
1:A:337:PHE:C	1:A:337:PHE:HD1	2.20	0.48
1:C:27:HIS:HE1	1:C:279:PHE:HA	1.76	0.48
1:C:196:MET:HE1	2:D:12:LEU:HD21	1.94	0.48
1:C:256:GLN:O	1:C:257:GLU:C	2.56	0.48
1:A:102:GLY:C	1:A:104:GLY:H	2.22	0.48
1:A:141:ILE:H	1:A:141:ILE:CD1	2.26	0.48
1:A:144:HIS:HB3	1:A:353:THR:HG23	1.95	0.48
1:A:164:ILE:HD13	1:A:164:ILE:C	2.38	0.48
1:A:181:VAL:CG2	1:A:287:LEU:HD11	2.43	0.48
1:A:196:MET:HE1	2:B:12:LEU:HD21	1.95	0.48
1:A:319:THR:N	1:A:320:ILE:HD12	2.26	0.48
1:A:396:SER:O	1:A:397:SER:C	2.56	0.48
1:C:311:GLU:CG	1:C:312:ILE:H	2.10	0.48
1:C:400:GLN:HA	1:C:400:GLN:NE2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:49:LEU:O	2:D:53:ILE:HG22	2.14	0.48
2:B:37:LEU:HD23	2:B:37:LEU:C	2.38	0.48
2:D:50:ALA:O	2:D:52:THR:N	2.47	0.48
1:A:23:ILE:HD12	1:A:23:ILE:C	2.38	0.48
1:A:97:VAL:CG2	1:A:113:ILE:HG21	2.42	0.48
1:A:256:GLN:HE21	1:A:256:GLN:CA	2.16	0.48
1:A:270:ILE:HG12	1:A:278:LEU:CB	2.43	0.48
1:A:402:ILE:O	1:A:403:GLU:C	2.56	0.48
1:C:122:LYS:HB2	1:C:122:LYS:NZ	2.27	0.48
1:C:373:PHE:HA	1:C:395:GLY:CA	2.44	0.48
1:A:1:MET:O	1:A:3:CYS:N	2.47	0.48
1:A:360:GLU:C	1:A:362:ASP:N	2.68	0.48
1:A:410:LYS:C	1:A:412:MET:N	2.71	0.48
1:C:88:LYS:O	1:C:234:LYS:NZ	2.47	0.48
1:C:157:LYS:HG2	1:C:157:LYS:O	2.13	0.48
1:C:396:SER:O	1:C:397:SER:C	2.56	0.48
1:A:58:LYS:O	1:A:59:TYR:C	2.54	0.47
1:A:308:VAL:HA	1:A:324:VAL:HA	1.95	0.47
1:A:350:ARG:HA	1:A:350:ARG:NE	2.29	0.47
1:C:181:VAL:CG2	1:C:287:LEU:HD11	2.43	0.47
1:C:248:GLN:NE2	1:C:248:GLN:O	2.46	0.47
1:A:102:GLY:HA3	1:C:151:VAL:O	2.13	0.47
1:A:184:GLU:O	1:A:285:CYS:HB2	2.14	0.47
1:A:400:GLN:HA	1:A:400:GLN:NE2	2.29	0.47
2:B:49:LEU:O	2:B:53:ILE:HG22	2.14	0.47
2:B:66:LEU:O	2:B:68:THR:N	2.46	0.47
1:C:1:MET:O	1:C:3:CYS:N	2.47	0.47
1:C:25:LEU:H	1:C:25:LEU:HG	1.52	0.47
1:C:356:PRO:O	1:C:357:ILE:HG22	2.14	0.47
1:C:378:ILE:CD1	1:C:389:LEU:HB3	2.44	0.47
2:D:37:LEU:HD23	2:D:37:LEU:C	2.38	0.47
1:A:245:ALA:O	1:A:246:LYS:O	2.32	0.47
1:A:252:VAL:O	1:A:253:LEU:CB	2.63	0.47
1:A:378:ILE:CD1	1:A:389:LEU:HB3	2.44	0.47
2:B:58:PHE:O	2:B:59:GLN:C	2.57	0.47
1:C:102:GLY:C	1:C:104:GLY:H	2.22	0.47
1:A:88:LYS:O	1:A:234:LYS:NZ	2.47	0.47
1:A:94:HIS:ND1	1:A:114:VAL:CG1	2.77	0.47
1:A:210:ARG:HG3	1:A:210:ARG:NH2	2.29	0.47
1:A:233:GLN:C	1:A:235:GLU:N	2.70	0.47
1:A:376:SER:C	1:A:377:TYR:HD2	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:HIS:C	1:C:146:GLY:H	2.22	0.47
1:C:187:PRO:HG2	1:C:187:PRO:O	2.13	0.47
1:C:188:ARG:O	1:C:188:ARG:HG2	2.15	0.47
1:C:242:ASN:O	1:C:243:PRO:O	2.33	0.47
1:C:350:ARG:NE	1:C:350:ARG:HA	2.29	0.47
1:C:410:LYS:C	1:C:412:MET:N	2.70	0.47
1:C:482:VAL:O	1:C:483:GLY:C	2.57	0.47
2:D:4:LEU:N	2:D:4:LEU:CD2	2.77	0.47
1:C:245:ALA:O	1:C:246:LYS:O	2.32	0.47
1:C:402:ILE:O	1:C:403:GLU:C	2.55	0.47
2:D:62:LEU:O	2:D:65:ILE:HG22	2.15	0.47
1:A:198:LEU:HD21	1:A:278:LEU:HD13	1.94	0.47
1:A:393:LYS:NZ	1:A:395:GLY:HA2	2.28	0.47
1:C:407:ARG:HG2	1:C:407:ARG:HH21	1.78	0.47
1:A:61:ILE:HD13	1:A:61:ILE:H	1.80	0.47
1:A:185:CYS:C	1:A:187:PRO:HD3	2.40	0.47
1:A:191:LEU:HD13	1:A:193:PHE:CZ	2.50	0.47
1:A:373:PHE:HA	1:A:395:GLY:CA	2.44	0.47
1:A:402:ILE:HG23	1:A:403:GLU:H	1.80	0.47
2:B:36:ILE:HD13	2:B:36:ILE:C	2.40	0.47
1:C:57:ARG:NH2	1:C:214:LEU:CD2	2.75	0.47
1:C:94:HIS:ND1	1:C:114:VAL:CG1	2.77	0.47
1:C:184:GLU:O	1:C:285:CYS:HB2	2.14	0.47
1:C:185:CYS:C	1:C:187:PRO:HD3	2.40	0.47
1:C:232:ILE:O	1:C:233:GLN:CG	2.62	0.47
1:C:233:GLN:C	1:C:235:GLU:N	2.70	0.47
1:C:326:TYR:HE2	1:C:329:ASP:O	1.98	0.47
1:C:376:SER:C	1:C:377:TYR:HD2	2.22	0.47
1:C:393:LYS:HG2	1:C:394:LYS:H	1.78	0.47
1:C:402:ILE:HG23	1:C:403:GLU:H	1.80	0.47
2:D:3:ALA:HB3	2:D:4:LEU:CD2	2.44	0.47
2:D:62:LEU:C	2:D:62:LEU:CD1	2.87	0.47
1:A:326:TYR:HE2	1:A:329:ASP:O	1.98	0.47
1:A:367:ILE:CG2	1:A:368:GLU:H	2.23	0.47
2:B:50:ALA:O	2:B:52:THR:N	2.47	0.47
1:C:162:ILE:O	1:C:162:ILE:HG12	2.14	0.47
1:C:261:HIS:O	1:C:264:LEU:N	2.48	0.47
1:C:410:LYS:O	1:C:412:MET:N	2.48	0.47
2:D:20:MET:O	2:D:21:SER:C	2.58	0.47
2:D:58:PHE:O	2:D:59:GLN:C	2.57	0.47
1:A:261:HIS:O	1:A:262:THR:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LYS:HG2	1:C:101:TRP:CE2	2.49	0.47
2:B:20:MET:O	2:B:21:SER:C	2.58	0.47
1:C:61:ILE:HD13	1:C:61:ILE:H	1.80	0.47
1:C:191:LEU:HD13	1:C:193:PHE:CZ	2.50	0.47
1:C:454:ILE:HG23	1:C:455:MET:N	2.23	0.47
1:C:494:GLN:O	1:C:495:ALA:C	2.57	0.47
1:A:151:VAL:O	1:C:102:GLY:HA3	2.14	0.47
1:A:232:ILE:O	1:A:233:GLN:CG	2.61	0.47
1:A:261:HIS:O	1:A:264:LEU:N	2.48	0.47
1:C:188:ARG:HG3	1:C:188:ARG:NH2	2.28	0.47
1:C:337:PHE:C	1:C:337:PHE:HD1	2.20	0.47
2:D:66:LEU:O	2:D:68:THR:N	2.47	0.47
1:A:360:GLU:C	1:A:362:ASP:H	2.23	0.46
1:A:399:GLY:O	1:A:402:ILE:HG23	2.15	0.46
2:B:62:LEU:O	2:B:65:ILE:HG22	2.15	0.46
1:C:32:THR:HA	1:C:41:LEU:O	2.15	0.46
1:C:124:ASN:OD1	1:C:124:ASN:C	2.58	0.46
2:D:36:ILE:HD13	2:D:36:ILE:C	2.40	0.46
1:A:27:HIS:HE1	1:A:279:PHE:HA	1.77	0.46
1:A:144:HIS:C	1:A:146:GLY:H	2.22	0.46
1:A:255:SER:OG	1:A:256:GLN:N	2.48	0.46
1:A:356:PRO:O	1:A:357:ILE:HG22	2.15	0.46
1:A:395:GLY:O	1:A:397:SER:N	2.48	0.46
1:A:410:LYS:O	1:A:411:ARG:C	2.56	0.46
1:A:485:VAL:O	1:A:489:LEU:HG	2.15	0.46
1:C:142:THR:OG1	1:C:143:PRO:HD2	2.16	0.46
1:C:354:VAL:O	1:C:355:ASN:O	2.33	0.46
1:C:393:LYS:CG	1:C:394:LYS:N	2.76	0.46
1:C:485:VAL:O	1:C:489:LEU:HG	2.15	0.46
1:A:39:PRO:O	1:A:40:THR:C	2.58	0.46
1:C:39:PRO:O	1:C:40:THR:C	2.58	0.46
1:A:115:THR:HB	1:A:248:GLN:HE22	1.80	0.46
1:C:102:GLY:O	1:C:103:ASN:C	2.59	0.46
1:C:122:LYS:NZ	1:C:122:LYS:CB	2.78	0.46
1:C:261:HIS:O	1:C:262:THR:C	2.58	0.46
1:C:360:GLU:C	1:C:362:ASP:H	2.23	0.46
1:A:15:VAL:HG23	1:A:16:SER:N	2.31	0.46
1:A:94:HIS:ND1	1:A:114:VAL:HG11	2.30	0.46
1:A:260:MET:HA	2:B:2:VAL:CB	2.46	0.46
1:A:366:ASN:N	1:A:366:ASN:OD1	2.49	0.46
1:A:461:VAL:O	1:A:462:ILE:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:GLN:O	1:A:495:ALA:C	2.57	0.46
1:C:20:TRP:O	1:C:424:SER:HB3	2.16	0.46
1:C:45:LEU:HD13	1:C:45:LEU:H	1.79	0.46
1:C:94:HIS:ND1	1:C:114:VAL:HG11	2.30	0.46
1:A:35:ALA:C	1:A:37:ASN:N	2.68	0.46
1:A:101:TRP:CE2	1:C:310:LYS:HG2	2.50	0.46
1:A:124:ASN:OD1	1:A:124:ASN:C	2.58	0.46
1:A:242:ASN:O	1:A:243:PRO:O	2.33	0.46
1:C:15:VAL:HG23	1:C:16:SER:N	2.31	0.46
2:D:62:LEU:O	2:D:66:LEU:HD13	2.16	0.46
1:A:102:GLY:O	1:A:103:ASN:C	2.59	0.46
1:A:147:GLU:HB3	1:A:148:GLU:H	1.59	0.46
1:A:162:ILE:O	1:A:162:ILE:HG12	2.14	0.46
1:A:188:ARG:HG2	1:A:188:ARG:O	2.15	0.46
2:B:63:ILE:C	2:B:63:ILE:CD1	2.87	0.46
1:A:70:THR:OG1	1:A:115:THR:HA	2.16	0.46
1:A:122:LYS:CB	1:A:122:LYS:NZ	2.79	0.46
1:A:350:ARG:HB3	1:A:370:GLU:HB3	1.98	0.46
1:A:354:VAL:O	1:A:355:ASN:O	2.33	0.46
1:C:166:PRO:CB	1:C:187:PRO:HG2	2.34	0.46
1:C:395:GLY:O	1:C:397:SER:N	2.48	0.46
1:A:313:ALA:O	1:A:314:GLU:HB3	2.16	0.46
1:A:20:TRP:O	1:A:424:SER:HB3	2.16	0.46
1:A:248:GLN:O	1:A:248:GLN:NE2	2.46	0.46
1:A:256:GLN:HA	1:A:256:GLN:NE2	2.17	0.46
1:A:313:ALA:C	1:A:314:GLU:HG3	2.41	0.46
1:A:384:PRO:HG2	1:A:386:GLN:NE2	2.27	0.46
1:C:115:THR:HB	1:C:248:GLN:HE22	1.80	0.46
1:C:210:ARG:HG3	1:C:210:ARG:NH2	2.29	0.46
1:C:252:VAL:O	1:C:253:LEU:CB	2.63	0.46
1:C:384:PRO:CG	1:C:386:GLN:HE21	2.27	0.46
1:C:461:VAL:HA	1:C:464:THR:HG22	1.97	0.46
2:D:51:TYR:CA	2:D:60:ARG:HD3	2.13	0.46
1:A:32:THR:HA	1:A:41:LEU:O	2.15	0.45
1:A:57:ARG:NH2	1:A:57:ARG:HG3	2.29	0.45
1:A:165:THR:HG22	1:A:167:GLN:H	1.81	0.45
1:A:227:GLN:O	1:A:227:GLN:CD	2.59	0.45
1:A:270:ILE:HG23	1:A:271:GLN:H	1.80	0.45
1:C:207:LEU:O	1:C:267:ALA:HB1	2.16	0.45
1:C:313:ALA:O	1:C:314:GLU:HB3	2.16	0.45
1:C:461:VAL:O	1:C:462:ILE:C	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:59:GLN:O	2:D:60:ARG:C	2.58	0.45
1:A:58:LYS:HB2	1:A:58:LYS:HZ2	1.81	0.45
1:A:142:THR:OG1	1:A:143:PRO:HD2	2.16	0.45
1:A:166:PRO:C	1:A:168:SER:N	2.74	0.45
1:A:166:PRO:CB	1:A:187:PRO:HG2	2.33	0.45
1:A:318:GLY:N	1:A:393:LYS:CE	2.78	0.45
1:A:410:LYS:O	1:A:412:MET:N	2.49	0.45
2:B:62:LEU:C	2:B:62:LEU:CD1	2.87	0.45
1:C:6:ILE:O	1:C:6:ILE:CG2	2.52	0.45
1:C:60:CYS:SG	1:C:219:PRO:HG3	2.56	0.45
1:C:399:GLY:O	1:C:402:ILE:HG23	2.16	0.45
2:D:63:ILE:C	2:D:63:ILE:CD1	2.87	0.45
2:B:3:ALA:HB3	2:B:4:LEU:CD2	2.44	0.45
2:B:4:LEU:N	2:B:4:LEU:CD2	2.77	0.45
1:C:283:LEU:HD13	1:C:284:LYS:O	2.16	0.45
1:A:1:MET:C	1:A:3:CYS:N	2.73	0.45
1:A:270:ILE:HD11	1:A:277:LEU:C	2.41	0.45
1:A:461:VAL:HA	1:A:464:THR:HG22	1.97	0.45
2:B:39:HIS:C	2:B:41:GLY:N	2.71	0.45
1:C:1:MET:C	1:C:3:CYS:N	2.73	0.45
1:C:74:CYS:C	1:C:77:GLN:NE2	2.74	0.45
1:C:100:GLY:HA2	1:C:108:PHE:HB2	1.99	0.45
1:C:260:MET:HA	2:D:2:VAL:CB	2.46	0.45
1:C:270:ILE:HD11	1:C:277:LEU:C	2.41	0.45
1:C:290:ASP:C	1:C:292:LEU:N	2.74	0.45
1:A:209:HIS:H	2:B:7:HIS:CE1	2.35	0.45
1:A:221:LEU:CG	1:A:222:PRO:CD	2.94	0.45
2:B:32:ILE:CD1	2:B:33:GLU:N	2.79	0.45
1:C:259:ALA:O	1:C:260:MET:C	2.59	0.45
1:C:351:LEU:HD23	1:C:351:LEU:HA	1.43	0.45
1:C:406:MET:O	1:C:408:GLY:N	2.49	0.45
1:A:306:PHE:CD1	1:A:306:PHE:N	2.84	0.45
1:A:489:LEU:O	1:A:493:VAL:HG13	2.16	0.45
2:B:34:THR:O	2:B:37:LEU:HD22	2.16	0.45
1:C:69:THR:HG22	1:C:70:THR:H	1.81	0.45
1:C:165:THR:O	1:C:167:GLN:N	2.50	0.45
1:C:165:THR:HG22	1:C:167:GLN:H	1.81	0.45
1:C:196:MET:HA	1:C:196:MET:CE	2.43	0.45
1:C:306:PHE:N	1:C:306:PHE:CD1	2.84	0.45
1:C:227:GLN:O	1:C:227:GLN:CD	2.60	0.45
1:C:366:ASN:N	1:C:366:ASN:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:39:HIS:C	2:D:41:GLY:N	2.71	0.45
1:A:15:VAL:HG13	1:A:35:ALA:HB1	1.99	0.45
1:A:188:ARG:HG3	1:A:188:ARG:NH2	2.28	0.45
1:A:221:LEU:HD22	1:A:231:TRP:CH2	2.51	0.45
1:A:283:LEU:HD13	1:A:284:LYS:O	2.16	0.45
1:A:320:ILE:CG1	1:A:371:PRO:HD2	2.47	0.45
1:A:377:TYR:HD1	1:A:388:LYS:HD2	1.81	0.45
2:B:62:LEU:O	2:B:66:LEU:HD13	2.16	0.45
1:C:57:ARG:NH2	1:C:57:ARG:HG3	2.29	0.45
1:C:193:PHE:O	1:C:195:GLU:N	2.50	0.45
1:A:119:PHE:O	1:A:119:PHE:CD2	2.70	0.45
1:A:196:MET:HA	1:A:196:MET:CE	2.43	0.45
1:A:259:ALA:O	1:A:260:MET:C	2.59	0.45
1:A:290:ASP:C	1:A:292:LEU:N	2.73	0.45
2:B:50:ALA:CA	2:B:63:ILE:HD11	2.46	0.45
1:C:200:GLN:N	1:C:272:MET:HE3	2.32	0.45
1:C:200:GLN:O	1:C:201:MET:HB2	2.17	0.45
1:C:221:LEU:HD22	1:C:231:TRP:CH2	2.52	0.45
1:C:270:ILE:HG23	1:C:271:GLN:H	1.81	0.45
1:C:320:ILE:CG1	1:C:371:PRO:HD2	2.47	0.45
1:C:489:LEU:O	1:C:493:VAL:HG13	2.17	0.45
2:D:34:THR:O	2:D:37:LEU:HD22	2.16	0.45
1:A:165:THR:O	1:A:167:GLN:N	2.49	0.45
1:C:9:ARG:O	1:C:10:ASP:CB	2.61	0.45
1:C:70:THR:OG1	1:C:115:THR:HA	2.16	0.45
1:A:193:PHE:O	1:A:195:GLU:N	2.50	0.44
1:A:393:LYS:CG	1:A:394:LYS:N	2.76	0.44
1:A:494:GLN:O	1:A:494:GLN:HG3	2.17	0.44
2:B:32:ILE:O	2:B:35:TRP:HB3	2.17	0.44
1:C:209:HIS:H	2:D:7:HIS:CE1	2.35	0.44
1:A:60:CYS:SG	1:A:219:PRO:HG3	2.58	0.44
2:B:59:GLN:O	2:B:60:ARG:C	2.59	0.44
1:C:62:GLU:HG3	1:C:62:GLU:O	2.17	0.44
1:C:205:ALA:O	1:C:270:ILE:HG22	2.18	0.44
1:C:350:ARG:HB3	1:C:370:GLU:HB3	1.98	0.44
1:C:377:TYR:HD1	1:C:388:LYS:HD2	1.81	0.44
1:A:69:THR:HG22	1:A:70:THR:H	1.81	0.44
1:A:99:ARG:HG2	1:A:103:ASN:OD1	2.18	0.44
1:A:170:ILE:H	1:A:170:ILE:CD1	2.25	0.44
1:A:200:GLN:N	1:A:272:MET:HE3	2.33	0.44
1:A:410:LYS:C	1:A:414:ILE:HD13	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:ARG:HG2	1:C:89:ARG:HH21	1.82	0.44
1:C:411:ARG:CD	1:C:422:PHE:CE1	3.01	0.44
1:C:493:VAL:HG23	1:C:494:GLN:N	2.33	0.44
1:A:100:GLY:HA2	1:A:108:PHE:HB2	1.99	0.44
1:A:200:GLN:O	1:A:201:MET:HB2	2.17	0.44
1:A:222:PRO:HG2	1:A:223:GLY:N	2.31	0.44
1:A:406:MET:O	1:A:408:GLY:N	2.50	0.44
1:A:481:LEU:HD13	1:A:481:LEU:C	2.43	0.44
1:A:493:VAL:HG23	1:A:494:GLN:N	2.33	0.44
2:B:6:PRO:O	2:B:8:VAL:N	2.51	0.44
1:C:119:PHE:CD2	1:C:119:PHE:O	2.70	0.44
1:C:166:PRO:C	1:C:168:SER:N	2.74	0.44
1:C:201:MET:HE2	1:C:202:GLU:HB2	1.99	0.44
1:C:355:ASN:O	1:C:355:ASN:OD1	2.36	0.44
1:C:481:LEU:HD13	1:C:481:LEU:C	2.43	0.44
1:A:20:TRP:HB3	1:A:425:LEU:CD2	2.47	0.44
1:A:56:LEU:O	1:A:56:LEU:CG	2.63	0.44
1:A:201:MET:HE2	1:A:202:GLU:HB2	1.99	0.44
1:A:229:SER:O	1:A:231:TRP:CD1	2.71	0.44
1:A:411:ARG:NE	1:A:422:PHE:CE1	2.86	0.44
1:A:420:TRP:CD1	1:A:434:LYS:HA	2.53	0.44
2:B:27:LYS:O	2:B:28:HIS:C	2.60	0.44
1:A:74:CYS:C	1:A:77:GLN:NE2	2.74	0.44
1:A:89:ARG:HH21	1:A:89:ARG:HG2	1.82	0.44
1:A:396:SER:O	1:A:398:ILE:N	2.51	0.44
1:C:75:PRO:C	1:C:77:GLN:HE21	2.25	0.44
1:C:319:THR:O	1:C:321:VAL:N	2.50	0.44
2:D:32:ILE:CD1	2:D:33:GLU:N	2.80	0.44
2:D:50:ALA:CA	2:D:63:ILE:HD11	2.46	0.44
1:A:181:VAL:HG22	1:A:287:LEU:HD11	1.99	0.44
1:A:207:LEU:O	1:A:267:ALA:HB1	2.17	0.44
1:A:411:ARG:CD	1:A:422:PHE:CE1	3.00	0.44
1:C:15:VAL:HG13	1:C:35:ALA:HB1	1.99	0.44
1:C:27:HIS:CE1	1:C:279:PHE:CA	2.99	0.44
1:C:460:GLY:O	1:C:482:VAL:HG13	2.18	0.44
2:D:39:HIS:O	2:D:40:PRO:C	2.60	0.44
1:A:140:VAL:O	1:A:140:VAL:CG2	2.66	0.44
1:C:313:ALA:C	1:C:314:GLU:HG3	2.42	0.44
1:C:420:TRP:CD1	1:C:434:LYS:HA	2.53	0.44
1:C:439:VAL:O	1:C:443:ILE:HG22	2.18	0.44
1:A:320:ILE:HD13	1:A:369:ALA:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:GLY:O	1:A:482:VAL:HG13	2.18	0.44
1:C:97:VAL:HG12	1:C:98:ASP:N	2.33	0.44
1:C:204:LYS:HE3	1:C:204:LYS:HB3	1.74	0.44
1:C:318:GLY:N	1:C:393:LYS:CE	2.79	0.44
1:C:494:GLN:O	1:C:494:GLN:HG3	2.17	0.44
1:A:46:ILE:O	1:A:47:GLU:C	2.61	0.43
1:C:181:VAL:HG22	1:C:287:LEU:HD11	1.99	0.43
1:C:221:LEU:HD12	1:C:221:LEU:HA	1.77	0.43
2:D:27:LYS:O	2:D:28:HIS:C	2.60	0.43
1:A:313:ALA:HB3	1:C:108:PHE:CZ	2.53	0.43
1:A:319:THR:O	1:A:321:VAL:N	2.51	0.43
1:A:327:GLU:CG	1:A:328:GLY:N	2.81	0.43
1:A:355:ASN:OD1	1:A:355:ASN:C	2.62	0.43
2:B:65:ILE:HD12	2:B:65:ILE:HA	1.93	0.43
1:C:106:GLY:C	1:C:107:LEU:HD23	2.44	0.43
1:C:320:ILE:HD13	1:C:369:ALA:O	2.18	0.43
1:C:468:MET:SD	1:C:468:MET:C	3.01	0.43
1:A:11:PHE:O	1:A:12:VAL:HG13	2.18	0.43
1:A:486:THR:C	1:A:488:TYR:N	2.76	0.43
1:C:51:LYS:HD3	1:C:51:LYS:N	2.33	0.43
1:A:80:PRO:HG3	1:A:113:ILE:CA	2.49	0.43
1:A:205:ALA:O	1:A:270:ILE:HG22	2.18	0.43
1:A:337:PHE:CE2	1:A:367:ILE:HG21	2.53	0.43
1:C:16:SER:HB2	1:C:425:LEU:HD23	2.01	0.43
1:C:59:TYR:CD2	1:C:218:LEU:HB2	2.52	0.43
1:C:140:VAL:O	1:C:140:VAL:CG2	2.66	0.43
1:C:317:HIS:HB3	1:C:393:LYS:HZ3	1.83	0.43
2:D:6:PRO:O	2:D:6:PRO:HG2	2.19	0.43
2:D:35:TRP:HH2	2:D:42:PHE:HD2	1.66	0.43
1:A:27:HIS:CE1	1:A:279:PHE:CA	3.00	0.43
1:A:45:LEU:C	1:A:45:LEU:CD2	2.90	0.43
1:A:51:LYS:HD3	1:A:51:LYS:N	2.33	0.43
2:B:71:ALA:C	2:B:72:PRO:O	2.61	0.43
1:C:221:LEU:CG	1:C:222:PRO:CD	2.94	0.43
1:C:222:PRO:HG2	1:C:223:GLY:N	2.31	0.43
1:C:464:THR:O	1:C:468:MET:HB2	2.18	0.43
2:D:66:LEU:O	2:D:70:VAL:HG23	2.19	0.43
1:A:108:PHE:CZ	1:C:313:ALA:HB3	2.53	0.43
1:A:355:ASN:O	1:A:355:ASN:OD1	2.35	0.43
1:A:464:THR:O	1:A:468:MET:HB2	2.19	0.43
1:A:467:GLY:O	1:A:470:SER:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:SER:O	1:C:231:TRP:CD1	2.71	0.43
1:C:247:LYS:O	1:C:248:GLN:CB	2.67	0.43
1:A:37:ASN:O	1:A:38:LYS:CB	2.66	0.43
1:A:61:ILE:CD1	1:A:123:LYS:O	2.61	0.43
1:A:97:VAL:HG12	1:A:98:ASP:N	2.33	0.43
1:A:454:ILE:CD1	1:A:455:MET:N	2.79	0.43
1:A:489:LEU:HD23	1:A:489:LEU:HA	1.79	0.43
2:B:35:TRP:HH2	2:B:42:PHE:HD2	1.66	0.43
1:C:64:LYS:HB3	1:C:64:LYS:HZ3	1.79	0.43
1:C:74:CYS:HB2	1:C:99:ARG:CZ	2.49	0.43
1:C:337:PHE:HE1	1:C:339:ILE:HG12	1.83	0.43
1:C:355:ASN:OD1	1:C:355:ASN:C	2.62	0.43
2:D:32:ILE:O	2:D:35:TRP:HB3	2.17	0.43
1:A:74:CYS:HB2	1:A:99:ARG:CZ	2.49	0.43
1:A:337:PHE:HE1	1:A:339:ILE:HG12	1.84	0.43
1:C:37:ASN:O	1:C:38:LYS:CB	2.66	0.43
1:C:396:SER:O	1:C:398:ILE:N	2.51	0.43
2:D:6:PRO:O	2:D:8:VAL:N	2.51	0.43
2:D:35:TRP:CE3	2:D:36:ILE:N	2.87	0.43
2:D:48:ILE:C	2:D:50:ALA:H	2.26	0.43
2:D:57:HIS:O	2:D:58:PHE:C	2.60	0.43
2:D:66:LEU:O	2:D:69:ALA:N	2.52	0.43
1:A:58:LYS:O	1:A:58:LYS:CG	2.67	0.43
1:A:75:PRO:C	1:A:77:GLN:HE21	2.25	0.43
1:C:11:PHE:HA	1:C:32:THR:O	2.19	0.43
1:C:411:ARG:NE	1:C:422:PHE:CE1	2.86	0.43
2:D:19:TRP:CD1	2:D:20:MET:SD	3.12	0.43
1:A:439:VAL:O	1:A:443:ILE:HG22	2.18	0.43
2:B:65:ILE:CG2	2:B:66:LEU:N	2.82	0.43
1:C:99:ARG:HG2	1:C:103:ASN:OD1	2.18	0.43
1:C:157:LYS:O	1:C:157:LYS:CG	2.67	0.43
1:C:229:SER:HA	1:C:231:TRP:CD1	2.53	0.43
1:C:454:ILE:HD13	1:C:455:MET:CA	2.48	0.43
1:A:62:GLU:HG3	1:A:62:GLU:O	2.18	0.42
1:A:101:TRP:CB	1:A:108:PHE:HD2	2.18	0.42
1:A:199:LEU:CD1	1:A:200:GLN:O	2.67	0.42
1:A:468:MET:C	1:A:468:MET:SD	3.02	0.42
1:C:11:PHE:O	1:C:12:VAL:HG13	2.19	0.42
1:C:80:PRO:HG3	1:C:113:ILE:CA	2.48	0.42
1:C:196:MET:HB3	1:C:207:LEU:CD1	2.49	0.42
1:C:275:GLY:O	1:C:276:ASN:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:PHE:CE2	1:C:367:ILE:HG21	2.54	0.42
1:C:467:GLY:O	1:C:470:SER:N	2.52	0.42
1:A:208:VAL:O	1:A:208:VAL:HG23	2.19	0.42
1:A:340:MET:HE2	1:A:345:ARG:HG3	2.01	0.42
1:A:360:GLU:O	1:A:362:ASP:N	2.52	0.42
1:A:426:GLY:HA3	1:A:431:SER:HB3	2.01	0.42
2:B:8:VAL:HG23	2:B:9:GLY:H	1.83	0.42
2:B:35:TRP:CE3	2:B:36:ILE:N	2.87	0.42
1:A:229:SER:HA	1:A:231:TRP:CD1	2.53	0.42
2:B:39:HIS:O	2:B:40:PRO:C	2.60	0.42
2:D:65:ILE:CG2	2:D:66:LEU:N	2.82	0.42
1:A:294:LEU:HD22	1:A:297:MET:HG2	2.02	0.42
1:A:345:ARG:HD2	1:A:345:ARG:N	2.35	0.42
1:A:414:ILE:HD12	1:A:414:ILE:N	2.34	0.42
1:A:417:ASP:C	1:A:419:ALA:H	2.28	0.42
2:B:19:TRP:CD1	2:B:20:MET:SD	3.12	0.42
1:C:98:ASP:O	1:C:99:ARG:C	2.62	0.42
1:C:294:LEU:HD22	1:C:297:MET:HG2	2.01	0.42
1:C:360:GLU:O	1:C:362:ASP:N	2.52	0.42
1:C:480:VAL:HG12	1:C:481:LEU:N	2.35	0.42
1:A:196:MET:HB3	1:A:207:LEU:CD1	2.49	0.42
1:A:270:ILE:HD12	1:A:271:GLN:HG2	2.00	0.42
1:A:309:VAL:HB	1:A:323:ARG:CG	2.48	0.42
1:A:313:ALA:O	1:A:314:GLU:CB	2.66	0.42
1:A:454:ILE:HD13	1:A:455:MET:CA	2.48	0.42
1:A:444:TYR:O	1:A:446:ALA:N	2.52	0.42
1:A:487:LEU:HD13	1:A:487:LEU:O	2.19	0.42
2:B:66:LEU:O	2:B:69:ALA:N	2.52	0.42
1:C:20:TRP:HB3	1:C:425:LEU:CD2	2.47	0.42
1:C:311:GLU:O	1:C:312:ILE:CG2	2.59	0.42
1:C:383:GLU:C	1:C:385:GLY:N	2.77	0.42
2:D:8:VAL:HG23	2:D:9:GLY:H	1.84	0.42
1:A:29:SER:O	1:A:30:CYS:O	2.38	0.42
1:A:103:ASN:O	1:A:103:ASN:ND2	2.52	0.42
1:A:125:MET:HG3	1:A:199:LEU:HD11	2.02	0.42
1:A:463:ILE:CG2	1:A:482:VAL:HG13	2.50	0.42
2:B:33:GLU:HA	2:B:36:ILE:CG2	2.50	0.42
1:C:46:ILE:O	1:C:47:GLU:C	2.61	0.42
1:C:103:ASN:O	1:C:103:ASN:ND2	2.52	0.42
1:C:125:MET:HG3	1:C:199:LEU:HD11	2.02	0.42
1:C:130:VAL:O	1:C:130:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:LYS:CE	1:C:418:THR:HB	2.50	0.42
1:C:345:ARG:HD2	1:C:345:ARG:N	2.35	0.42
1:C:346:HIS:O	1:C:347:VAL:O	2.37	0.42
1:C:426:GLY:HA3	1:C:431:SER:HB3	2.01	0.42
2:D:65:ILE:CG2	2:D:66:LEU:HD12	2.50	0.42
2:D:71:ALA:C	2:D:72:PRO:O	2.62	0.42
1:A:27:HIS:H	1:A:45:LEU:CD1	2.32	0.42
1:A:106:GLY:C	1:A:107:LEU:HD23	2.45	0.42
1:A:271:GLN:OE1	1:A:271:GLN:HA	2.19	0.42
1:A:294:LEU:HD23	1:A:296:GLY:N	2.34	0.42
1:A:384:PRO:CG	1:A:386:GLN:HE21	2.27	0.42
1:A:463:ILE:CA	1:A:466:ILE:HG22	2.49	0.42
2:B:6:PRO:O	2:B:6:PRO:HG2	2.18	0.42
2:B:40:PRO:O	2:B:41:GLY:C	2.63	0.42
2:B:48:ILE:C	2:B:50:ALA:H	2.25	0.42
1:C:208:VAL:O	1:C:208:VAL:HG23	2.19	0.42
1:C:210:ARG:HG3	1:C:210:ARG:HH21	1.85	0.42
1:C:240:PHE:CD1	1:C:250:VAL:CG1	3.03	0.42
1:C:255:SER:OG	1:C:256:GLN:N	2.48	0.42
1:C:277:LEU:HD12	1:C:279:PHE:CE2	2.53	0.42
1:C:463:ILE:CG2	1:C:482:VAL:HG13	2.50	0.42
1:A:25:LEU:H	1:A:25:LEU:HG	1.51	0.42
1:A:142:THR:HA	1:A:143:PRO:HD3	1.72	0.42
1:A:210:ARG:HG3	1:A:210:ARG:HH21	1.85	0.42
1:A:221:LEU:HG	1:A:222:PRO:HD3	2.00	0.42
1:A:346:HIS:O	1:A:347:VAL:O	2.37	0.42
2:B:57:HIS:O	2:B:58:PHE:C	2.60	0.42
1:C:185:CYS:CB	1:C:187:PRO:HD3	2.50	0.42
1:C:294:LEU:HD23	1:C:296:GLY:N	2.34	0.42
1:C:295:LYS:NZ	1:C:295:LYS:HB2	2.35	0.42
1:C:384:PRO:HG2	1:C:386:GLN:NE2	2.28	0.42
1:A:11:PHE:HA	1:A:32:THR:O	2.19	0.42
1:A:41:LEU:CB	1:A:43:PHE:HE1	2.32	0.42
1:A:157:LYS:O	1:A:157:LYS:CG	2.67	0.42
1:A:240:PHE:CD1	1:A:250:VAL:CG1	3.02	0.42
1:A:247:LYS:O	1:A:248:GLN:CB	2.67	0.42
1:A:275:GLY:O	1:A:276:ASN:C	2.62	0.42
1:A:284:LYS:CE	1:A:418:THR:HB	2.50	0.42
1:A:350:ARG:HB2	1:A:350:ARG:NH2	2.35	0.42
1:A:455:MET:O	1:A:456:LYS:C	2.63	0.42
1:A:458:LEU:HD13	1:A:458:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:SER:O	1:C:30:CYS:O	2.37	0.42
1:C:108:PHE:CD1	1:C:108:PHE:C	2.98	0.42
1:A:16:SER:HB2	1:A:425:LEU:HD23	2.02	0.41
1:A:367:ILE:O	1:A:368:GLU:HG2	2.20	0.41
1:A:383:GLU:C	1:A:385:GLY:N	2.77	0.41
2:B:65:ILE:CG2	2:B:66:LEU:HD12	2.50	0.41
2:B:66:LEU:O	2:B:70:VAL:HG23	2.20	0.41
1:C:271:GLN:OE1	1:C:271:GLN:HA	2.20	0.41
1:C:331:SER:HA	1:C:332:PRO:HD3	1.92	0.41
1:C:444:TYR:O	1:C:446:ALA:N	2.53	0.41
2:D:40:PRO:O	2:D:41:GLY:C	2.62	0.41
1:A:43:PHE:CE2	1:A:141:ILE:CG2	3.03	0.41
1:A:74:CYS:SG	1:A:75:PRO:N	2.93	0.41
1:A:99:ARG:NH1	1:A:105:CYS:CB	2.76	0.41
1:A:311:GLU:O	1:A:312:ILE:CG2	2.58	0.41
1:A:487:LEU:O	1:A:491:VAL:HG13	2.20	0.41
1:C:22:ASP:HB2	1:C:424:SER:HA	2.02	0.41
1:C:41:LEU:CB	1:C:43:PHE:HE1	2.32	0.41
1:C:66:THR:C	1:C:68:THR:H	2.28	0.41
1:C:256:GLN:HA	1:C:256:GLN:NE2	2.17	0.41
1:C:422:PHE:HD2	1:C:422:PHE:HA	1.67	0.41
1:C:458:LEU:HD13	1:C:458:LEU:O	2.20	0.41
1:C:475:LEU:HG	1:C:476:SER:H	1.85	0.41
1:A:23:ILE:CD1	1:A:285:CYS:SG	3.08	0.41
1:A:41:LEU:CD2	1:A:143:PRO:HA	2.51	0.41
1:A:51:LYS:O	1:A:52:GLN:HB2	2.20	0.41
1:A:64:LYS:HB3	1:A:64:LYS:HZ3	1.81	0.41
1:A:295:LYS:NZ	1:A:295:LYS:HB2	2.35	0.41
1:A:384:PRO:CG	1:A:386:GLN:NE2	2.83	0.41
2:B:38:ARG:CG	2:B:39:HIS:CE1	3.04	0.41
1:C:74:CYS:SG	1:C:77:GLN:NE2	2.93	0.41
1:C:132:PRO:O	1:C:135:LEU:HB2	2.20	0.41
1:C:350:ARG:CZ	1:C:350:ARG:CB	2.98	0.41
2:D:33:GLU:HA	2:D:36:ILE:CG2	2.50	0.41
1:A:98:ASP:O	1:A:99:ARG:C	2.62	0.41
1:A:185:CYS:C	1:A:187:PRO:CD	2.93	0.41
1:A:444:TYR:C	1:A:446:ALA:N	2.77	0.41
2:B:35:TRP:O	2:B:38:ARG:N	2.53	0.41
1:C:100:GLY:O	1:C:103:ASN:CB	2.65	0.41
1:C:185:CYS:C	1:C:187:PRO:CD	2.94	0.41
1:C:394:LYS:O	1:C:396:SER:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:TYR:N	1:A:178:TYR:HD2	2.17	0.41
1:A:284:LYS:HG3	1:A:285:CYS:N	2.35	0.41
1:A:408:GLY:O	1:A:409:ALA:C	2.64	0.41
1:C:23:ILE:CD1	1:C:285:CYS:SG	3.08	0.41
1:C:75:PRO:HG3	1:C:110:LYS:O	2.20	0.41
1:C:135:LEU:HD22	1:C:135:LEU:HA	1.62	0.41
1:C:402:ILE:C	1:C:404:THR:N	2.77	0.41
2:D:35:TRP:O	2:D:38:ARG:N	2.54	0.41
1:A:74:CYS:SG	1:A:77:GLN:NE2	2.93	0.41
1:A:101:TRP:HZ3	1:C:321:VAL:HB	1.85	0.41
1:A:142:THR:OG1	1:A:143:PRO:CD	2.69	0.41
1:A:186:SER:O	1:A:188:ARG:N	2.53	0.41
1:A:196:MET:HB3	1:A:207:LEU:HD11	2.03	0.41
1:A:277:LEU:HD12	1:A:279:PHE:CE2	2.54	0.41
2:B:56:THR:HG1	2:B:59:GLN:HB2	1.77	0.41
1:C:309:VAL:HB	1:C:323:ARG:CG	2.49	0.41
1:C:340:MET:HE2	1:C:345:ARG:HG3	2.01	0.41
1:C:384:PRO:CG	1:C:386:GLN:NE2	2.83	0.41
1:C:400:GLN:O	1:C:401:MET:C	2.64	0.41
1:C:489:LEU:HA	1:C:489:LEU:HD23	1.80	0.41
1:A:130:VAL:HG23	1:A:130:VAL:O	2.20	0.41
1:A:221:LEU:HD12	1:A:221:LEU:HA	1.77	0.41
1:A:320:ILE:O	1:A:368:GLU:HA	2.20	0.41
1:A:321:VAL:O	1:A:321:VAL:HG23	2.21	0.41
1:C:27:HIS:H	1:C:45:LEU:CD1	2.33	0.41
1:C:43:PHE:CE2	1:C:141:ILE:CG2	3.03	0.41
1:C:96:MET:HA	1:C:111:GLY:O	2.20	0.41
1:C:142:THR:OG1	1:C:143:PRO:CD	2.69	0.41
1:C:270:ILE:HD12	1:C:271:GLN:HG2	2.01	0.41
1:C:315:THR:O	1:C:315:THR:HG23	2.19	0.41
1:C:320:ILE:O	1:C:368:GLU:HA	2.21	0.41
1:C:345:ARG:CD	1:C:345:ARG:N	2.82	0.41
1:C:414:ILE:HD12	1:C:414:ILE:N	2.35	0.41
1:C:487:LEU:O	1:C:491:VAL:HG13	2.21	0.41
2:D:54:GLY:O	2:D:55:THR:HB	2.20	0.41
1:A:45:LEU:H	1:A:45:LEU:CD1	2.34	0.41
1:A:71:ASP:O	1:A:113:ILE:HG13	2.21	0.41
1:A:82:LEU:H	1:A:82:LEU:HD12	1.86	0.41
1:A:204:LYS:HE3	1:A:204:LYS:HB3	1.73	0.41
1:A:386:GLN:NE2	1:A:386:GLN:HA	2.36	0.41
1:A:453:TRP:O	1:A:454:ILE:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:VAL:HG12	1:A:481:LEU:N	2.35	0.41
2:B:42:PHE:O	2:B:43:THR:C	2.63	0.41
2:B:54:GLY:O	2:B:55:THR:HB	2.20	0.41
1:C:1:MET:CG	1:C:151:VAL:HA	2.45	0.41
1:C:41:LEU:CD2	1:C:143:PRO:HA	2.51	0.41
1:C:253:LEU:O	1:C:253:LEU:CD2	2.69	0.41
1:C:350:ARG:HB2	1:C:350:ARG:NH2	2.35	0.41
1:C:386:GLN:NE2	1:C:386:GLN:HA	2.36	0.41
1:C:389:LEU:C	1:C:389:LEU:HD13	2.46	0.41
1:C:417:ASP:C	1:C:419:ALA:H	2.27	0.41
1:A:1:MET:CG	1:A:151:VAL:HA	2.45	0.41
1:A:75:PRO:HG3	1:A:110:LYS:O	2.20	0.41
1:A:82:LEU:HD12	1:A:82:LEU:N	2.36	0.41
1:A:96:MET:HA	1:A:111:GLY:O	2.20	0.41
1:A:108:PHE:CD1	1:A:108:PHE:C	2.98	0.41
1:A:253:LEU:O	1:A:253:LEU:CD2	2.69	0.41
1:A:301:MET:O	1:A:302:CYS:O	2.39	0.41
1:A:317:HIS:HB3	1:A:393:LYS:NZ	2.36	0.41
1:A:367:ILE:N	1:A:367:ILE:CD1	2.74	0.41
1:A:391:TRP:O	1:A:392:PHE:CB	2.66	0.41
1:C:125:MET:HB2	1:C:201:MET:CE	2.51	0.41
1:C:178:TYR:N	1:C:178:TYR:HD2	2.17	0.41
1:C:186:SER:O	1:C:188:ARG:N	2.53	0.41
1:C:199:LEU:CD1	1:C:200:GLN:O	2.68	0.41
1:C:201:MET:C	1:C:203:ASN:N	2.79	0.41
1:C:284:LYS:HG3	1:C:285:CYS:N	2.36	0.41
1:C:319:THR:O	1:C:320:ILE:C	2.63	0.41
1:C:367:ILE:O	1:C:368:GLU:HG2	2.20	0.41
1:C:398:ILE:C	1:C:400:GLN:N	2.76	0.41
1:C:402:ILE:O	1:C:405:THR:N	2.53	0.41
1:C:471:ARG:HE	1:C:471:ARG:HB3	1.69	0.41
1:C:487:LEU:HD13	1:C:487:LEU:O	2.21	0.41
2:D:35:TRP:HH2	2:D:42:PHE:CD2	2.39	0.41
2:D:48:ILE:O	2:D:51:TYR:N	2.54	0.41
2:D:50:ALA:HB1	2:D:63:ILE:HD11	2.03	0.41
1:A:53:PRO:HB2	1:A:129:VAL:O	2.21	0.41
1:A:125:MET:HB2	1:A:201:MET:CE	2.51	0.41
1:A:306:PHE:HZ	1:A:381:GLY:CA	2.22	0.41
1:A:353:THR:O	1:A:353:THR:HG22	2.20	0.41
1:A:357:ILE:O	1:A:357:ILE:CG2	2.65	0.41
1:A:402:ILE:O	1:A:405:THR:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ARG:CZ	1:A:411:ARG:HB2	2.51	0.41
1:C:53:PRO:HB2	1:C:129:VAL:O	2.21	0.41
1:C:82:LEU:HD12	1:C:82:LEU:N	2.36	0.41
1:C:196:MET:HB3	1:C:207:LEU:HD11	2.03	0.41
1:C:353:THR:O	1:C:353:THR:HG22	2.21	0.41
1:C:362:ASP:O	1:C:363:SER:C	2.64	0.41
1:C:411:ARG:CZ	1:C:411:ARG:HB2	2.51	0.41
1:C:455:MET:O	1:C:456:LYS:C	2.63	0.41
2:D:32:ILE:HD12	2:D:32:ILE:C	2.46	0.41
2:D:37:LEU:HD21	2:D:38:ARG:CZ	2.51	0.41
1:A:22:ASP:CB	1:A:424:SER:HA	2.51	0.40
1:A:41:LEU:HA	1:A:41:LEU:HD23	1.80	0.40
1:A:57:ARG:HA	1:A:57:ARG:HD3	1.83	0.40
1:A:132:PRO:O	1:A:135:LEU:HB2	2.21	0.40
1:A:310:LYS:HG2	1:C:101:TRP:NE1	2.36	0.40
1:A:384:PRO:C	1:A:386:GLN:N	2.78	0.40
1:A:436:LEU:C	1:A:438:GLN:N	2.78	0.40
1:A:472:SER:O	1:A:474:SER:N	2.54	0.40
2:B:32:ILE:HD12	2:B:32:ILE:C	2.46	0.40
1:C:57:ARG:HD3	1:C:57:ARG:HA	1.83	0.40
1:C:367:ILE:CG2	1:C:368:GLU:H	2.23	0.40
1:A:22:ASP:HB2	1:A:424:SER:HA	2.02	0.40
1:A:101:TRP:NE1	1:C:310:LYS:HG2	2.36	0.40
1:A:122:LYS:HB2	1:A:122:LYS:NZ	2.27	0.40
1:A:185:CYS:CB	1:A:187:PRO:HD3	2.51	0.40
1:A:284:LYS:HE3	1:A:418:THR:HB	2.03	0.40
2:B:44:ILE:O	2:B:45:MET:C	2.64	0.40
2:B:48:ILE:O	2:B:51:TYR:N	2.54	0.40
1:C:1:MET:HE3	1:C:1:MET:CA	2.51	0.40
1:C:45:LEU:H	1:C:45:LEU:CD1	2.34	0.40
1:C:61:ILE:CD1	1:C:123:LYS:O	2.62	0.40
1:C:313:ALA:O	1:C:314:GLU:CB	2.66	0.40
1:C:335:ILE:O	1:C:335:ILE:HG22	2.18	0.40
1:A:46:ILE:HD11	1:A:140:VAL:HG11	2.03	0.40
1:A:131:GLN:NE2	1:A:131:GLN:H	2.20	0.40
1:A:315:THR:O	1:A:315:THR:HG23	2.20	0.40
1:A:319:THR:O	1:A:320:ILE:C	2.64	0.40
1:A:425:LEU:HD22	1:A:425:LEU:N	2.37	0.40
1:A:440:PHE:HA	1:A:443:ILE:HG22	2.04	0.40
2:B:50:ALA:HA	2:B:63:ILE:CD1	2.52	0.40
1:C:51:LYS:O	1:C:52:GLN:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:ASP:O	1:C:113:ILE:HG13	2.21	0.40
1:C:147:GLU:HB3	1:C:148:GLU:H	1.59	0.40
1:C:440:PHE:HA	1:C:443:ILE:HG22	2.04	0.40
1:A:8:ASN:CB	1:A:28:GLY:O	2.70	0.40
1:A:373:PHE:HA	1:A:395:GLY:HA3	2.04	0.40
2:B:37:LEU:HD21	2:B:38:ARG:CZ	2.51	0.40
2:B:64:PHE:O	2:B:65:ILE:C	2.65	0.40
1:C:8:ASN:CB	1:C:28:GLY:O	2.70	0.40
1:C:317:HIS:HB3	1:C:393:LYS:NZ	2.36	0.40
2:D:14:THR:O	2:D:15:ALA:C	2.65	0.40
2:D:23:GLU:O	2:D:27:LYS:HB2	2.22	0.40
2:D:38:ARG:CG	2:D:39:HIS:CE1	3.04	0.40
1:A:21:VAL:HG21	1:A:289:MET:HE2	2.04	0.40
1:A:198:LEU:HD12	1:A:272:MET:HE1	2.04	0.40
1:A:333:CYS:H	1:A:358:VAL:HG23	1.87	0.40
1:A:396:SER:O	1:A:399:GLY:N	2.54	0.40
1:A:400:GLN:O	1:A:401:MET:C	2.63	0.40
1:C:46:ILE:HB	1:C:47:GLU:H	1.66	0.40
1:C:200:GLN:CA	1:C:272:MET:HE3	2.52	0.40
2:D:42:PHE:O	2:D:43:THR:C	2.64	0.40
2:D:45:MET:HA	2:D:48:ILE:HD12	2.04	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	493/495 (100%)	228 (46%)	144 (29%)	121 (24%)	0	0
1	C	493/495 (100%)	227 (46%)	144 (29%)	122 (25%)	0	0
2	B	70/75 (93%)	33 (47%)	23 (33%)	14 (20%)	0	1
2	D	70/75 (93%)	33 (47%)	23 (33%)	14 (20%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1126/1140 (99%)	521 (46%)	334 (30%)	271 (24%)	0 0

All (271) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	A	30	CYS
1	A	57	ARG
1	A	74	CYS
1	A	77	GLN
1	A	88	LYS
1	A	134	ASN
1	A	147	GLU
1	A	154	ASP
1	A	188	ARG
1	A	203	ASN
1	A	217	PRO
1	A	222	PRO
1	A	225	ASP
1	A	233	GLN
1	A	238	VAL
1	A	243	PRO
1	A	246	LYS
1	A	255	SER
1	A	257	GLU
1	A	270	ILE
1	A	272	MET
1	A	274	SER
1	A	279	PHE
1	A	300	SER
1	A	302	CYS
1	A	310	LYS
1	A	314	GLU
1	A	342	LEU
1	A	344	LYS
1	A	346	HIS
1	A	347	VAL
1	A	355	ASN
1	A	357	ILE
1	A	383	GLU
1	A	386	GLN
1	A	394	LYS

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Mol	Chain	Res	Type
1	A	396	SER
1	A	397	SER
1	A	417	ASP
1	A	429	PHE
1	A	435	ALA
1	A	444	TYR
1	A	468	MET
1	A	493	VAL
1	A	494	GLN
2	B	15	ALA
2	B	21	SER
2	B	56	THR
2	B	57	HIS
1	C	16	SER
1	C	30	CYS
1	C	57	ARG
1	C	74	CYS
1	C	77	GLN
1	C	88	LYS
1	C	134	ASN
1	C	147	GLU
1	C	154	ASP
1	C	188	ARG
1	C	203	ASN
1	C	217	PRO
1	C	222	PRO
1	C	225	ASP
1	C	233	GLN
1	C	238	VAL
1	C	243	PRO
1	C	246	LYS
1	C	255	SER
1	C	257	GLU
1	C	270	ILE
1	C	272	MET
1	C	274	SER
1	C	279	PHE
1	C	300	SER
1	C	302	CYS
1	C	310	LYS
1	C	314	GLU
1	C	342	LEU

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Mol	Chain	Res	Type
1	C	344	LYS
1	C	346	HIS
1	C	347	VAL
1	C	355	ASN
1	C	357	ILE
1	C	383	GLU
1	C	386	GLN
1	C	394	LYS
1	C	396	SER
1	C	397	SER
1	C	417	ASP
1	C	429	PHE
1	C	435	ALA
1	C	444	TYR
1	C	468	MET
1	C	493	VAL
1	C	494	GLN
2	D	15	ALA
2	D	21	SER
2	D	56	THR
2	D	57	HIS
1	A	2	ARG
1	A	10	ASP
1	A	40	THR
1	A	46	ILE
1	A	58	LYS
1	A	68	THR
1	A	99	ARG
1	A	110	LYS
1	A	128	LYS
1	A	143	PRO
1	A	193	PHE
1	A	211	GLN
1	A	276	ASN
1	A	296	GLY
1	A	317	HIS
1	A	356	PRO
1	A	372	PRO
1	A	374	GLY
1	A	418	THR
1	A	443	ILE
1	A	447	ALA

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Mol	Chain	Res	Type
1	A	473	THR
1	A	483	GLY
1	A	484	VAL
1	A	485	VAL
2	B	7	HIS
2	B	22	SER
1	C	2	ARG
1	C	10	ASP
1	C	40	THR
1	C	46	ILE
1	C	58	LYS
1	C	68	THR
1	C	99	ARG
1	C	110	LYS
1	C	128	LYS
1	C	143	PRO
1	C	193	PHE
1	C	211	GLN
1	C	276	ASN
1	C	296	GLY
1	C	317	HIS
1	C	356	PRO
1	C	372	PRO
1	C	374	GLY
1	C	418	THR
1	C	443	ILE
1	C	447	ALA
1	C	473	THR
1	C	483	GLY
1	C	484	VAL
1	C	485	VAL
2	D	7	HIS
2	D	22	SER
1	A	27	HIS
1	A	37	ASN
1	A	103	ASN
1	A	108	PHE
1	A	192	ASP
1	A	204	LYS
1	A	221	LEU
1	A	256	GLN
1	A	261	HIS

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Mol	Chain	Res	Type
1	A	331	SER
1	A	334	LYS
1	A	371	PRO
1	A	413	ALA
1	A	430	THR
1	A	470	SER
1	A	474	SER
2	B	51	TYR
2	B	66	LEU
1	C	4	ILE
1	C	27	HIS
1	C	37	ASN
1	C	103	ASN
1	C	108	PHE
1	C	192	ASP
1	C	204	LYS
1	C	221	LEU
1	C	256	GLN
1	C	261	HIS
1	C	331	SER
1	C	334	LYS
1	C	371	PRO
1	C	413	ALA
1	C	430	THR
1	C	470	SER
1	C	474	SER
1	C	491	VAL
2	D	51	TYR
1	A	4	ILE
1	A	18	GLY
1	A	38	LYS
1	A	76	THR
1	A	201	MET
1	A	229	SER
1	A	289	MET
1	A	316	GLN
1	A	354	VAL
1	A	363	SER
1	A	425	LEU
1	A	491	VAL
2	B	2	VAL
2	B	46	ALA

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Mol	Chain	Res	Type
1	C	18	GLY
1	C	38	LYS
1	C	76	THR
1	C	201	MET
1	C	229	SER
1	C	289	MET
1	C	316	GLN
1	C	354	VAL
1	C	363	SER
1	C	425	LEU
2	D	2	VAL
2	D	46	ALA
2	D	66	LEU
1	A	7	SER
1	A	75	PRO
1	A	123	LYS
1	A	126	LYS
1	A	144	HIS
1	A	195	GLU
1	A	227	GLN
1	A	228	GLY
1	A	311	GLU
1	A	343	GLU
1	A	365	VAL
1	A	445	GLY
2	B	44	ILE
2	B	67	LEU
1	C	7	SER
1	C	75	PRO
1	C	123	LYS
1	C	126	LYS
1	C	144	HIS
1	C	195	GLU
1	C	227	GLN
1	C	228	GLY
1	C	311	GLU
1	C	343	GLU
1	C	365	VAL
1	C	445	GLY
2	D	44	ILE
1	A	36	LYS
1	A	248	GLN

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Mol	Chain	Res	Type
1	A	487	LEU
2	B	55	THR
1	C	36	LYS
1	C	248	GLN
1	C	407	ARG
1	C	487	LEU
2	D	55	THR
2	D	67	LEU
1	A	320	ILE
2	B	8	VAL
1	C	320	ILE
2	D	8	VAL
1	A	395	GLY
1	C	395	GLY
1	A	382	VAL
1	C	382	VAL
1	A	223	GLY
1	C	223	GLY
1	A	12	VAL
1	A	266	GLY
1	A	482	VAL
1	C	12	VAL
1	C	266	GLY
1	C	482	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	420/420 (100%)	333 (79%)	87 (21%)	1	7
1	C	420/420 (100%)	333 (79%)	87 (21%)	1	7
2	B	57/60 (95%)	48 (84%)	9 (16%)	2	15
2	D	57/60 (95%)	48 (84%)	9 (16%)	2	15
All	All	954/960 (99%)	762 (80%)	192 (20%)	3	8

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	20	TRP
1	A	25	LEU
1	A	38	LYS
1	A	45	LEU
1	A	46	ILE
1	A	48	THR
1	A	51	LYS
1	A	55	THR
1	A	58	LYS
1	A	61	ILE
1	A	64	LYS
1	A	65	LEU
1	A	70	THR
1	A	75	PRO
1	A	77	GLN
1	A	82	LEU
1	A	98	ASP
1	A	107	LEU
1	A	113	ILE
1	A	116	CYS
1	A	122	LYS
1	A	125	MET
1	A	126	LYS
1	A	131	GLN
1	A	135	LEU
1	A	139	ILE
1	A	141	ILE
1	A	157	LYS
1	A	158	HIS
1	A	162	ILE
1	A	164	ILE
1	A	170	ILE
1	A	175	LEU
1	A	196	MET
1	A	198	LEU
1	A	204	LYS
1	A	207	LEU
1	A	211	GLN
1	A	217	PRO
1	A	220	TRP
1	A	233	GLN

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Mol	Chain	Res	Type
1	A	240	PHE
1	A	244	HIS
1	A	247	LYS
1	A	248	GLN
1	A	250	VAL
1	A	256	GLN
1	A	264	LEU
1	A	270	ILE
1	A	277	LEU
1	A	279	PHE
1	A	280	THR
1	A	283	LEU
1	A	295	LYS
1	A	299	TYR
1	A	306	PHE
1	A	311	GLU
1	A	312	ILE
1	A	320	ILE
1	A	335	ILE
1	A	348	LEU
1	A	351	LEU
1	A	352	ILE
1	A	358	VAL
1	A	359	THR
1	A	365	VAL
1	A	367	ILE
1	A	371	PRO
1	A	388	LYS
1	A	389	LEU
1	A	390	ASN
1	A	400	GLN
1	A	402	ILE
1	A	422	PHE
1	A	431	SER
1	A	432	ILE
1	A	434	LYS
1	A	438	GLN
1	A	448	PHE
1	A	451	VAL
1	A	454	ILE
1	A	457	ILE
1	A	466	ILE

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Mol	Chain	Res	Type
1	A	480	VAL
1	A	484	VAL
1	A	492	MET
2	B	2	VAL
2	B	4	LEU
2	B	6	PRO
2	B	8	VAL
2	B	14	THR
2	B	26	TRP
2	B	36	ILE
2	B	37	LEU
2	B	39	HIS
1	C	1	MET
1	C	20	TRP
1	C	25	LEU
1	C	38	LYS
1	C	45	LEU
1	C	46	ILE
1	C	48	THR
1	C	51	LYS
1	C	55	THR
1	C	58	LYS
1	C	61	ILE
1	C	64	LYS
1	C	65	LEU
1	C	70	THR
1	C	75	PRO
1	C	77	GLN
1	C	82	LEU
1	C	98	ASP
1	C	107	LEU
1	C	113	ILE
1	C	116	CYS
1	C	122	LYS
1	C	125	MET
1	C	126	LYS
1	C	131	GLN
1	C	135	LEU
1	C	139	ILE
1	C	141	ILE
1	C	157	LYS
1	C	158	HIS

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Mol	Chain	Res	Type
1	C	162	ILE
1	C	164	ILE
1	C	170	ILE
1	C	175	LEU
1	C	196	MET
1	C	198	LEU
1	C	204	LYS
1	C	207	LEU
1	C	211	GLN
1	C	217	PRO
1	C	220	TRP
1	C	233	GLN
1	C	240	PHE
1	C	244	HIS
1	C	247	LYS
1	C	248	GLN
1	C	250	VAL
1	C	256	GLN
1	C	264	LEU
1	C	270	ILE
1	C	277	LEU
1	C	279	PHE
1	C	280	THR
1	C	283	LEU
1	C	295	LYS
1	C	299	TYR
1	C	306	PHE
1	C	311	GLU
1	C	312	ILE
1	C	320	ILE
1	C	335	ILE
1	C	348	LEU
1	C	351	LEU
1	C	352	ILE
1	C	358	VAL
1	C	359	THR
1	C	365	VAL
1	C	367	ILE
1	C	371	PRO
1	C	388	LYS
1	C	389	LEU
1	C	390	ASN

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Mol	Chain	Res	Type
1	C	400	GLN
1	C	402	ILE
1	C	422	PHE
1	C	431	SER
1	C	432	ILE
1	C	434	LYS
1	C	438	GLN
1	C	448	PHE
1	C	451	VAL
1	C	454	ILE
1	C	457	ILE
1	C	466	ILE
1	C	480	VAL
1	C	484	VAL
1	C	492	MET
2	D	2	VAL
2	D	4	LEU
2	D	6	PRO
2	D	8	VAL
2	D	14	THR
2	D	26	TRP
2	D	36	ILE
2	D	37	LEU
2	D	39	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	77	GLN
1	A	83	ASN
1	A	131	GLN
1	A	167	GLN
1	A	200	GLN
1	A	211	GLN
1	A	230	ASN
1	A	233	GLN
1	A	242	ASN
1	A	248	GLN
1	A	256	GLN
1	A	282	HIS
1	A	386	GLN

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Mol	Chain	Res	Type
1	A	390	ASN
1	A	400	GLN
2	B	7	HIS
1	C	27	HIS
1	C	77	GLN
1	C	83	ASN
1	C	131	GLN
1	C	167	GLN
1	C	200	GLN
1	C	211	GLN
1	C	230	ASN
1	C	233	GLN
1	C	242	ASN
1	C	248	GLN
1	C	256	GLN
1	C	261	HIS
1	C	282	HIS
1	C	386	GLN
1	C	390	ASN
1	C	400	GLN
2	D	7	HIS

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](#)

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	1	1,3	14,14,15	0.58	0	17,19,21	0.78	0
3	NAG	E	2	3	14,14,15	0.61	0	17,19,21	0.82	1 (5%)
3	NAG	F	1	1,3	14,14,15	0.59	0	17,19,21	0.77	0
3	NAG	F	2	3	14,14,15	0.60	0	17,19,21	0.81	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	1,3	-	6/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	6/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	NAG	C2-N2-C7	-2.27	119.86	122.90
3	F	2	NAG	C2-N2-C7	-2.24	119.90	122.90

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	E	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6

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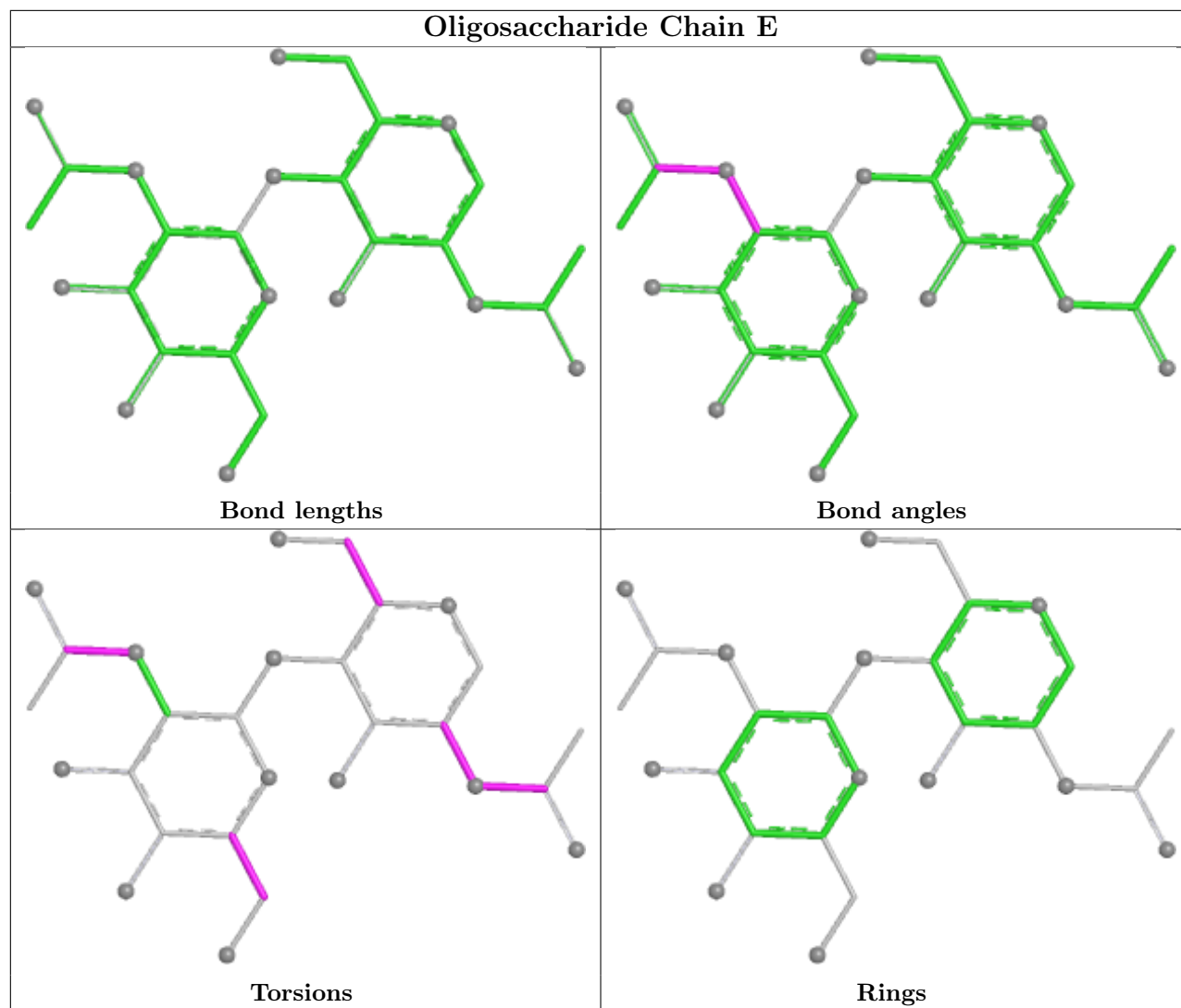
Mol	Chain	Res	Type	Atoms
3	F	2	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C3-C2-N2-C7
3	F	1	NAG	C3-C2-N2-C7
3	E	1	NAG	C1-C2-N2-C7
3	F	1	NAG	C1-C2-N2-C7

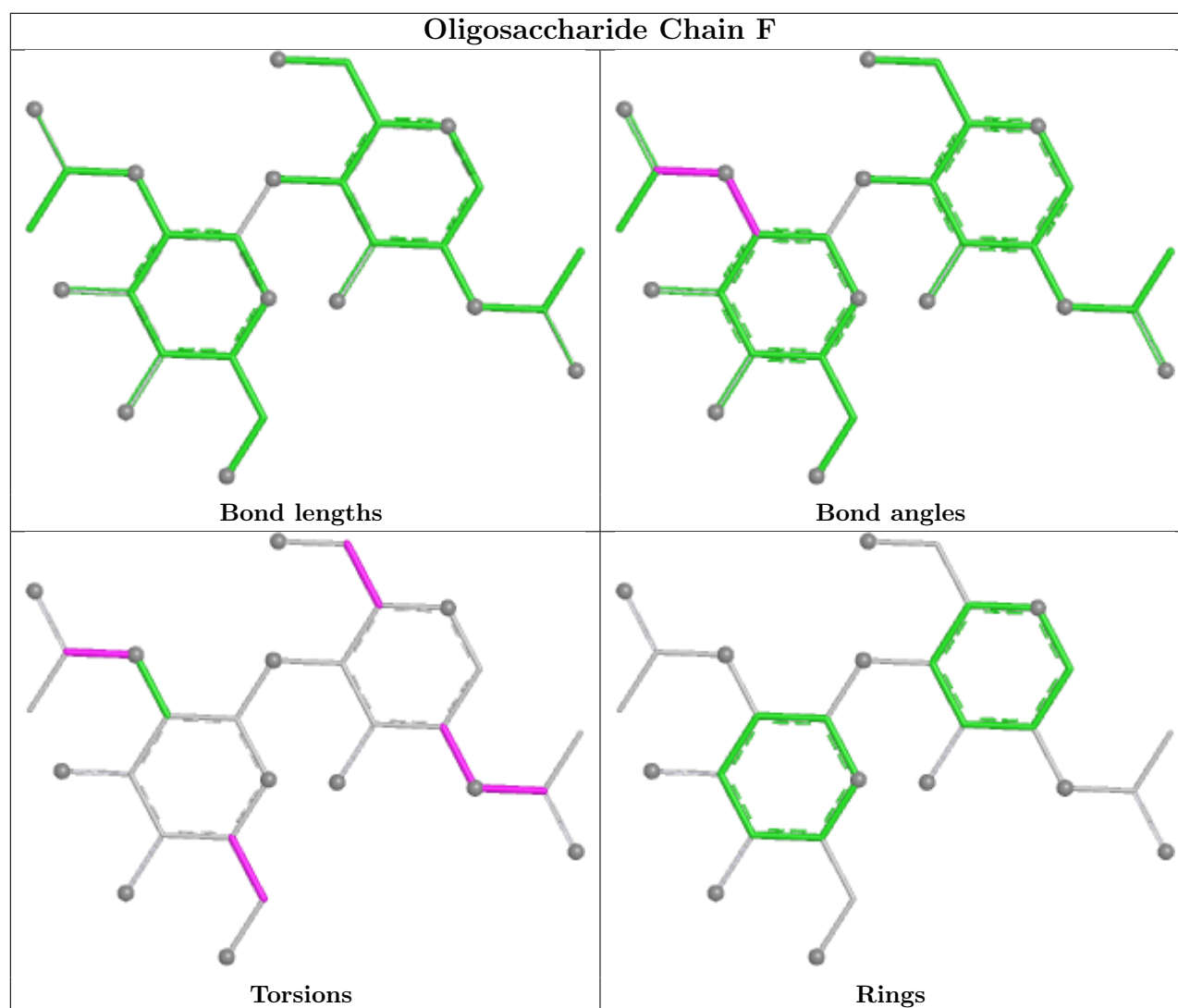
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1	NAG	3	0
3	F	1	NAG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	C	501	1	14,14,15	0.53	0	17,19,21	0.88	1 (5%)
4	NAG	A	501	1	14,14,15	0.53	0	17,19,21	0.87	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	501	1	-	4/6/23/26	0/1/1/1
4	NAG	A	501	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	NAG	C2-N2-C7	-2.78	119.17	122.90
4	A	501	NAG	C2-N2-C7	-2.73	119.23	122.90

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	NAG	C8-C7-N2-C2
4	A	501	NAG	O7-C7-N2-C2
4	C	501	NAG	C8-C7-N2-C2
4	C	501	NAG	O7-C7-N2-C2
4	A	501	NAG	O5-C5-C6-O6
4	C	501	NAG	O5-C5-C6-O6
4	A	501	NAG	C4-C5-C6-O6
4	C	501	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

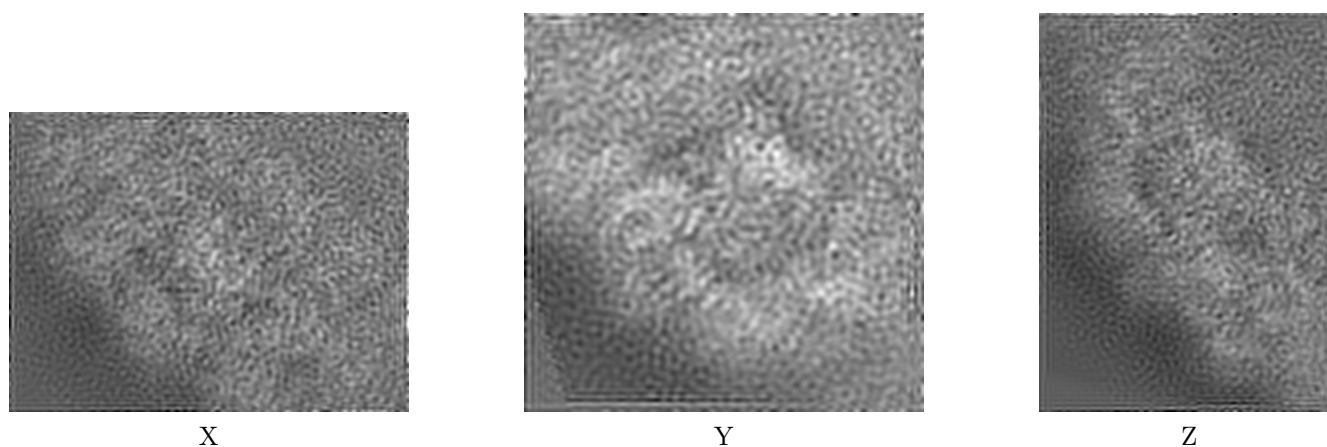
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5499. 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](#)

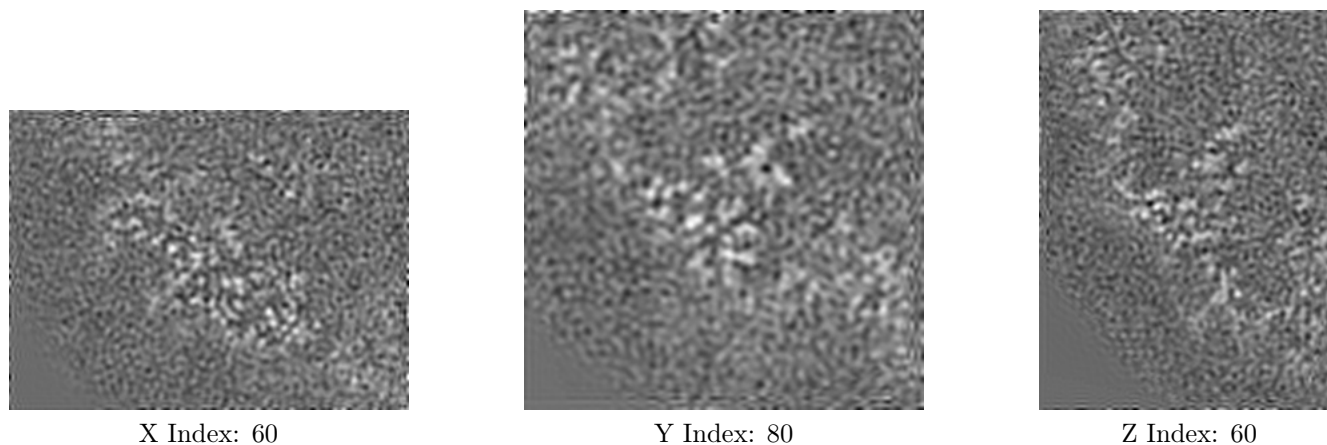
6.1.1 Primary map



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

6.2 Central slices [i](#)

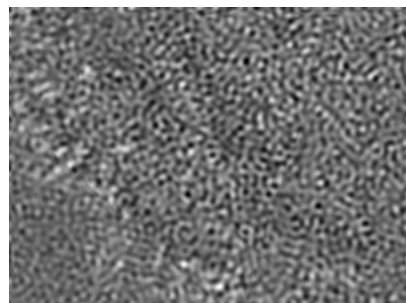
6.2.1 Primary map



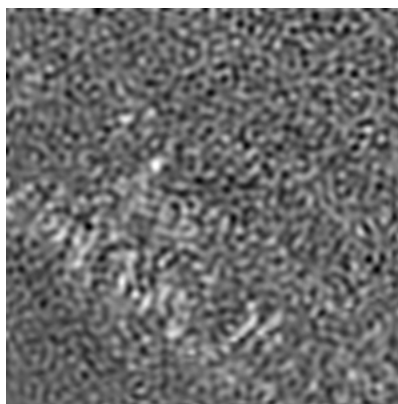
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

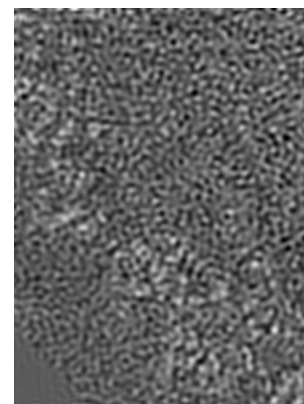
6.3.1 Primary map



X Index: 119



Y Index: 159

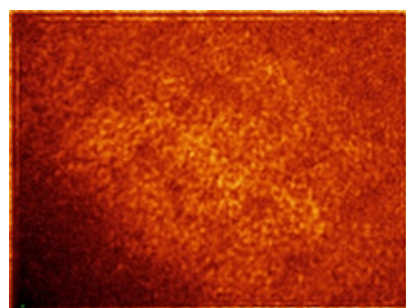


Z Index: 119

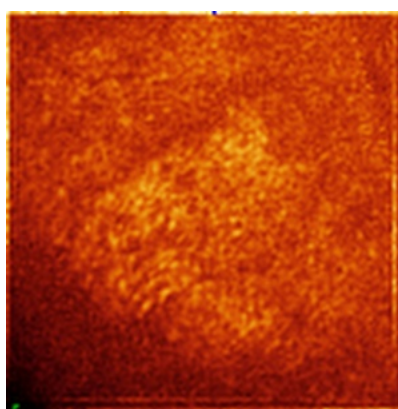
The images above show the largest variance slices of the map in three orthogonal directions.

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

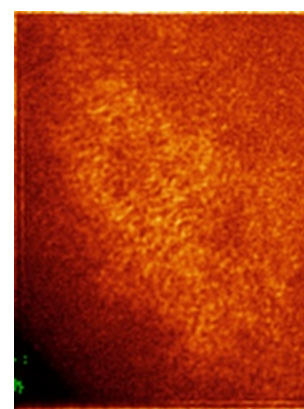
6.4.1 Primary map



X



Y

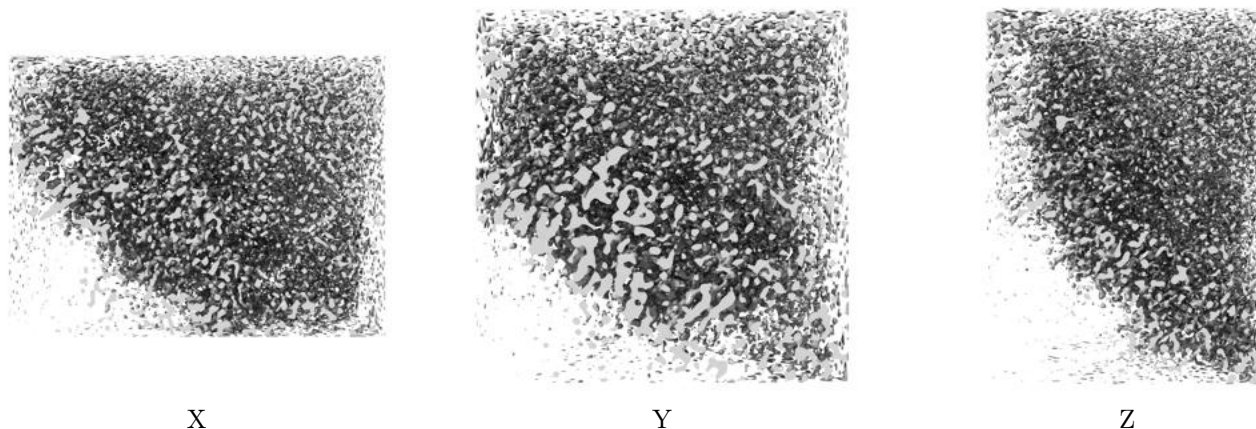


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

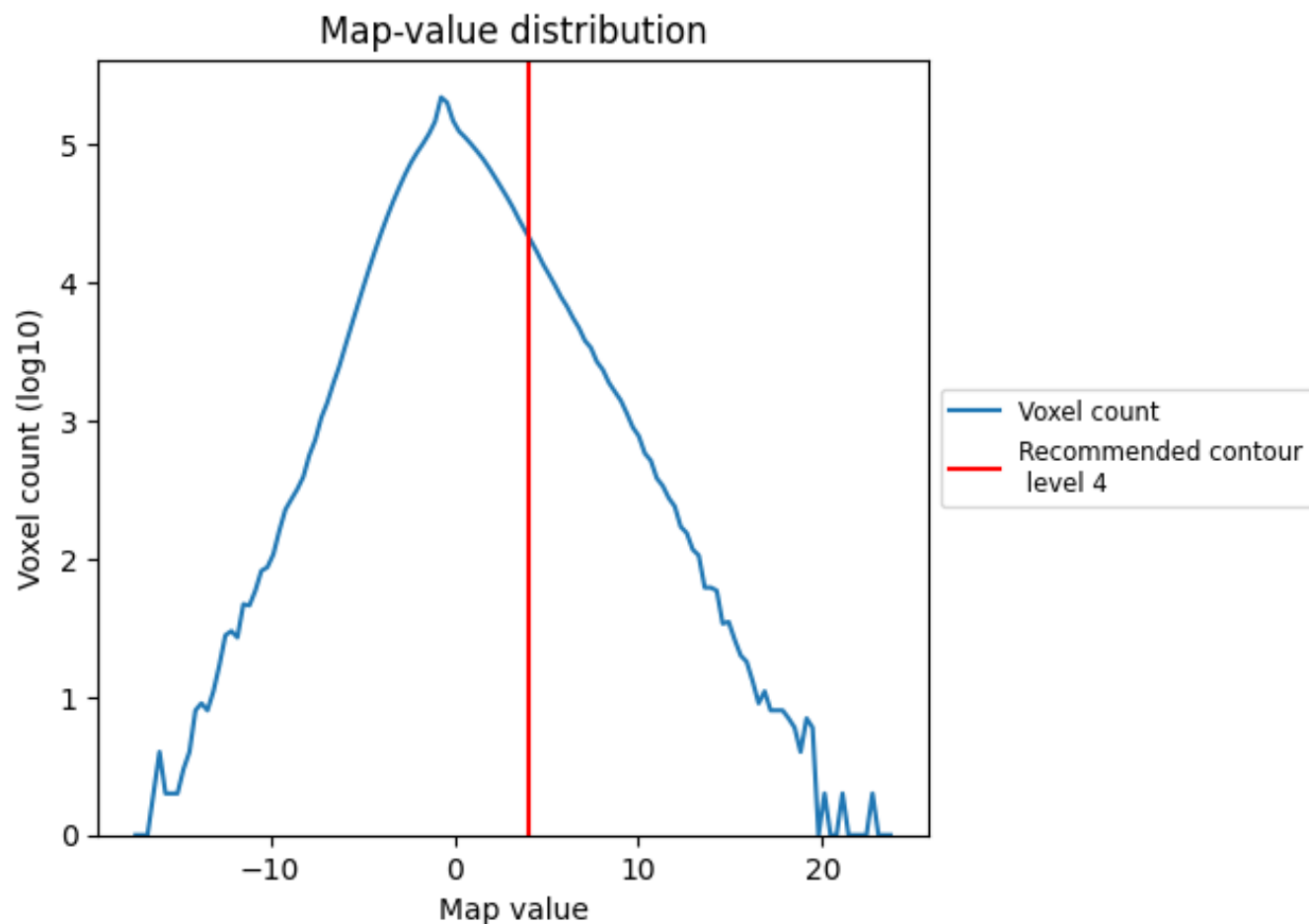
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

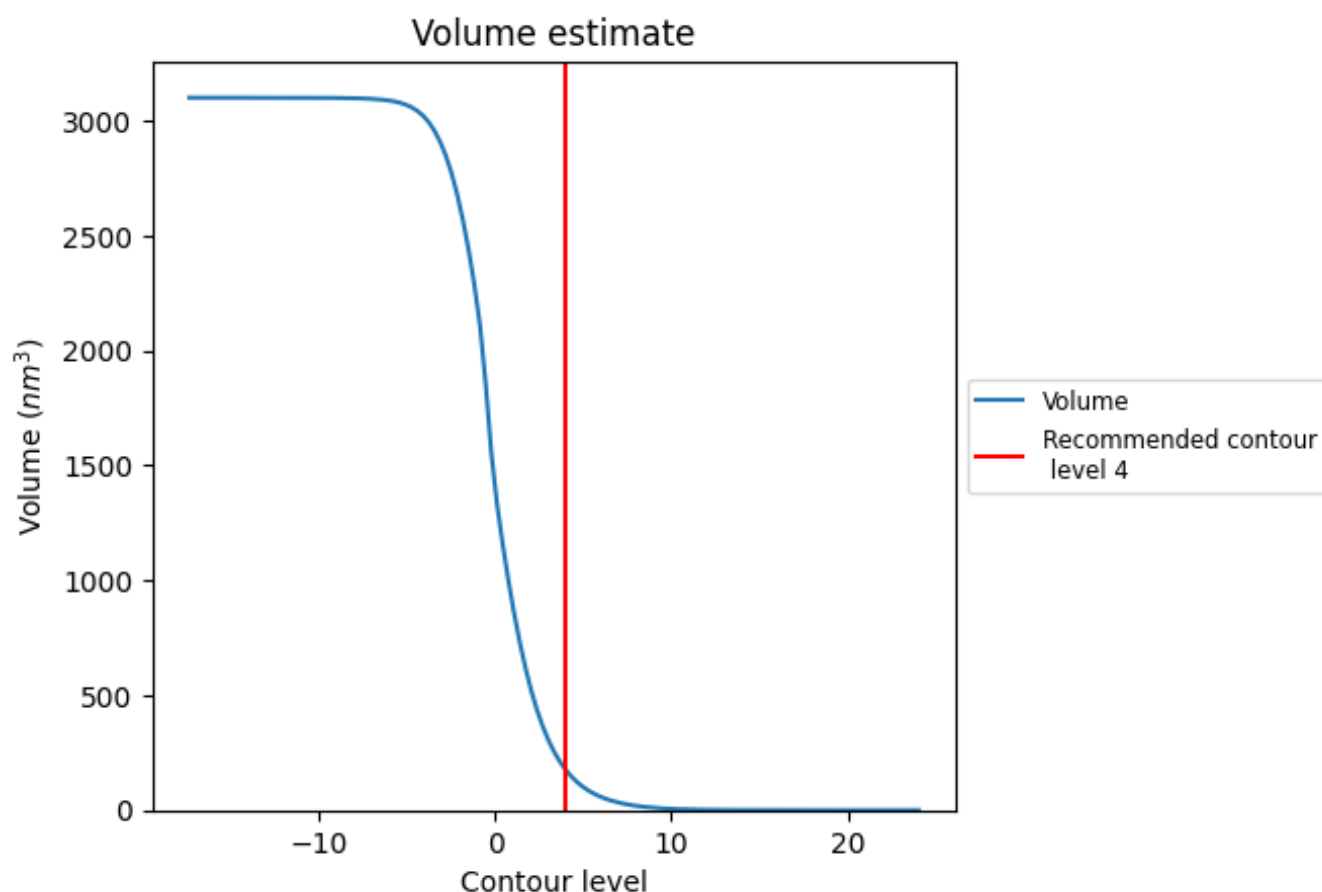
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 177 nm³; this corresponds to an approximate mass of 160 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

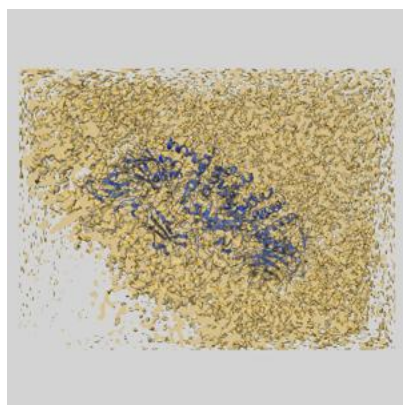
8 Fourier-Shell correlation ⓘ

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

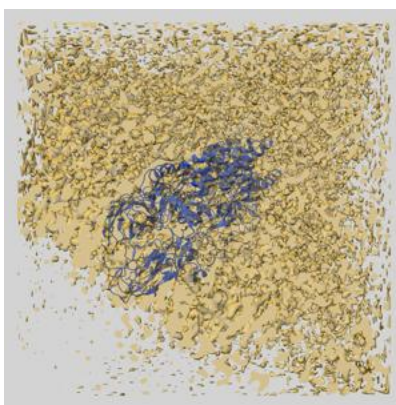
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5499 and PDB model 3J2P. Per-residue inclusion information can be found in section [3](#) on page [6](#).

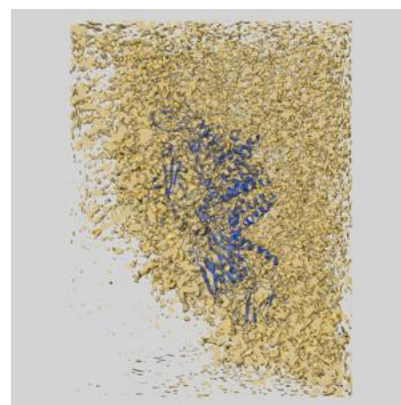
9.1 Map-model overlay [i](#)



X



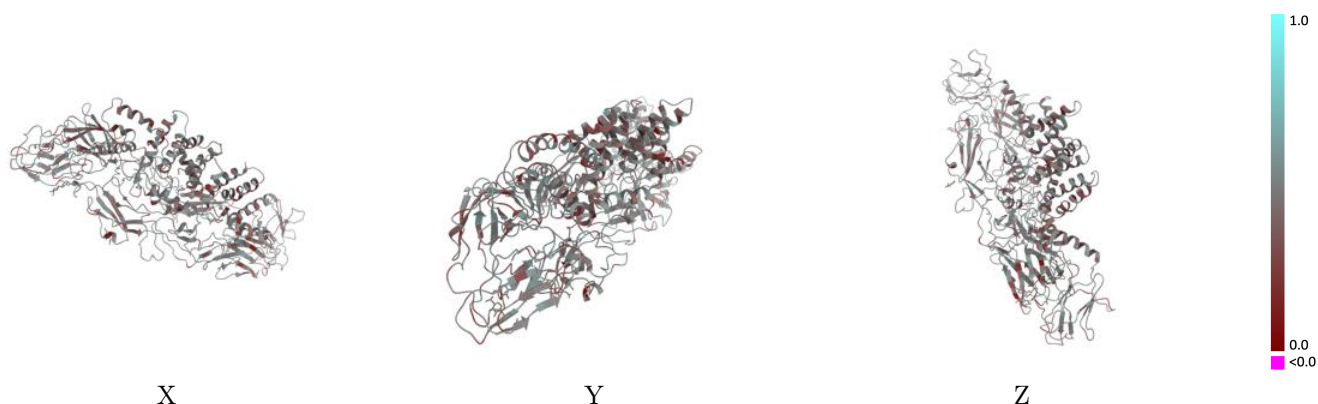
Y



Z

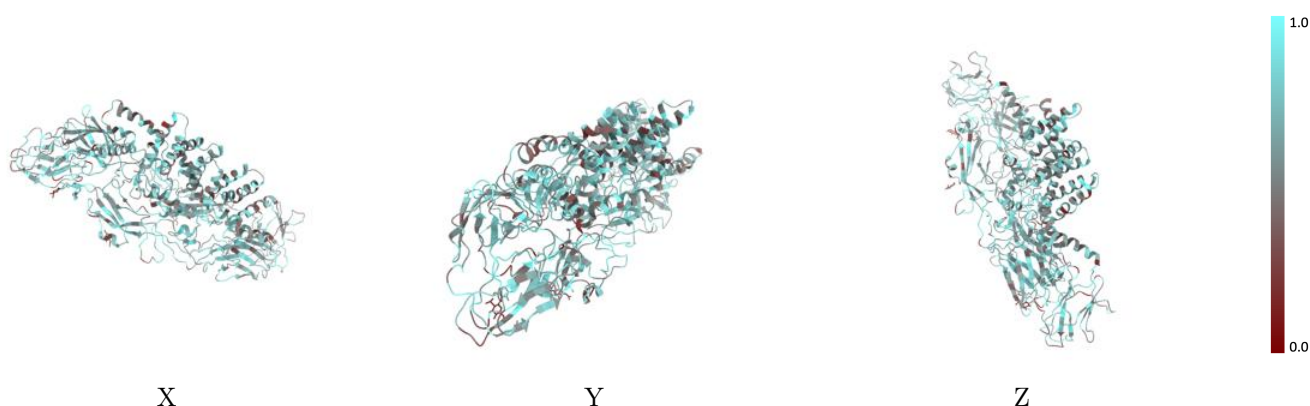
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



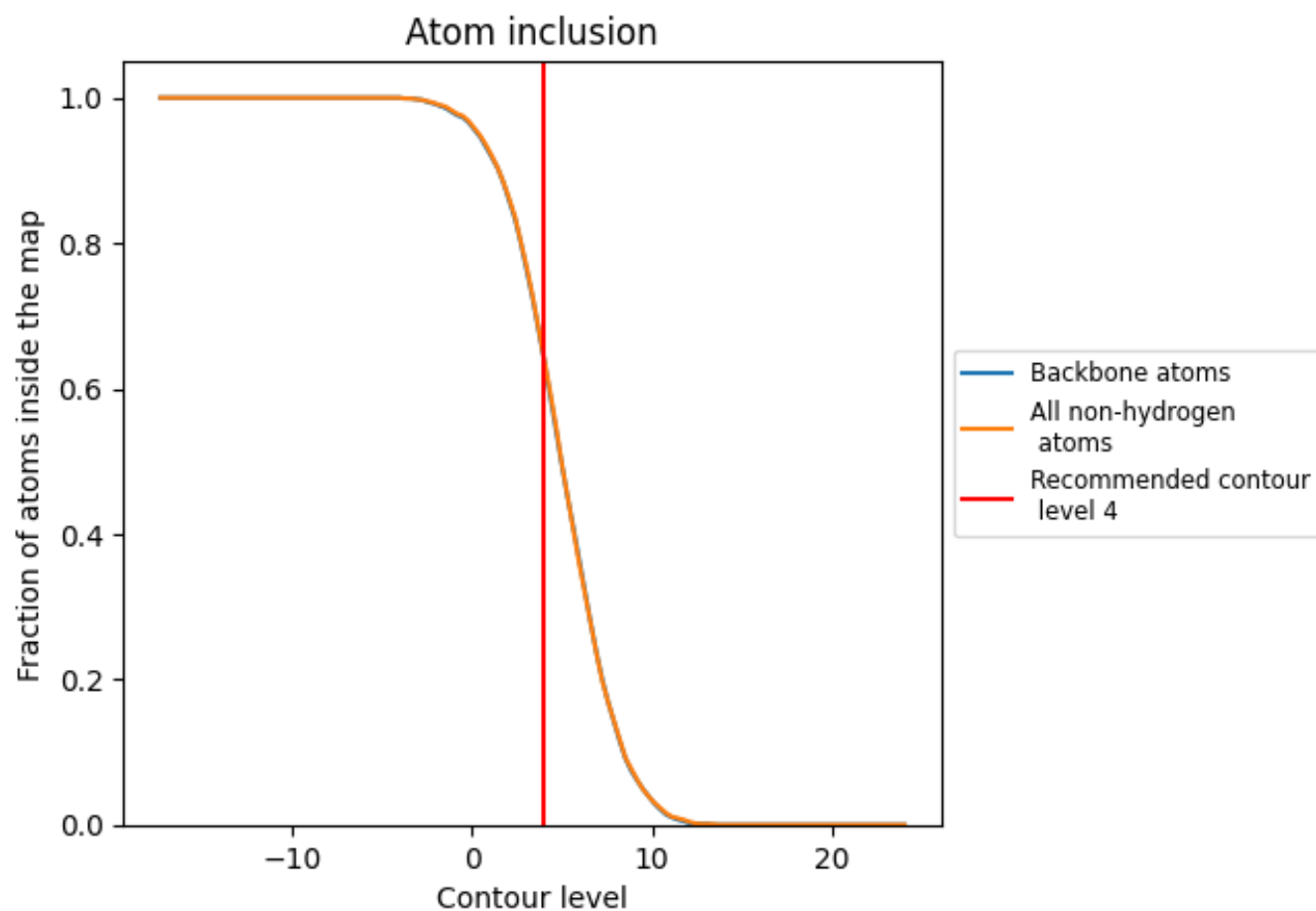
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6410	0.4450
A	0.6450	0.4450
B	0.6480	0.4450
C	0.6480	0.4450
D	0.6450	0.4460
E	0.3930	0.4390
F	0.4290	0.4420

1.0

0.0

<0.0