



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 11:23 PM UTC

PDB ID : 3JA8 / pdb_00003ja8
EMDB ID : EMD-6338
Title : Cryo-EM structure of the MCM2-7 double hexamer
Authors : Li, N.; Zhai, Y.; Zhang, Y.; Li, W.; Yang, M.; Lei, J.; Tye, B.K.; Gao, N.
Deposited on : 2015-05-09
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

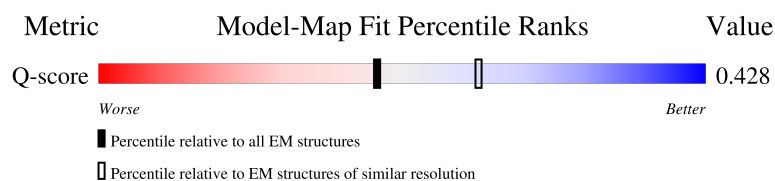
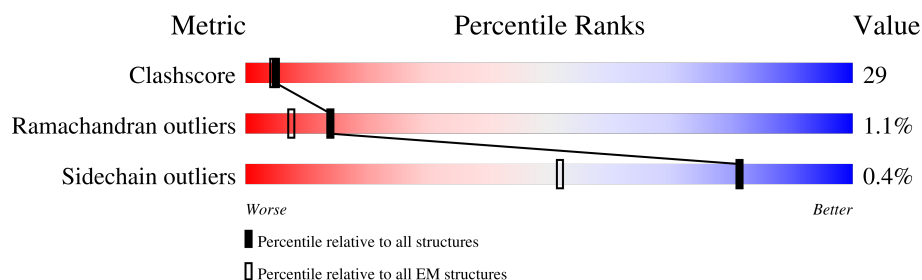
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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	2	868	
2	3	971	
3	4	933	
4	5	775	

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Mol	Chain	Length	Quality of chain
5	6	1017	
6	7	845	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	ADP	6	2001	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 29838 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Minichromosome Maintenance 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	603	Total	C	N	O	S	0	0
			4714	2974	842	881	17		

- Molecule 2 is a protein called Minichromosome Maintenance 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	605	Total	C	N	O	S	0	0
			4745	2990	846	896	13		

- Molecule 3 is a protein called Minichromosome Maintenance 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	640	Total	C	N	O	S	0	0
			5081	3194	879	981	27		

- Molecule 4 is a protein called Minichromosome Maintenance 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	633	Total	C	N	O	S	0	0
			4962	3112	855	971	24		

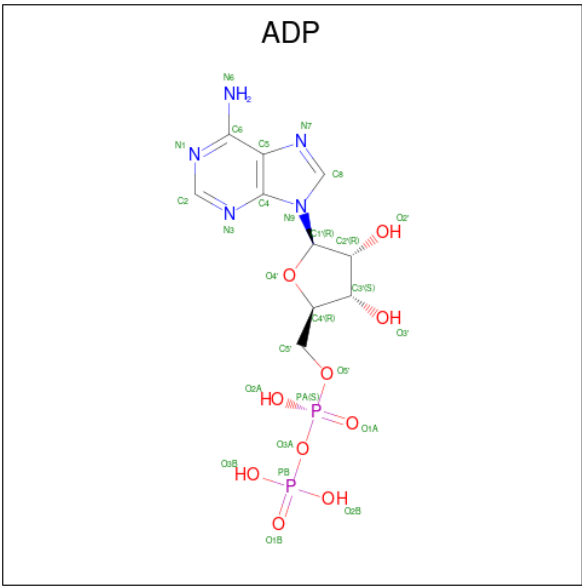
- Molecule 5 is a protein called Minichromosome Maintenance 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	616	Total	C	N	O	S	0	0
			4742	2985	841	896	20		

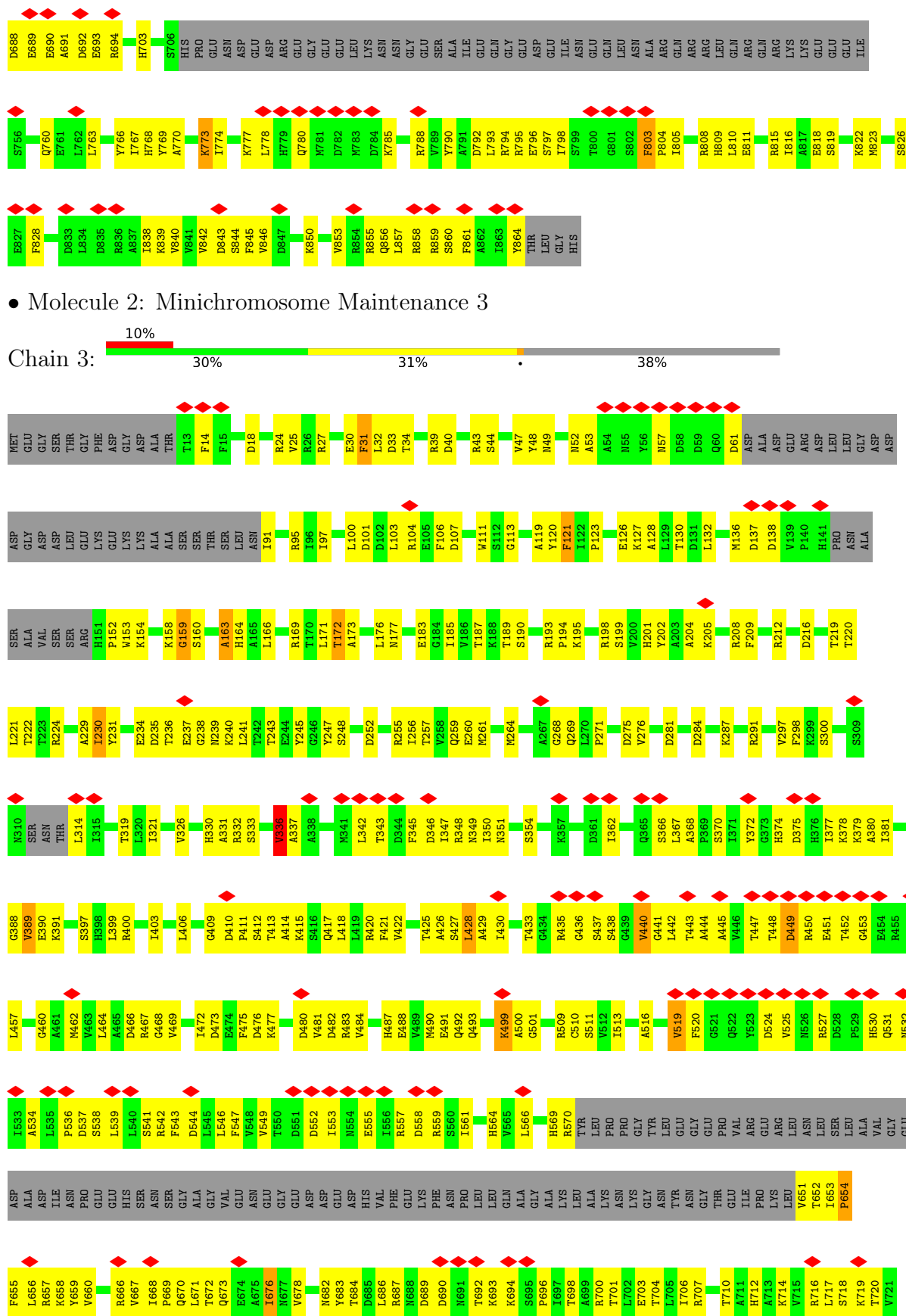
- Molecule 6 is a protein called Minichromosome Maintenance 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	689	Total	C	N	O	S	0	0
			5432	3419	940	1042	31		

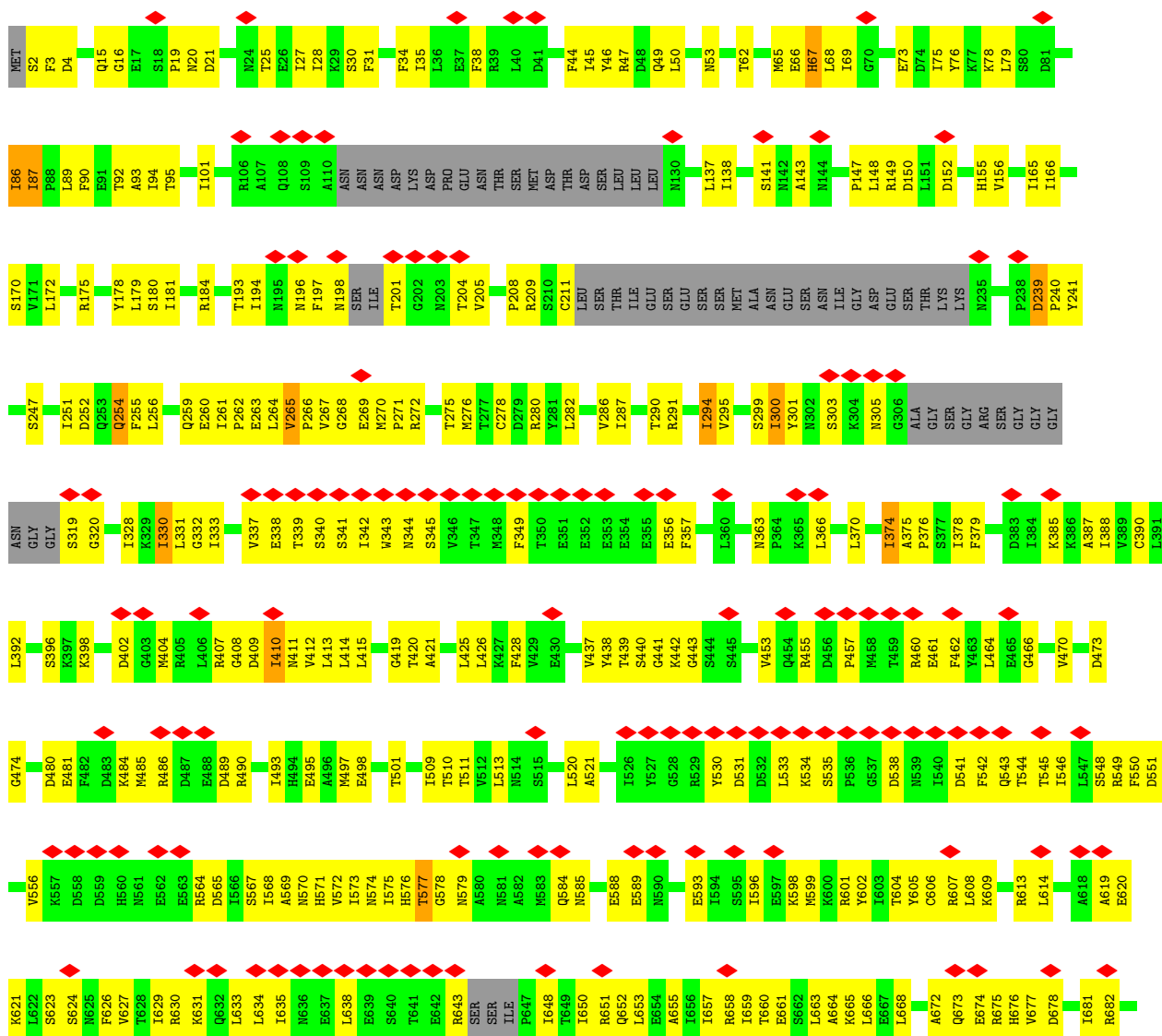
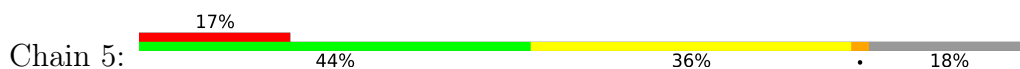
- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

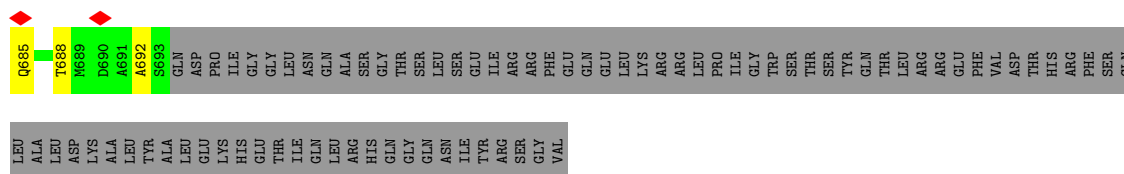


Mol	Chain	Residues	Atoms					AltConf
7	2	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	3	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	4	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	5	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	6	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	7	1	Total	C	N	O	P	0
			27	10	5	10	2	

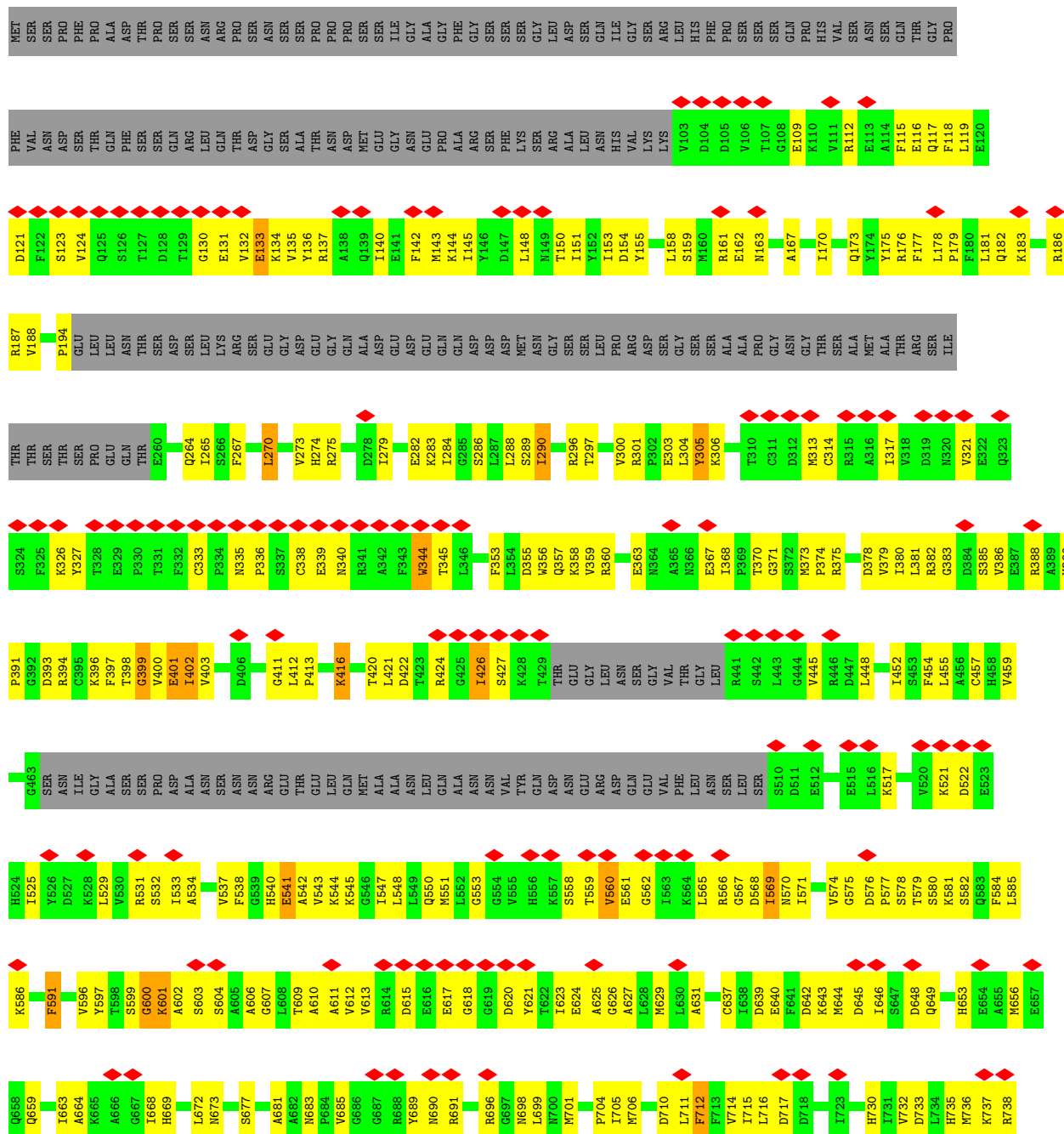
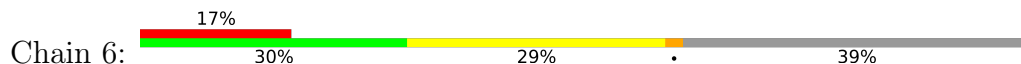


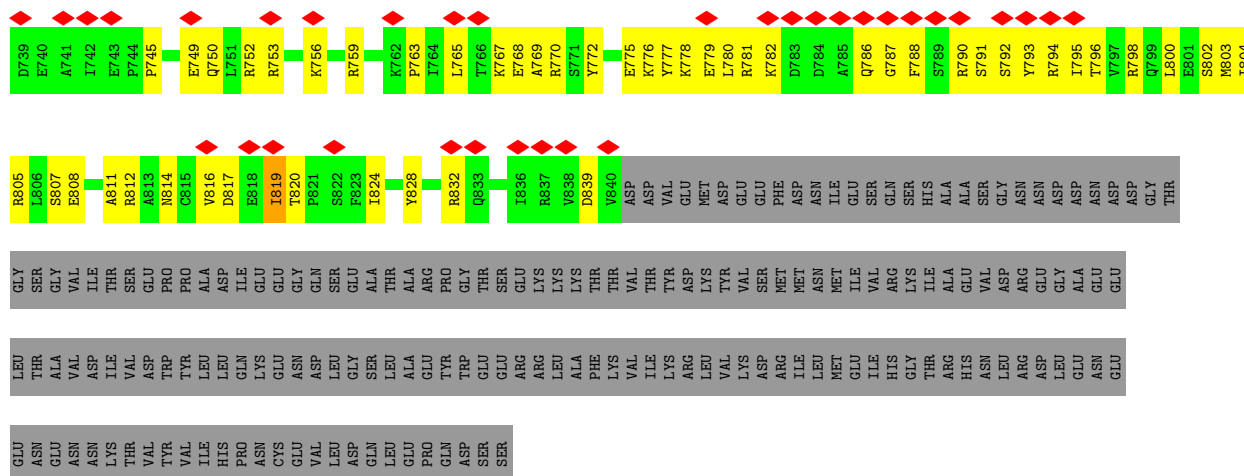
● Molecule 4: Minichromosome Maintenance 5



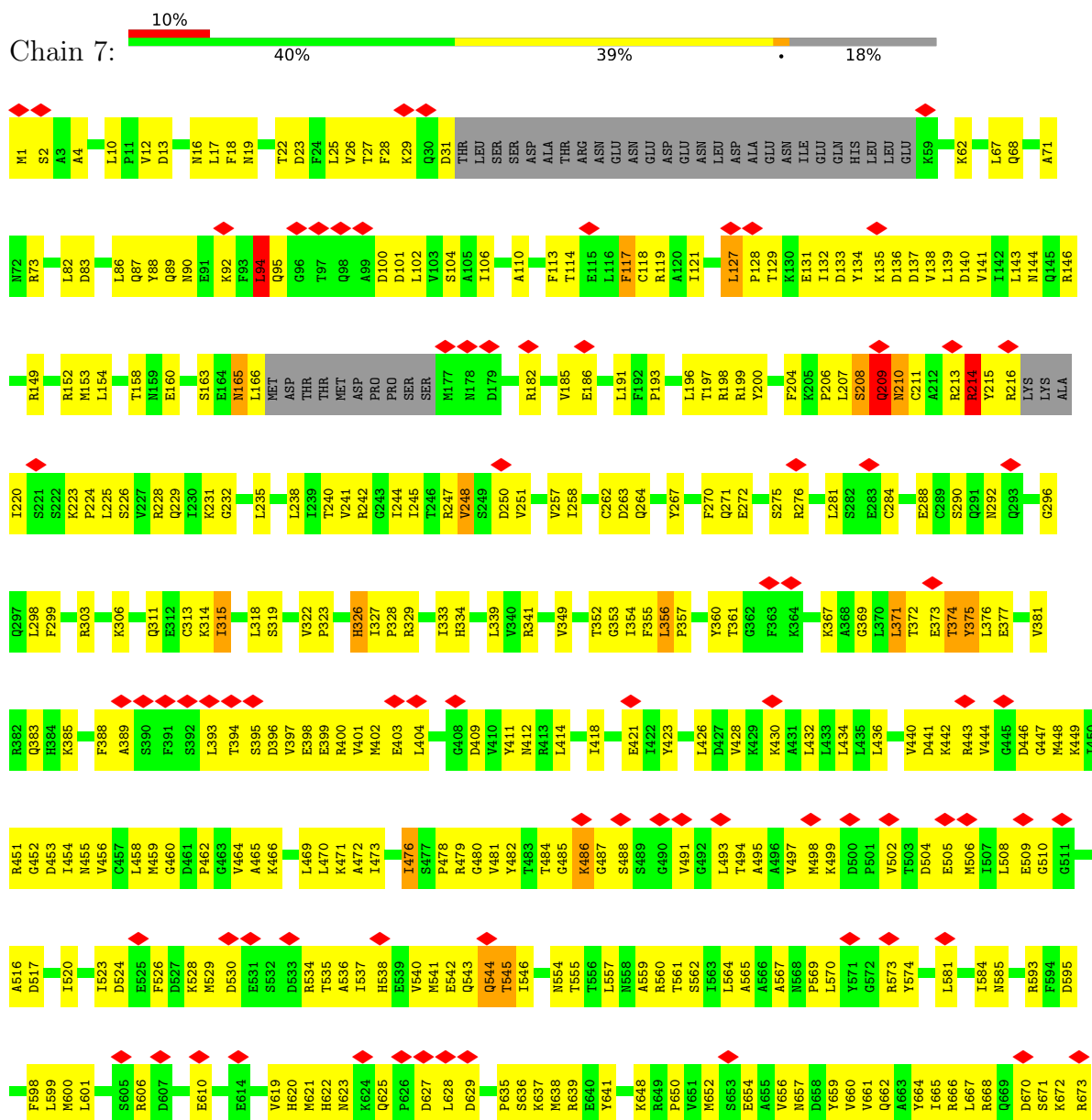


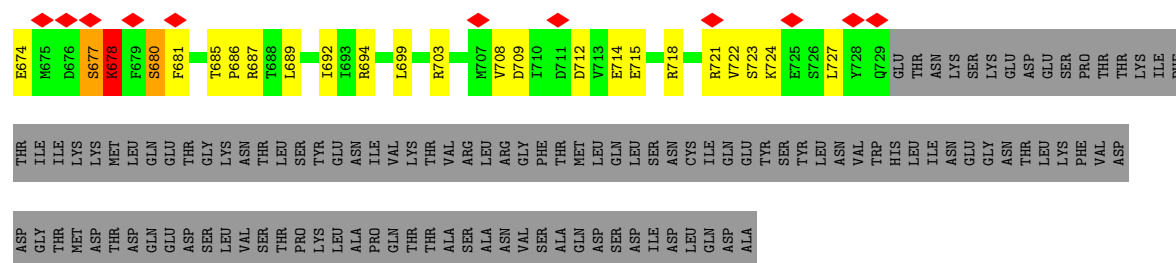
• Molecule 5: Minichromosome Maintenance 6





• Molecule 6: Minichromosome Maintenance 7





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	85365	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	CTFFIND	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	22	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	22500	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	32.028	Depositor
Minimum map value	-16.136	Depositor
Average map value	-0.058	Depositor
Map value standard deviation	0.697	Depositor
Recommended contour level	5	Depositor
Map size ($\text{\AA}$)	396.00003, 396.00003, 396.00003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.32, 1.32, 1.32	Depositor

5 Model quality

5.1 Standard geometry

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

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	2	0.53	0/4794	1.03	24/6479 (0.4%)
2	3	0.63	0/4827	1.03	22/6545 (0.3%)
3	4	0.59	0/5154	1.05	25/6967 (0.4%)
4	5	0.60	0/5032	0.99	17/6799 (0.3%)
5	6	0.53	0/4812	1.03	19/6497 (0.3%)
6	7	0.62	0/5514	1.03	22/7450 (0.3%)
All	All	0.59	0/30133	1.03	129/40737 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2	0	4
2	3	0	2
3	4	0	3
5	6	0	5
6	7	0	5
All	All	0	19

There are no bond length outliers.

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	7	356	LEU	CA-C-N	11.60	132.44	120.14
6	7	356	LEU	C-N-CA	11.60	132.44	120.14
1	2	570	GLY	N-CA-C	9.56	126.42	114.37
5	6	401	GLU	N-CA-C	9.35	121.08	111.07
6	7	486	LYS	N-CA-C	9.12	124.14	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	654	PRO	CA-N-CD	-9.04	99.35	112.00
1	2	371	GLY	CA-C-N	8.84	130.88	119.84
1	2	371	GLY	C-N-CA	8.84	130.88	119.84
3	4	686	LEU	CA-C-N	-8.75	110.71	119.90
3	4	686	LEU	C-N-CA	-8.75	110.71	119.90
3	4	714	GLU	N-CA-C	8.67	122.36	111.69
3	4	679	GLY	N-CA-C	8.21	122.57	112.64
5	6	333	CYS	CA-C-N	7.84	128.00	120.31
5	6	333	CYS	C-N-CA	7.84	128.00	120.31
3	4	376	CYS	CA-C-N	7.81	135.75	121.70
3	4	376	CYS	C-N-CA	7.81	135.75	121.70
1	2	366	ASN	CA-C-N	7.74	135.64	121.70
1	2	366	ASN	C-N-CA	7.74	135.64	121.70
6	7	208	SER	N-CA-C	-7.41	95.03	110.80
6	7	542	GLU	N-CA-C	-7.37	104.02	113.16
6	7	210	ASN	N-CA-C	-7.33	103.29	111.28
6	7	214	ARG	N-CA-C	7.22	119.16	111.28
5	6	399	GLY	N-CA-C	7.15	130.12	113.18
2	3	668	ILE	CA-C-N	7.06	127.21	119.87
2	3	668	ILE	C-N-CA	7.06	127.21	119.87
4	5	577	THR	N-CA-C	-7.00	98.54	108.96
6	7	648	LYS	N-CA-C	6.95	119.88	111.40
6	7	677	SER	CB-CA-C	-6.89	107.59	115.79
2	3	343	THR	CB-CA-C	-6.89	107.59	115.79
2	3	14	PHE	CB-CA-C	-6.83	108.69	116.54
6	7	267	TYR	CB-CA-C	-6.82	107.67	115.79
3	4	714	GLU	CA-C-N	6.78	133.91	121.70
3	4	714	GLU	C-N-CA	6.78	133.91	121.70
3	4	406	VAL	CA-C-N	6.76	126.90	119.87
3	4	406	VAL	C-N-CA	6.76	126.90	119.87
4	5	239	ASP	CA-C-N	6.73	128.25	119.84
4	5	239	ASP	C-N-CA	6.73	128.25	119.84
5	6	620	ASP	CB-CA-C	-6.65	108.92	116.63
2	3	163	ALA	N-CA-C	6.64	119.86	111.69
3	4	527	ALA	CA-C-N	6.52	125.96	118.85
3	4	527	ALA	C-N-CA	6.52	125.96	118.85
2	3	163	ALA	CA-C-N	6.51	133.41	121.70
2	3	163	ALA	C-N-CA	6.51	133.41	121.70
5	6	601	LYS	N-CA-C	6.49	122.08	111.37
1	2	439	ASN	N-CA-C	-6.49	105.00	113.17
1	2	213	SER	N-CA-C	-6.47	104.14	111.07
5	6	402	ILE	N-CA-C	6.18	122.19	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	6	340	ASN	CA-C-N	6.17	132.80	121.70
5	6	340	ASN	C-N-CA	6.17	132.80	121.70
2	3	208	ARG	CB-CA-C	-6.14	107.74	116.34
1	2	341	CYS	CB-CA-C	-6.10	108.53	115.79
6	7	326	HIS	CB-CA-C	-6.08	107.87	115.89
6	7	94	LEU	N-CA-C	6.06	120.83	111.56
4	5	255	PHE	N-CA-C	6.05	117.99	110.91
6	7	209	GLN	N-CA-C	-6.05	94.06	111.00
3	4	559	ARG	CB-CA-C	-6.05	108.60	115.79
5	6	601	LYS	CA-C-N	-6.05	113.52	122.41
5	6	601	LYS	C-N-CA	-6.05	113.52	122.41
2	3	166	LEU	N-CA-C	6.03	119.00	110.50
2	3	449	ASP	CB-CA-C	-6.00	109.07	117.23
2	3	336	VAL	CA-C-N	5.99	132.48	121.70
2	3	336	VAL	C-N-CA	5.99	132.48	121.70
2	3	499	LYS	N-CA-C	5.97	118.31	111.02
5	6	712	PHE	N-CA-C	5.97	119.03	111.69
1	2	521	GLY	N-CA-C	5.96	118.01	110.38
5	6	270	LEU	CA-C-N	5.92	125.54	119.56
5	6	270	LEU	C-N-CA	5.92	125.54	119.56
5	6	416	LYS	CA-C-N	5.92	125.83	119.85
5	6	416	LYS	C-N-CA	5.92	125.83	119.85
1	2	301	PRO	CA-C-O	-5.86	114.45	121.48
4	5	87	ILE	CA-C-N	-5.86	112.83	119.28
4	5	87	ILE	C-N-CA	-5.86	112.83	119.28
4	5	330	ILE	N-CA-C	5.81	116.17	107.51
1	2	412	ALA	CB-CA-C	-5.80	109.90	116.63
3	4	659	ALA	CB-CA-C	-5.77	109.93	116.63
3	4	181	TRP	N-CA-C	5.75	118.01	111.11
6	7	117	PHE	N-CA-C	-5.73	105.03	111.28
3	4	685	ASN	CB-CA-C	-5.71	108.99	115.79
6	7	127	LEU	CA-C-N	-5.68	112.75	119.84
6	7	127	LEU	C-N-CA	-5.68	112.75	119.84
6	7	677	SER	N-CA-C	5.67	119.76	109.32
4	5	300	ILE	N-CA-C	5.67	116.84	108.45
5	6	368	ILE	CA-C-N	5.64	125.82	119.90
5	6	368	ILE	C-N-CA	5.64	125.82	119.90
4	5	254	GLN	N-CA-C	5.62	120.14	112.04
3	4	402	THR	CA-C-N	5.56	125.18	119.56
3	4	402	THR	C-N-CA	5.56	125.18	119.56
4	5	86	ILE	N-CA-C	5.56	115.76	110.53
1	2	644	CYS	N-CA-C	5.51	118.02	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	773	LYS	N-CA-C	5.49	118.09	111.40
4	5	374	ILE	N-CA-C	5.44	116.17	110.62
2	3	336	VAL	CA-C-O	-5.38	114.06	120.78
2	3	121	PHE	N-CA-C	5.37	118.99	112.23
4	5	280	ARG	CB-CA-C	-5.32	110.00	117.23
3	4	355	THR	N-CA-C	5.29	119.84	113.17
1	2	365	THR	N-CA-C	5.28	122.05	110.80
3	4	288	ASN	CB-CA-C	-5.28	110.05	117.23
2	3	123	PRO	N-CA-C	5.27	117.13	110.70
2	3	31	PHE	N-CA-C	-5.25	100.68	109.24
2	3	510	CYS	N-CA-C	5.25	117.64	110.24
1	2	443	GLY	N-CA-C	5.25	120.91	111.62
6	7	208	SER	CA-C-N	5.24	131.13	121.70
6	7	208	SER	C-N-CA	5.24	131.13	121.70
4	5	419	GLY	N-CA-C	-5.24	108.09	115.32
3	4	588	GLY	N-CA-C	5.19	118.03	112.33
1	2	441	LYS	CA-C-N	5.18	131.03	121.70
1	2	441	LYS	C-N-CA	5.18	131.03	121.70
4	5	67	HIS	N-CA-C	-5.18	105.70	112.23
3	4	628	VAL	N-CA-C	5.17	115.48	107.78
3	4	202	LYS	CB-CA-C	-5.17	110.20	117.23
6	7	703	ARG	N-CA-C	-5.16	106.83	113.23
4	5	341	SER	N-CA-C	-5.16	106.94	113.18
1	2	393	ALA	CA-C-N	5.16	124.82	119.56
1	2	393	ALA	C-N-CA	5.16	124.82	119.56
6	7	275	SER	CB-CA-C	-5.15	109.13	116.34
4	5	265	VAL	CA-C-N	-5.14	113.41	119.84
4	5	265	VAL	C-N-CA	-5.14	113.41	119.84
3	4	264	TYR	CA-C-N	5.13	124.31	118.97
3	4	264	TYR	C-N-CA	5.13	124.31	118.97
1	2	334	LEU	N-CA-C	5.10	117.57	111.71
1	2	444	PHE	CA-C-N	-5.08	114.34	119.83
1	2	444	PHE	C-N-CA	-5.08	114.34	119.83
2	3	159	GLY	CA-C-O	-5.08	117.67	122.39
6	7	193	PRO	O-C-N	5.06	123.64	121.31
2	3	387	GLY	N-CA-C	5.05	125.16	113.18
1	2	263	CYS	CA-C-N	5.02	124.63	119.56
1	2	263	CYS	C-N-CA	5.02	124.63	119.56
5	6	591	PHE	N-CA-C	5.02	116.60	111.03
2	3	336	VAL	CB-CA-C	5.01	119.51	111.29

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	367	CYS	Peptide
1	2	372	PRO	Peptide
1	2	436	GLY	Peptide
1	2	803	PHE	Peptide
2	3	172	THR	Peptide
2	3	428	LEU	Peptide
3	4	352	CYS	Peptide
3	4	373	ARG	Peptide
3	4	408	ASP	Peptide
5	6	133	GLU	Peptide
5	6	338	CYS	Peptide
5	6	344	TRP	Peptide
5	6	398	THR	Peptide
5	6	600	GLY	Peptide
6	7	165	ASN	Peptide
6	7	545	THR	Peptide
6	7	678	LYS	Peptide
6	7	680	SER	Peptide
6	7	94	LEU	Peptide

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	2	4714	0	4730	268	0
2	3	4745	0	4793	323	0
3	4	5081	0	5125	351	0
4	5	4962	0	4994	279	0
5	6	4742	0	4692	332	0
6	7	5432	0	5495	369	0
7	2	27	0	12	1	0
7	3	27	0	12	4	0
7	4	27	0	12	6	0
7	5	27	0	12	7	0
7	6	27	0	12	10	0
7	7	27	0	12	6	0
All	All	29838	0	29901	1754	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 29.

All (1754) 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)
2:3:653:ILE:CD1	4:5:402:ASP:HB3	1.36	1.53
2:3:653:ILE:HD13	4:5:402:ASP:CB	1.55	1.36
2:3:652:THR:C	2:3:654:PRO:HD3	1.52	1.32
2:3:653:ILE:CD1	4:5:402:ASP:CB	2.11	1.26
6:7:214:ARG:HG3	6:7:215:TYR:C	1.64	1.19
5:6:355:ASP:OD2	5:6:383:GLY:N	1.80	1.13
2:3:653:ILE:HD11	4:5:402:ASP:HB3	1.19	1.09
1:2:327:ARG:NH1	4:5:269:GLU:OE2	1.85	1.08
2:3:652:THR:C	2:3:654:PRO:CD	2.25	1.08
1:2:298:SER:O	1:2:319:ARG:NH1	1.87	1.08
2:3:366:SER:CB	2:3:651:VAL:HG13	1.83	1.07
2:3:366:SER:HB3	2:3:651:VAL:HG13	1.09	1.06
2:3:43:ARG:HH12	2:3:137:ASP:HB2	1.17	1.05
2:3:654:PRO:HD2	2:3:655:PHE:H	1.17	1.05
6:7:662:GLN:HB3	6:7:666:ARG:HH12	1.18	1.05
2:3:652:THR:O	2:3:654:PRO:HD2	1.57	1.04
2:3:652:THR:O	2:3:654:PRO:CD	2.05	1.04
6:7:453:ASP:OD2	6:7:562:SER:OG	1.75	1.04
4:5:442:LYS:NZ	4:5:484:LYS:O	1.92	1.02
6:7:149:ARG:NH1	6:7:152:ARG:HH11	1.59	1.00
2:3:409:GLY:O	2:3:415:LYS:NZ	1.95	1.00
6:7:460:GLY:O	6:7:466:LYS:NZ	1.94	0.99
1:2:614:ASP:OD1	1:2:617:ARG:NH1	1.96	0.99
3:4:506:LEU:HB3	3:4:510:ARG:HH12	1.28	0.99
2:3:234:GLU:OE2	2:3:240:LYS:NZ	1.95	0.98
5:6:566:ARG:NH1	5:6:656:MET:O	1.97	0.98
3:4:315:ARG:HH12	6:7:251:VAL:N	1.60	0.98
2:3:569:HIS:O	4:5:398:LYS:NZ	1.97	0.97
2:3:653:ILE:CD1	4:5:402:ASP:CA	2.41	0.97
6:7:118:CYS:SG	6:7:198:ARG:NH1	2.37	0.97
1:2:656:ARG:HH11	5:6:794:ARG:HA	1.28	0.96
6:7:715:GLU:OE2	6:7:718:ARG:NH1	1.96	0.96
4:5:349:PHE:HB3	4:5:601:ARG:HH21	1.30	0.96
2:3:653:ILE:HD13	4:5:402:ASP:HB3	1.09	0.95
1:2:522:GLY:O	1:2:822:LYS:NZ	1.99	0.95
2:3:420:ARG:NH1	4:5:495:GLU:OE2	1.99	0.95
2:3:391:LYS:NZ	6:7:623:ASN:OD1	2.00	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:519:VAL:HG22	2:3:534:ALA:HB2	1.47	0.94
6:7:214:ARG:HB2	6:7:214:ARG:NH2	1.82	0.94
3:4:315:ARG:HH12	6:7:251:VAL:H	0.99	0.94
2:3:195:LYS:NZ	6:7:369:GLY:O	2.00	0.94
4:5:426:LEU:HD21	4:5:520:LEU:HD22	1.50	0.93
2:3:366:SER:HB3	2:3:651:VAL:CG1	1.98	0.93
3:4:647:GLU:OE2	3:4:655:SER:N	2.02	0.93
2:3:43:ARG:NH1	2:3:137:ASP:HB2	1.85	0.91
5:6:575:GLY:O	5:6:581:LYS:NZ	2.04	0.91
2:3:389:VAL:HG12	2:3:390:GLU:H	1.32	0.90
3:4:428:ARG:HH12	3:4:482:GLU:HG3	1.36	0.90
6:7:94:LEU:HB2	6:7:95:GLN:HB2	1.52	0.90
1:2:433:ASN:HB2	1:2:434:TYR:HB2	1.52	0.90
5:6:183:LYS:HG2	5:6:186:ARG:HH11	1.34	0.90
5:6:355:ASP:HB3	5:6:356:TRP:HA	1.54	0.90
6:7:208:SER:HB3	6:7:209:GLN:CB	2.02	0.89
2:3:216:ASP:OD1	2:3:219:THR:N	2.06	0.89
4:5:606:CYS:O	4:5:665:LYS:NZ	2.05	0.89
2:3:519:VAL:HB	2:3:527:ARG:HH12	1.38	0.88
5:6:691:ARG:HH11	5:6:716:LEU:HD22	1.38	0.88
4:5:375:ALA:HB1	4:5:378:ILE:HB	1.56	0.87
5:6:778:LYS:HG2	5:6:782:LYS:HZ2	1.39	0.87
5:6:133:GLU:HB3	5:6:134:LYS:HA	1.55	0.86
4:5:551:ASP:OD2	4:5:658:ARG:NH2	2.09	0.86
3:4:202:LYS:HA	3:4:224:LEU:HA	1.57	0.86
3:4:557:ARG:HH11	3:4:668:ARG:NH2	1.74	0.86
6:7:315:ILE:HD13	6:7:333:ILE:HD12	1.57	0.86
3:4:211:GLU:OE2	3:4:212:ARG:NH1	2.10	0.85
2:3:255:ARG:NH2	2:3:275:ASP:OD2	2.07	0.85
6:7:288:GLU:O	6:7:292:ASN:ND2	2.09	0.85
2:3:212:ARG:HH11	2:3:229:ALA:HB1	1.39	0.85
5:6:586:LYS:NZ	5:6:597:TYR:OH	2.09	0.85
2:3:24:ARG:NH1	2:3:120:TYR:HB3	1.91	0.85
1:2:425:GLU:HB3	1:2:457:LYS:HB2	1.59	0.84
5:6:778:LYS:O	5:6:782:LYS:NZ	2.09	0.84
3:4:666:ASN:HD22	3:4:668:ARG:HH22	1.26	0.84
1:2:656:ARG:NH1	5:6:794:ARG:HA	1.91	0.84
1:2:327:ARG:NH1	1:2:420:PRO:HD3	1.92	0.84
3:4:731:ASP:O	6:7:442:LYS:NZ	2.10	0.84
5:6:296:ARG:HE	5:6:613:VAL:HG21	1.43	0.84
1:2:543:GLY:HA3	1:2:549:LYS:HD3	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:558:SER:HB3	5:6:559:THR:HA	1.57	0.84
2:3:653:ILE:N	2:3:654:PRO:HD3	1.91	0.84
6:7:73:ARG:NH1	6:7:136:ASP:OD1	2.10	0.83
5:6:737:LYS:O	5:6:738:ARG:NH1	2.11	0.83
2:3:654:PRO:HD2	2:3:655:PHE:N	1.91	0.83
1:2:299:ASP:HA	1:2:319:ARG:NH1	1.93	0.83
2:3:368:ALA:HB2	2:3:378:LYS:HE2	1.60	0.83
6:7:16:ASN:ND2	6:7:100:ASP:OD2	2.12	0.83
3:4:506:LEU:HB3	3:4:510:ARG:NH1	1.93	0.83
5:6:621:TYR:HB3	5:6:668:ILE:HD13	1.61	0.83
1:2:297:ILE:HG22	1:2:298:SER:H	1.43	0.83
6:7:73:ARG:O	6:7:199:ARG:NH1	2.11	0.83
4:5:197:PHE:HZ	4:5:251:ILE:HD11	1.45	0.82
5:6:296:ARG:HH12	5:6:360:ARG:NH1	1.76	0.82
2:3:653:ILE:HD13	4:5:402:ASP:CA	2.05	0.82
1:2:690:GLU:OE2	1:2:694:ARG:NE	2.13	0.82
3:4:432:ARG:NH1	3:4:586:PRO:O	2.12	0.82
2:3:559:ARG:HH21	4:5:627:VAL:HG21	1.45	0.81
3:4:489:LYS:NZ	3:4:497:GLU:HB2	1.94	0.81
6:7:453:ASP:OD1	6:7:454:ILE:N	2.13	0.81
6:7:529:MET:HE1	6:7:537:ILE:HD12	1.61	0.81
3:4:602:THR:HA	3:4:619:GLY:HA3	1.63	0.81
3:4:651:GLN:NE2	5:6:597:TYR:OH	2.13	0.81
1:2:243:GLU:OE2	1:2:298:SER:OG	1.98	0.80
2:3:291:ARG:HH11	4:5:511:THR:HG22	1.46	0.80
3:4:362:ARG:NH1	6:7:263:ASP:OD2	2.14	0.80
3:4:334:ARG:NH2	3:4:617:GLU:OE2	2.14	0.80
3:4:326:ILE:HD12	3:4:439:PHE:HB2	1.63	0.80
5:6:828:TYR:OH	5:6:832:ARG:NH2	2.13	0.80
5:6:796:THR:HG22	5:6:798:ARG:H	1.46	0.80
6:7:662:GLN:HB3	6:7:666:ARG:NH1	1.97	0.80
3:4:188:GLN:O	3:4:190:CYS:N	2.14	0.80
4:5:264:LEU:HB2	4:5:265:VAL:HG22	1.64	0.80
6:7:208:SER:HB3	6:7:209:GLN:CG	2.11	0.80
3:4:234:ARG:NH1	3:4:284:ILE:HG13	1.95	0.80
3:4:401:GLU:OE2	3:4:413:HIS:HB3	1.80	0.80
1:2:401:ARG:HG3	5:6:390:LYS:NZ	1.95	0.80
1:2:309:LEU:O	1:2:310:ARG:NH1	2.13	0.79
1:2:839:LYS:HZ3	1:2:864:TYR:HA	1.46	0.79
3:4:650:GLU:CD	3:4:796:ARG:HH12	1.90	0.79
2:3:437:SER:HB3	2:3:438:SER:HA	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:443:ARG:HH12	6:7:449:LYS:NZ	1.81	0.79
2:3:654:PRO:CD	2:3:655:PHE:H	1.95	0.79
3:4:315:ARG:NH1	6:7:251:VAL:H	1.79	0.79
4:5:608:LEU:HD11	4:5:609:LYS:NZ	1.97	0.79
3:4:408:ASP:CG	3:4:409:GLY:HA2	2.08	0.78
1:2:274:VAL:HG13	1:2:277:GLU:OE2	1.82	0.78
6:7:361:THR:HG21	6:7:367:LYS:HD2	1.64	0.78
3:4:519:TYR:HD1	3:4:811:MET:HE1	1.49	0.78
3:4:604:TYR:HE2	6:7:554:ASN:HD21	1.29	0.78
5:6:790:ARG:NH1	5:6:839:ASP:OD2	2.16	0.78
5:6:597:TYR:OH	5:6:639:ASP:OD2	2.01	0.78
6:7:504:ASP:HB3	6:7:505:GLU:HB3	1.66	0.78
5:6:689:TYR:HA	5:6:690:ASN:HB2	1.64	0.78
2:3:366:SER:CB	2:3:651:VAL:CG1	2.59	0.77
3:4:713:ASP:HB2	3:4:716:ASN:HB2	1.65	0.77
6:7:87:GLN:HE22	6:7:214:ARG:NH1	1.81	0.77
2:3:559:ARG:HE	4:5:627:VAL:HG11	1.50	0.77
3:4:406:VAL:HG23	6:7:560:ARG:HH12	1.49	0.77
1:2:339:PHE:HB2	1:2:348:LEU:HD23	1.65	0.77
2:3:336:VAL:HG12	2:3:337:ALA:HA	1.66	0.77
5:6:183:LYS:CG	5:6:186:ARG:HH11	1.98	0.77
5:6:691:ARG:NH1	5:6:716:LEU:HD22	2.00	0.77
1:2:502:ALA:HB3	1:2:512:LYS:HE2	1.67	0.77
3:4:616:LEU:HD23	5:6:373:MET:HE2	1.67	0.77
2:3:653:ILE:CD1	4:5:402:ASP:HA	2.15	0.76
1:2:327:ARG:HH12	1:2:420:PRO:HD3	1.49	0.76
2:3:230:ILE:HG22	2:3:231:TYR:H	1.51	0.76
4:5:170:SER:O	4:5:254:GLN:NE2	2.17	0.76
5:6:792:SER:HA	5:6:793:TYR:HB2	1.67	0.76
6:7:214:ARG:N	6:7:215:TYR:HA	2.00	0.76
5:6:580:SER:N	7:6:2001:ADP:O1A	2.17	0.75
5:6:691:ARG:HE	5:6:716:LEU:HD13	1.48	0.75
6:7:677:SER:OG	6:7:678:LYS:N	2.19	0.75
2:3:653:ILE:HD11	4:5:402:ASP:CB	1.95	0.75
6:7:530:ASP:O	6:7:534:ARG:NH1	2.18	0.75
6:7:23:ASP:O	6:7:27:THR:OG1	2.02	0.75
2:3:212:ARG:NH1	2:3:229:ALA:HB1	2.02	0.75
4:5:407:ARG:NH2	4:5:658:ARG:HH12	1.85	0.75
6:7:86:LEU:HD12	6:7:216:ARG:HG2	1.69	0.75
3:4:352:CYS:N	3:4:373:ARG:O	2.19	0.75
2:3:414:ALA:N	7:3:2001:ADP:O1A	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:455:ASN:ND2	6:7:541:MET:SD	2.60	0.74
1:2:523:VAL:HG12	1:2:525:LYS:HB3	1.68	0.74
6:7:87:GLN:HE22	6:7:214:ARG:HH12	1.33	0.74
2:3:291:ARG:NH1	4:5:511:THR:HG22	2.02	0.74
4:5:538:ASP:H	4:5:544:THR:HG22	1.52	0.74
1:2:507:GLY:HA3	1:2:512:LYS:HE3	1.70	0.74
2:3:684:THR:HG21	6:7:610:GLU:OE2	1.87	0.74
5:6:426:ILE:HG22	5:6:427:SER:H	1.51	0.74
6:7:443:ARG:NH1	6:7:449:LYS:NZ	2.35	0.74
3:4:594:LYS:HG3	6:7:535:THR:HG21	1.68	0.74
4:5:204:THR:HG22	4:5:205:VAL:HG23	1.69	0.74
5:6:776:LYS:O	5:6:779:GLU:HG2	1.88	0.74
6:7:214:ARG:HG3	6:7:215:TYR:O	1.86	0.74
6:7:247:ARG:HG2	6:7:314:LYS:HZ1	1.52	0.74
2:3:553:ILE:HB	4:5:630:ARG:HD2	1.68	0.74
5:6:296:ARG:NH1	5:6:360:ARG:NH1	2.36	0.74
1:2:253:LYS:HE2	1:2:256:LEU:HD11	1.68	0.74
3:4:333:LEU:HD12	3:4:398:LYS:HZ2	1.52	0.74
5:6:533:ILE:HD12	5:6:544:LYS:HB3	1.70	0.73
3:4:561:ASP:O	3:4:803:ARG:NH2	2.22	0.73
2:3:519:VAL:HB	2:3:527:ARG:NH1	2.03	0.73
3:4:764:GLU:HA	3:4:767:LYS:NZ	2.02	0.73
3:4:348:LYS:HB3	3:4:353:ASP:OD2	1.89	0.73
4:5:608:LEU:HD11	4:5:609:LYS:HZ2	1.53	0.73
5:6:819:ILE:HG22	5:6:820:THR:H	1.54	0.73
2:3:362:ILE:CG2	2:3:651:VAL:HG21	2.17	0.73
3:4:234:ARG:HE	3:4:291:TYR:HE2	1.36	0.73
5:6:538:PHE:H	7:6:2001:ADP:HN62	1.35	0.73
5:6:566:ARG:HH21	5:6:659:GLN:HB2	1.52	0.73
2:3:314:LEU:O	4:5:175:ARG:NH2	2.21	0.72
3:4:712:VAL:HG22	6:7:672:LYS:NZ	2.03	0.72
4:5:379:PHE:H	7:5:2001:ADP:HN62	1.34	0.72
4:5:455:ARG:NH1	4:5:460:ARG:HB3	2.02	0.72
6:7:208:SER:HB3	6:7:209:GLN:HB2	1.69	0.72
5:6:582:SER:HA	5:6:585:LEU:HD12	1.69	0.72
6:7:154:LEU:HD21	6:7:191:LEU:HD11	1.71	0.72
2:3:159:GLY:HA2	2:3:160:SER:HB2	1.71	0.72
3:4:484:GLU:O	3:4:488:ASN:N	2.21	0.72
3:4:512:VAL:HG13	3:4:515:ARG:NH1	2.03	0.72
6:7:214:ARG:HB2	6:7:214:ARG:HH21	1.51	0.72
1:2:300:PHE:O	1:2:302:THR:OG1	2.06	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:198:ARG:NH2	6:7:200:TYR:OH	2.20	0.72
6:7:73:ARG:HD2	6:7:140:ASP:OD2	1.90	0.72
6:7:214:ARG:HG3	6:7:215:TYR:CA	2.18	0.72
3:4:458:LYS:NZ	5:6:413:PRO:HB3	2.04	0.72
7:4:2001:ADP:O3A	6:7:687:ARG:NH2	2.22	0.72
4:5:588:GLU:O	4:5:593:GLU:N	2.23	0.72
2:3:163:ALA:H	2:3:164:HIS:HB2	1.55	0.72
3:4:370:ARG:HB2	3:4:371:CYS:HB2	1.70	0.72
3:4:592:SER:HA	3:4:632:ASP:HB2	1.71	0.72
6:7:73:ARG:NH1	6:7:140:ASP:OD2	2.23	0.72
2:3:49:ASN:OD1	2:3:91:ILE:N	2.22	0.72
2:3:722:ASN:OD1	2:3:723:LYS:N	2.21	0.72
3:4:353:ASP:OD1	3:4:354:HIS:N	2.23	0.71
3:4:527:ALA:HB3	3:4:537:LYS:NZ	2.05	0.71
5:6:183:LYS:NZ	5:6:186:ARG:NH1	2.38	0.71
2:3:449:ASP:OD1	2:3:453:GLY:HA2	1.90	0.71
6:7:165:ASN:HB3	6:7:166:LEU:HA	1.71	0.71
2:3:113:GLY:HA3	2:3:121:PHE:CE2	2.26	0.71
6:7:228:ARG:NH2	6:7:327:ILE:O	2.23	0.71
6:7:385:LYS:HA	6:7:639:ARG:NH1	2.06	0.71
2:3:347:ILE:O	2:3:351:ASN:ND2	2.24	0.71
3:4:610:ASP:OD1	3:4:611:THR:N	2.23	0.71
6:7:443:ARG:HH12	6:7:449:LYS:HZ1	1.37	0.71
3:4:557:ARG:HH11	3:4:668:ARG:HH21	1.39	0.70
3:4:701:ARG:NH2	7:6:2001:ADP:O3B	2.24	0.70
3:4:767:LYS:HG2	5:6:732:VAL:HG11	1.72	0.70
3:4:188:GLN:C	3:4:190:CYS:H	2.00	0.70
3:4:575:SER:OG	7:4:2001:ADP:O2A	2.06	0.70
1:2:242:LEU:HB3	1:2:295:VAL:HG12	1.74	0.70
2:3:440:VAL:HG21	2:3:482:ASP:OD2	1.91	0.70
6:7:374:THR:OG1	6:7:375:TYR:N	2.19	0.70
2:3:362:ILE:CG2	2:3:651:VAL:CG2	2.69	0.70
4:5:407:ARG:CZ	4:5:658:ARG:HH12	2.04	0.70
6:7:146:ARG:NH1	6:7:196:LEU:HD21	2.06	0.70
6:7:149:ARG:NH1	6:7:152:ARG:NH1	2.37	0.70
2:3:689:ASP:O	2:3:692:THR:OG1	2.10	0.70
1:2:325:THR:HG22	1:2:326:ARG:H	1.56	0.69
2:3:400:ARG:NH2	2:3:544:ASP:OD1	2.24	0.69
1:2:766:TYR:OH	1:2:823:MET:O	2.10	0.69
1:2:843:ASP:OD1	1:2:844:SER:N	2.25	0.69
2:3:212:ARG:NH1	2:3:229:ALA:O	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:420:ARG:NH2	4:5:501:THR:OG1	2.21	0.69
3:4:259:HIS:ND1	6:7:135:LYS:HE3	2.06	0.69
3:4:349:CYS:H	3:4:353:ASP:CG	2.01	0.69
6:7:482:TYR:OH	6:7:524:ASP:OD2	2.03	0.69
1:2:441:LYS:HA	1:2:442:ASN:HB2	1.74	0.69
3:4:512:VAL:HG13	3:4:515:ARG:HH12	1.57	0.69
5:6:288:LEU:H	5:6:399:GLY:HA3	1.57	0.69
1:2:299:ASP:HA	1:2:319:ARG:HH12	1.55	0.69
1:2:839:LYS:NZ	1:2:864:TYR:HA	2.07	0.69
4:5:78:LYS:HG3	4:5:86:ILE:HD11	1.74	0.69
5:6:301:ARG:NH2	5:6:618:GLY:O	2.25	0.69
1:2:241:SER:OG	1:2:413:ASP:OD2	2.10	0.69
2:3:654:PRO:O	2:3:658:LYS:NZ	2.26	0.69
3:4:428:ARG:NH1	3:4:482:GLU:HA	2.06	0.69
3:4:483:GLN:HG3	3:4:484:GLU:H	1.56	0.69
5:6:123:SER:HB2	5:6:135:VAL:H	1.57	0.69
2:3:113:GLY:HA3	2:3:121:PHE:HE2	1.57	0.69
2:3:451:GLU:HG3	2:3:452:THR:HG23	1.75	0.69
1:2:495:ASP:CG	1:2:509:ARG:HH12	2.00	0.69
3:4:727:LEU:N	3:4:728:TYR:HB3	2.09	0.68
2:3:520:PHE:HE1	4:5:542:PHE:HB3	1.58	0.68
3:4:354:HIS:HD2	3:4:372:GLU:HG3	1.57	0.68
3:4:774:TYR:OH	3:4:778:ARG:NH2	2.26	0.68
4:5:375:ALA:H	4:5:385:LYS:HE3	1.58	0.68
1:2:780:GLN:NE2	4:5:577:THR:O	2.27	0.68
6:7:484:THR:HG23	6:7:487:GLY:HA2	1.76	0.68
2:3:53:ALA:O	2:3:57:ASN:ND2	2.27	0.68
2:3:260:GLU:OE2	2:3:271:PRO:HA	1.94	0.68
6:7:498:MET:HE3	6:7:509:GLU:HB3	1.76	0.68
3:4:489:LYS:HZ1	3:4:497:GLU:HB2	1.59	0.68
5:6:609:THR:HG22	5:6:610:ALA:H	1.59	0.68
1:2:583:ASP:HB3	1:2:587:LYS:HE3	1.76	0.68
2:3:570:ARG:HB3	4:5:613:ARG:HH21	1.58	0.68
3:4:714:GLU:H	3:4:715:LYS:HB3	1.58	0.68
3:4:830:ARG:HD3	3:4:833:ILE:HD12	1.76	0.67
4:5:375:ALA:N	4:5:385:LYS:HE3	2.09	0.67
4:5:461:GLU:HG2	4:5:462:PHE:H	1.59	0.67
4:5:570:ASN:O	4:5:574:ASN:ND2	2.27	0.67
5:6:625:ALA:HB3	5:6:626:GLY:HA2	1.74	0.67
6:7:459:MET:C	6:7:466:LYS:HZ3	2.01	0.67
2:3:410:ASP:O	2:3:413:THR:OG1	2.11	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:716:ARG:HH22	2:3:724:VAL:HB	1.57	0.67
5:6:540:HIS:O	5:6:542:ALA:N	2.27	0.67
5:6:600:GLY:HA2	5:6:602:ALA:N	2.08	0.67
6:7:247:ARG:HG2	6:7:314:LYS:NZ	2.08	0.67
1:2:549:LYS:HE3	7:2:2001:ADP:O2B	1.94	0.67
3:4:563:ASN:ND2	3:4:649:MET:SD	2.68	0.67
5:6:759:ARG:HA	5:6:812:ARG:HH21	1.59	0.67
6:7:388:PHE:HB2	6:7:389:ALA:HA	1.75	0.67
4:5:178:TYR:HD1	4:5:193:THR:HG22	1.59	0.67
6:7:228:ARG:HE	6:7:329:ARG:HG3	1.59	0.67
2:3:163:ALA:HB3	2:3:164:HIS:HD1	1.59	0.67
2:3:48:TYR:O	2:3:52:ASN:ND2	2.24	0.67
5:6:575:GLY:N	5:6:581:LYS:HZ3	1.92	0.67
4:5:166:ILE:HD12	4:5:286:VAL:HG11	1.77	0.67
5:6:183:LYS:HZ2	5:6:186:ARG:NH1	1.93	0.67
2:3:101:ASP:HA	2:3:104:ARG:HH21	1.59	0.67
6:7:104:SER:OG	6:7:216:ARG:NH1	2.27	0.67
1:2:601:LYS:NZ	1:2:643:ARG:HD2	2.11	0.66
2:3:276:VAL:HG22	2:3:321:ILE:HB	1.77	0.66
6:7:428:VAL:HG21	6:7:600:MET:HE2	1.77	0.66
6:7:652:MET:HG2	6:7:708:VAL:HG11	1.77	0.66
1:2:338:LYS:HE2	1:2:379:LYS:HB2	1.77	0.66
2:3:651:VAL:O	2:3:651:VAL:HG12	1.94	0.66
5:6:696:ARG:HA	5:6:706:MET:HE1	1.78	0.66
5:6:767:LYS:HE3	5:6:769:ALA:HB3	1.77	0.66
6:7:444:VAL:HG22	6:7:448:MET:H	1.60	0.66
5:6:781:ARG:HG2	5:6:795:ILE:HB	1.78	0.66
6:7:593:ARG:HG2	6:7:687:ARG:NH1	2.10	0.66
1:2:394:PRO:O	5:6:673:ASN:ND2	2.28	0.66
3:4:717:ASP:OD2	6:7:668:ARG:HG2	1.96	0.66
5:6:179:PRO:HA	5:6:182:GLN:NE2	2.10	0.66
1:2:309:LEU:H	1:2:310:ARG:NH1	1.94	0.66
1:2:678:ASP:OD1	1:2:679:ILE:N	2.29	0.66
5:6:399:GLY:HA2	5:6:454:PHE:CZ	2.31	0.66
2:3:24:ARG:HH12	2:3:120:TYR:HB3	1.58	0.65
6:7:149:ARG:HG3	6:7:153:MET:HE3	1.78	0.65
2:3:163:ALA:N	2:3:164:HIS:HB2	2.10	0.65
2:3:476:ASP:O	2:3:483:ARG:NH1	2.29	0.65
2:3:696:PRO:HB3	6:7:573:ARG:HH12	1.62	0.65
5:6:143:MET:HE2	5:6:150:THR:H	1.61	0.65
6:7:220:ILE:HA	6:7:223:LYS:HZ1	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:393:LEU:HA	6:7:394:THR:HB	1.77	0.65
6:7:670:ASP:OD1	6:7:671:SER:N	2.30	0.65
3:4:226:TYR:OH	3:4:247:ASN:ND2	2.22	0.65
2:3:95:ARG:NE	2:3:281:ASP:OD2	2.27	0.65
2:3:33:ASP:CB	2:3:39:ARG:HH11	2.09	0.65
2:3:189:THR:HG22	2:3:190:SER:H	1.61	0.65
3:4:714:GLU:N	3:4:715:LYS:HB3	2.11	0.65
6:7:543:GLN:HG3	6:7:544:GLN:H	1.60	0.65
2:3:476:ASP:HA	2:3:483:ARG:HH12	1.61	0.65
3:4:532:GLU:HG2	3:4:533:LEU:H	1.59	0.65
4:5:301:TYR:CE1	4:5:303:SER:HB3	2.31	0.65
2:3:524:ASP:OD1	2:3:532:ASN:ND2	2.30	0.65
3:4:509:ILE:HD11	3:4:749:MET:HE2	1.77	0.65
5:6:541:GLU:O	5:6:545:LYS:NZ	2.28	0.65
2:3:553:ILE:HD11	4:5:634:LEU:HD13	1.80	0.64
2:3:119:ALA:HA	2:3:221:LEU:HD22	1.79	0.64
2:3:525:VAL:HG11	2:3:552:ASP:OD2	1.97	0.64
3:4:360:ILE:HG13	3:4:365:ILE:HG12	1.79	0.64
4:5:149:ARG:NH1	4:5:272:ARG:HE	1.95	0.64
6:7:67:LEU:HD11	6:7:121:ILE:HG23	1.79	0.64
3:4:370:ARG:HH12	5:6:426:ILE:CG1	2.10	0.64
3:4:650:GLU:OE1	3:4:796:ARG:NH1	2.31	0.64
3:4:703:ASP:OD1	3:4:800:SER:OG	2.08	0.64
5:6:596:VAL:HG23	5:6:631:ALA:HB2	1.79	0.64
5:6:776:LYS:HD3	5:6:828:TYR:HB2	1.79	0.64
1:2:601:LYS:NZ	1:2:643:ARG:NH1	2.45	0.64
4:5:209:ARG:HA	4:5:239:ASP:HB3	1.78	0.64
1:2:811:GLU:OE2	1:2:815:ARG:NH1	2.31	0.64
2:3:542:ARG:NH1	2:3:700:ARG:NH1	2.45	0.64
3:4:408:ASP:OD2	3:4:409:GLY:HA2	1.97	0.64
6:7:220:ILE:HA	6:7:223:LYS:NZ	2.13	0.64
6:7:662:GLN:CB	6:7:666:ARG:HH12	2.02	0.64
1:2:289:ILE:HG22	1:2:290:HIS:CD2	2.33	0.64
2:3:268:GLY:O	2:3:269:GLN:HG3	1.97	0.64
3:4:573:SER:N	7:4:2001:ADP:O1A	2.25	0.64
5:6:300:VAL:HG22	5:6:357:GLN:HB3	1.78	0.64
5:6:531:ARG:HD2	5:6:745:PRO:HG3	1.80	0.64
5:6:752:ARG:C	5:6:756:LYS:HZ3	2.05	0.64
6:7:149:ARG:HH11	6:7:152:ARG:HE	1.46	0.64
6:7:423:TYR:O	7:7:2001:ADP:N6	2.31	0.64
1:2:286:TYR:HE2	1:2:293:ILE:HD11	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:505:ILE:HG22	1:2:507:GLY:H	1.62	0.64
3:4:471:ASP:OD1	3:4:472:LYS:N	2.31	0.64
4:5:172:LEU:HD13	4:5:252:ASP:OD2	1.98	0.64
1:2:401:ARG:HG3	5:6:390:LYS:HZ2	1.61	0.63
1:2:792:ASP:O	1:2:859:ARG:NH1	2.31	0.63
1:2:401:ARG:HG3	5:6:390:LYS:HZ3	1.62	0.63
1:2:524:PRO:HB2	1:2:525:LYS:HA	1.79	0.63
2:3:100:LEU:HB3	2:3:111:TRP:HZ3	1.62	0.63
2:3:400:ARG:HG3	2:3:493:GLN:OE1	1.98	0.63
4:5:392:LEU:O	4:5:607:ARG:NH2	2.30	0.63
5:6:183:LYS:HG2	5:6:186:ARG:NH1	2.11	0.63
5:6:775:GLU:O	5:6:779:GLU:N	2.31	0.63
4:5:457:PRO:O	4:5:460:ARG:NH2	2.31	0.63
2:3:390:GLU:HG2	2:3:509:ARG:HH12	1.64	0.63
3:4:186:SER:HB2	3:4:189:GLU:OE2	1.98	0.63
3:4:233:MET:HE3	3:4:239:SER:HA	1.81	0.63
1:2:505:ILE:HD13	1:2:552:ILE:HG13	1.79	0.63
2:3:654:PRO:CD	2:3:655:PHE:N	2.58	0.63
4:5:564:ARG:O	4:5:567:SER:OG	2.13	0.63
6:7:226:SER:HB3	6:7:229:GLN:HG2	1.80	0.63
1:2:526:ASN:HA	1:2:532:SER:HA	1.81	0.63
2:3:199:SER:OG	2:3:201:HIS:NE2	2.32	0.63
3:4:234:ARG:HH12	3:4:284:ILE:HG13	1.62	0.63
2:3:701:THR:O	2:3:704:THR:OG1	2.14	0.63
6:7:538:HIS:CD2	6:7:593:ARG:HE	2.17	0.63
1:2:540:LEU:HB2	1:2:677:PHE:CD2	2.33	0.62
2:3:445:ALA:HB3	2:3:499:LYS:HD2	1.81	0.62
4:5:178:TYR:CD1	4:5:193:THR:HG22	2.33	0.62
6:7:668:ARG:HH12	6:7:685:THR:HA	1.64	0.62
1:2:383:ARG:HE	1:2:411:LEU:HD23	1.64	0.62
1:2:816:ILE:O	1:2:819:SER:OG	2.16	0.62
5:6:355:ASP:HB3	5:6:356:TRP:CA	2.24	0.62
1:2:309:LEU:H	1:2:310:ARG:HH12	1.47	0.62
3:4:428:ARG:NH1	3:4:482:GLU:HG3	2.10	0.62
1:2:796:GLU:OE1	1:2:859:ARG:NE	2.30	0.62
3:4:365:ILE:HD12	5:6:448:LEU:HD21	1.82	0.62
3:4:444:ILE:HG21	5:6:411:GLY:HA2	1.81	0.62
3:4:658:LYS:HB3	5:6:604:SER:H	1.63	0.62
6:7:208:SER:OG	6:7:209:GLN:HA	2.00	0.62
6:7:211:CYS:O	6:7:214:ARG:HB3	2.00	0.62
1:2:235:GLY:HA2	1:2:283:TYR:HE2	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:734:ARG:O	2:3:738:LEU:N	2.24	0.62
3:4:651:GLN:HE21	5:6:586:LYS:NZ	1.97	0.62
4:5:165:ILE:HD11	4:5:291:ARG:NH1	2.15	0.62
1:2:319:ARG:HE	1:2:427:THR:HG22	1.64	0.62
1:2:338:LYS:NZ	1:2:376:ASN:HD21	1.97	0.62
2:3:269:GLN:HE21	4:5:287:ILE:HG23	1.64	0.62
4:5:388:ILE:HD11	4:5:425:LEU:HD21	1.82	0.62
6:7:491:VAL:HA	6:7:494:THR:HG22	1.80	0.62
2:3:467:ARG:NH1	2:3:509:ARG:CZ	2.63	0.61
6:7:357:PRO:HA	6:7:374:THR:HA	1.81	0.61
6:7:543:GLN:O	6:7:545:THR:N	2.33	0.61
3:4:458:LYS:HZ3	5:6:413:PRO:HB3	1.63	0.61
3:4:543:GLN:HA	3:4:562:ILE:HD11	1.82	0.61
4:5:147:PRO:HG2	4:5:150:ASP:HB2	1.82	0.61
4:5:357:PHE:CE1	4:5:598:LYS:HE2	2.36	0.61
1:2:616:ASP:O	1:2:619:SER:OG	2.15	0.61
3:4:408:ASP:C	3:4:410:GLN:H	2.07	0.61
1:2:778:LEU:HG	4:5:577:THR:HG22	1.82	0.61
5:6:550:GLN:HA	5:6:569:ILE:HG21	1.81	0.61
5:6:566:ARG:HH12	5:6:656:MET:C	2.04	0.61
5:6:412:LEU:HB3	5:6:416:LYS:NZ	2.15	0.61
5:6:522:ASP:HB2	5:6:525:ILE:HG23	1.82	0.61
6:7:680:SER:HB2	6:7:681:PHE:HA	1.81	0.61
3:4:519:TYR:CD1	3:4:811:MET:HE1	2.33	0.61
6:7:149:ARG:NH1	6:7:152:ARG:HE	1.97	0.61
2:3:30:GLU:O	2:3:34:THR:N	2.27	0.61
5:6:575:GLY:C	5:6:581:LYS:HZ1	2.03	0.61
6:7:465:ALA:HA	7:7:2001:ADP:H5'1	1.83	0.61
6:7:718:ARG:HA	6:7:721:ARG:NH1	2.14	0.61
2:3:27:ARG:NH2	2:3:107:ASP:OD1	2.33	0.61
5:6:611:ALA:H	5:6:624:GLU:HG2	1.66	0.61
1:2:212:LYS:HG3	1:2:274:VAL:CG1	2.31	0.61
3:4:196:ASN:OD1	3:4:197:PHE:N	2.34	0.61
4:5:626:PHE:CG	4:5:653:LEU:HD12	2.36	0.61
2:3:119:ALA:HB1	2:3:222:THR:HG22	1.82	0.61
3:4:688:VAL:O	3:4:691:ASN:N	2.33	0.61
4:5:441:GLY:HA3	4:5:443:GLY:N	2.16	0.60
1:2:212:LYS:HE3	1:2:274:VAL:HB	1.83	0.60
3:4:475:ASP:OD1	3:4:476:VAL:N	2.33	0.60
5:6:382:ARG:HH11	5:6:455:LEU:HD21	1.64	0.60
6:7:526:PHE:HB3	6:7:567:ALA:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:444:ALA:HA	2:3:499:LYS:HZ1	1.66	0.60
3:4:515:ARG:HG2	3:4:517:ASP:OD1	2.01	0.60
3:4:758:ILE:HG22	3:4:760:PRO:HD3	1.84	0.60
2:3:370:SER:OG	4:5:404:MET:SD	2.58	0.60
1:2:343:LYS:HZ3	1:2:371:GLY:CA	2.15	0.60
1:2:382:TYR:HD2	4:5:156:VAL:HG21	1.66	0.60
1:2:653:ASN:O	1:2:658:ASN:ND2	2.34	0.60
3:4:548:THR:N	3:4:806:GLU:OE2	2.33	0.60
5:6:296:ARG:HH12	5:6:360:ARG:HH11	1.47	0.60
1:2:687:VAL:HG13	1:2:692:ASP:OD2	2.02	0.60
2:3:428:LEU:HB3	2:3:429:ALA:CA	2.31	0.60
5:6:750:GLN:HA	5:6:753:ARG:NH1	2.16	0.60
6:7:248:VAL:HG23	6:7:313:CYS:HB3	1.83	0.60
5:6:183:LYS:NZ	5:6:186:ARG:HH12	2.00	0.60
6:7:451:ARG:O	6:7:694:ARG:NH2	2.32	0.60
1:2:335:LYS:HB3	1:2:381:VAL:O	2.02	0.60
1:2:684:ARG:HB3	1:2:685:ASP:HA	1.83	0.60
3:4:292:ASP:HA	3:4:293:LEU:HD12	1.83	0.60
3:4:493:ASN:O	3:4:494:GLU:HG2	2.00	0.60
4:5:196:ASN:OD1	4:5:197:PHE:N	2.34	0.60
5:6:610:ALA:HB3	5:6:663:ILE:HD13	1.84	0.60
5:6:803:MET:HE1	5:6:828:TYR:HA	1.82	0.60
6:7:224:PRO:HB2	6:7:242:ARG:HE	1.67	0.60
6:7:235:LEU:HD23	6:7:357:PRO:HG3	1.84	0.60
6:7:454:ILE:HG23	6:7:595:ASP:OD2	2.02	0.60
2:3:127:LYS:O	2:3:130:THR:OG1	2.19	0.59
2:3:557:ARG:O	2:3:561:ILE:HG12	2.02	0.59
4:5:531:ASP:HA	4:5:534:LYS:HD3	1.84	0.59
3:4:236:LEU:HB3	3:4:238:THR:HG23	1.84	0.59
4:5:31:PHE:CE1	4:5:90:PHE:HE1	2.19	0.59
5:6:778:LYS:HG2	5:6:782:LYS:NZ	2.14	0.59
5:6:794:ARG:H	5:6:795:ILE:HA	1.67	0.59
6:7:470:LEU:HD21	6:7:564:LEU:HD22	1.84	0.59
3:4:666:ASN:HD22	3:4:668:ARG:NH2	1.97	0.59
3:4:682:TYR:O	3:4:691:ASN:ND2	2.35	0.59
5:6:794:ARG:HB2	5:6:796:THR:N	2.16	0.59
6:7:132:ILE:HD13	6:7:144:ASN:HD22	1.67	0.59
6:7:434:LEU:HD21	6:7:699:LEU:HD23	1.84	0.59
2:3:185:ILE:HD13	2:3:291:ARG:HG2	1.84	0.59
3:4:315:ARG:NH1	6:7:251:VAL:HG12	2.16	0.59
3:4:635:ASP:O	3:4:642:ARG:NH2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:301:TYR:HE1	4:5:303:SER:HB3	1.67	0.59
4:5:685:GLN:OE1	4:5:688:THR:OG1	2.20	0.59
1:2:212:LYS:HZ1	1:2:275:ALA:HB2	1.68	0.59
4:5:197:PHE:CZ	4:5:251:ILE:HD11	2.32	0.59
5:6:109:GLU:O	5:6:112:ARG:HB3	2.02	0.59
5:6:159:SER:HA	5:6:167:ALA:HB2	1.82	0.59
2:3:330:HIS:HD2	2:3:336:VAL:O	1.85	0.59
3:4:231:ASN:O	3:4:234:ARG:HG2	2.02	0.59
3:4:803:ARG:O	3:4:806:GLU:HG2	2.02	0.59
5:6:175:TYR:HA	5:6:178:LEU:HD13	1.85	0.59
5:6:274:HIS:ND1	5:6:288:LEU:HD11	2.18	0.59
5:6:301:ARG:O	5:6:356:TRP:N	2.28	0.59
6:7:486:LYS:N	6:7:487:GLY:HA3	2.17	0.59
2:3:204:ALA:HB1	2:3:205:LYS:HD2	1.84	0.59
3:4:406:VAL:CG2	6:7:560:ARG:HH12	2.15	0.59
5:6:553:GLY:O	5:6:812:ARG:NH1	2.36	0.59
2:3:372:TYR:OH	2:3:561:ILE:O	2.21	0.59
3:4:559:ARG:NE	3:4:668:ARG:HD3	2.17	0.59
3:4:827:ARG:O	3:4:831:SER:N	2.34	0.59
2:3:43:ARG:HB2	2:3:136:MET:HE2	1.83	0.59
2:3:472:ILE:HG21	2:3:475:PHE:HD1	1.68	0.59
2:3:33:ASP:HB2	2:3:39:ARG:HH11	1.68	0.58
2:3:336:VAL:CG1	2:3:337:ALA:HA	2.33	0.58
2:3:428:LEU:HB3	2:3:429:ALA:HA	1.85	0.58
2:3:672:THR:HG21	2:3:720:THR:HB	1.85	0.58
3:4:833:ILE:HA	3:4:836:TYR:CD2	2.38	0.58
1:2:508:HIS:HB2	1:2:511:ILE:HG22	1.84	0.58
2:3:390:GLU:HB2	2:3:509:ARG:HH22	1.68	0.58
3:4:488:ASN:OD1	3:4:489:LYS:N	2.33	0.58
5:6:808:GLU:O	5:6:812:ARG:HG2	2.03	0.58
1:2:330:VAL:HG23	4:5:272:ARG:HH12	1.68	0.58
2:3:257:THR:HA	2:3:275:ASP:HA	1.85	0.58
3:4:489:LYS:HZ3	3:4:497:GLU:HB2	1.64	0.58
3:4:547:GLY:HA3	3:4:560:GLY:HA2	1.85	0.58
4:5:410:ILE:O	4:5:411:ASN:ND2	2.36	0.58
6:7:113:PHE:O	6:7:117:PHE:HB2	2.03	0.58
6:7:353:GLY:HA3	6:7:377:GLU:O	2.02	0.58
2:3:18:ASP:OD1	2:3:18:ASP:N	2.35	0.58
2:3:194:PRO:HG2	6:7:372:THR:OG1	2.04	0.58
4:5:663:LEU:HG	4:5:666:LEU:HD12	1.86	0.58
2:3:493:GLN:HE21	2:3:509:ARG:HA	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:343:TRP:CG	4:5:344:ASN:H	2.21	0.58
5:6:585:LEU:HD13	5:6:639:ASP:OD1	2.03	0.58
2:3:441:GLY:HA3	2:3:462:MET:HB3	1.85	0.58
3:4:253:GLN:O	3:4:254:THR:OG1	2.19	0.58
3:4:625:ASP:OD1	3:4:668:ARG:HG2	2.04	0.58
5:6:551:MET:HE1	5:6:591:PHE:HE2	1.69	0.58
6:7:385:LYS:HG2	6:7:639:ARG:NH1	2.19	0.58
5:6:183:LYS:HA	5:6:186:ARG:HE	1.69	0.58
6:7:440:VAL:HG21	6:7:650:PRO:HD2	1.85	0.58
3:4:517:ASP:O	3:4:520:SER:OG	2.14	0.58
4:5:259:GLN:HE21	4:5:271:PRO:HG2	1.67	0.58
4:5:549:ARG:HA	4:5:651:ARG:HH21	1.68	0.58
4:5:643:ARG:NH1	4:5:692:ALA:HA	2.18	0.58
5:6:385:SER:OG	5:6:457:CYS:O	2.17	0.58
3:4:477:ASP:OD1	3:4:478:THR:N	2.37	0.58
4:5:420:THR:HG23	4:5:556:VAL:HG11	1.85	0.58
5:6:356:TRP:HZ3	5:6:358:LYS:HB2	1.68	0.58
5:6:561:GLU:N	5:6:562:GLY:HA3	2.18	0.58
6:7:214:ARG:HB2	6:7:214:ARG:CZ	2.34	0.57
6:7:584:ILE:HD12	6:7:681:PHE:HZ	1.68	0.57
5:6:359:VAL:HG23	5:6:379:VAL:HG13	1.86	0.57
5:6:820:THR:O	5:6:824:ILE:HG12	2.04	0.57
2:3:362:ILE:HG22	2:3:651:VAL:HG22	1.85	0.57
3:4:243:LEU:HD23	3:4:244:ASP:H	1.69	0.57
6:7:635:PRO:HA	6:7:638:MET:HE2	1.86	0.57
1:2:605:LEU:HD23	1:2:647:ILE:HB	1.85	0.57
4:5:621:LYS:O	4:5:624:SER:OG	2.21	0.57
6:7:248:VAL:HG22	6:7:311:GLN:HE21	1.69	0.57
2:3:257:THR:HG22	2:3:275:ASP:HB3	1.87	0.57
5:6:750:GLN:HA	5:6:753:ARG:HH11	1.70	0.57
6:7:541:MET:HB2	6:7:593:ARG:HD3	1.85	0.57
6:7:699:LEU:HB2	6:7:712:ASP:OD1	2.04	0.57
1:2:622:GLU:OE2	1:2:626:GLN:NE2	2.37	0.57
3:4:527:ALA:HB3	3:4:537:LYS:HZ2	1.68	0.57
6:7:393:LEU:HD13	6:7:395:SER:HB3	1.86	0.57
3:4:422:GLU:HB3	3:4:494:GLU:OE2	2.04	0.57
1:2:495:ASP:OD1	1:2:509:ARG:NH2	2.35	0.57
2:3:542:ARG:HH12	2:3:700:ARG:NH1	2.01	0.57
4:5:92:THR:HA	4:5:95:THR:HG22	1.86	0.57
4:5:572:VAL:HA	4:5:575:ILE:HD12	1.86	0.57
2:3:682:ASN:OD1	2:3:734:ARG:NH1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:219:THR:HB	1:2:223:GLY:HA2	1.87	0.57
1:2:405:HIS:HB2	5:6:621:TYR:CE1	2.40	0.57
1:2:688:ASP:HB3	1:2:691:ALA:HB3	1.85	0.57
3:4:569:ASP:O	3:4:572:THR:OG1	2.19	0.57
4:5:259:GLN:NE2	4:5:271:PRO:HG2	2.20	0.57
5:6:314:CYS:N	5:6:336:PRO:O	2.38	0.57
6:7:143:LEU:HD22	6:7:199:ARG:HB2	1.85	0.57
4:5:49:GLN:NE2	4:5:62:THR:OG1	2.37	0.56
4:5:79:LEU:HA	4:5:86:ILE:HD12	1.86	0.56
6:7:86:LEU:CD1	6:7:216:ARG:HG2	2.34	0.56
2:3:291:ARG:HD2	2:3:331:ALA:HB3	1.87	0.56
3:4:502:THR:HG22	3:4:503:ASP:H	1.70	0.56
5:6:270:LEU:HD12	5:6:289:SER:HB2	1.86	0.56
5:6:273:VAL:HG22	5:6:396:LYS:NZ	2.20	0.56
5:6:335:ASN:H	5:6:339:GLU:HA	1.70	0.56
5:6:711:LEU:HG	5:6:712:PHE:H	1.69	0.56
6:7:228:ARG:HH22	6:7:326:HIS:HB3	1.70	0.56
6:7:257:VAL:HG12	6:7:272:GLU:HA	1.86	0.56
1:2:235:GLY:HA2	1:2:283:TYR:CE2	2.40	0.56
1:2:686:LEU:HD12	5:6:788:PHE:HZ	1.71	0.56
2:3:425:THR:HA	2:3:657:ARG:HH11	1.70	0.56
2:3:547:PHE:HE1	2:3:736:ALA:HB2	1.71	0.56
3:4:239:SER:OG	3:4:240:ASN:N	2.38	0.56
3:4:505:ASP:O	3:4:509:ILE:HD12	2.05	0.56
4:5:148:LEU:HD23	4:5:260:GLU:HB3	1.87	0.56
5:6:297:THR:HA	5:6:359:VAL:HG12	1.88	0.56
6:7:411:TYR:CE2	6:7:430:LYS:HE2	2.40	0.56
1:2:557:GLU:OE2	1:2:565:PHE:CD1	2.59	0.56
4:5:421:ALA:HA	7:5:2001:ADP:H5'2	1.86	0.56
3:4:349:CYS:N	3:4:353:ASP:OD1	2.34	0.56
5:6:134:LYS:HZ3	5:6:137:ARG:HD2	1.70	0.56
6:7:182:ARG:O	6:7:186:GLU:HG2	2.04	0.56
1:2:855:ARG:HG3	1:2:858:ARG:HH21	1.70	0.56
5:6:344:TRP:CB	5:6:345:THR:HA	2.36	0.56
2:3:284:ASP:OD1	6:7:329:ARG:NH2	2.39	0.56
4:5:464:LEU:HD11	4:5:470:VAL:HG21	1.87	0.56
1:2:339:PHE:HE1	1:2:375:VAL:HG22	1.71	0.56
2:3:367:LEU:HD12	2:3:378:LYS:HB3	1.88	0.56
2:3:399:LEU:HD22	6:7:620:HIS:CE1	2.41	0.56
2:3:491:GLU:CD	2:3:700:ARG:HH22	2.14	0.56
3:4:764:GLU:HA	3:4:767:LYS:HZ1	1.67	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:540:HIS:C	5:6:542:ALA:H	2.13	0.56
1:2:290:HIS:O	1:2:292:GLU:N	2.38	0.56
1:2:323:VAL:HG22	1:2:423:GLU:HG3	1.87	0.56
1:2:506:TYR:OH	1:2:694:ARG:HD3	2.05	0.56
1:2:308:GLU:OE1	1:2:310:ARG:NH2	2.39	0.56
1:2:580:VAL:HG21	1:2:636:ILE:HG21	1.88	0.56
6:7:208:SER:HB3	6:7:209:GLN:HG3	1.88	0.56
6:7:401:VAL:HG13	6:7:641:TYR:HD1	1.71	0.56
1:2:229:ALA:HA	1:2:232:ARG:HG2	1.87	0.55
1:2:689:GLU:OE2	5:6:778:LYS:HD3	2.06	0.55
2:3:475:PHE:HB3	2:3:516:ALA:HB2	1.87	0.55
3:4:764:GLU:HA	3:4:767:LYS:HZ3	1.68	0.55
6:7:281:LEU:HD12	6:7:298:LEU:HD11	1.88	0.55
6:7:601:LEU:HD21	6:7:727:LEU:HA	1.88	0.55
1:2:296:ARG:O	1:2:455:SER:OG	2.24	0.55
2:3:202:TYR:HD1	2:3:209:PHE:CE1	2.25	0.55
3:4:428:ARG:CZ	3:4:485:LEU:HD12	2.36	0.55
3:4:527:ALA:HB1	3:4:530:ILE:HD13	1.86	0.55
5:6:134:LYS:N	5:6:135:VAL:HA	2.21	0.55
5:6:791:SER:OG	5:6:839:ASP:OD1	2.17	0.55
3:4:646:HIS:HA	3:4:701:ARG:NH1	2.21	0.55
5:6:543:VAL:HG21	5:6:715:ILE:HD11	1.88	0.55
1:2:808:ARG:HG2	7:5:2001:ADP:H4'	1.88	0.55
2:3:362:ILE:HG22	2:3:651:VAL:CG2	2.35	0.55
2:3:493:GLN:HE21	2:3:509:ARG:CA	2.19	0.55
4:5:409:ASP:OD1	4:5:410:ILE:HG12	2.06	0.55
4:5:437:VAL:HG12	4:5:439:THR:HG23	1.87	0.55
5:6:356:TRP:CZ3	5:6:358:LYS:HB2	2.41	0.55
5:6:776:LYS:HG3	5:6:779:GLU:OE2	2.07	0.55
6:7:421:GLU:HA	6:7:625:GLN:HE22	1.72	0.55
2:3:346:ASP:HA	2:3:349:ASN:HD22	1.72	0.55
2:3:558:ASP:OD2	4:5:627:VAL:HA	2.05	0.55
3:4:345:ALA:O	3:4:357:ALA:HB1	2.06	0.55
3:4:370:ARG:HH22	5:6:426:ILE:HG13	1.71	0.55
4:5:485:MET:HE3	4:5:490:ARG:HA	1.88	0.55
1:2:410:LEU:HD22	1:2:456:ILE:HD11	1.87	0.55
2:3:375:ASP:O	2:3:379:LYS:HG3	2.06	0.55
2:3:655:PHE:HA	2:3:658:LYS:NZ	2.21	0.55
2:3:690:ASP:HA	2:3:693:LYS:HB2	1.89	0.55
4:5:86:ILE:O	4:5:89:LEU:N	2.39	0.55
5:6:412:LEU:HB3	5:6:416:LYS:HZ1	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:661:VAL:O	6:7:665:ILE:HD12	2.07	0.55
2:3:706:ILE:HD13	6:7:620:HIS:HD2	1.72	0.55
4:5:35:ILE:HD11	4:5:94:ILE:HG13	1.89	0.55
5:6:115:PHE:O	5:6:118:PHE:HB3	2.07	0.55
3:4:400:GLN:HE22	6:7:555:THR:HA	1.71	0.55
5:6:132:VAL:HG22	5:6:133:GLU:OE1	2.06	0.55
5:6:534:ALA:HB3	5:6:544:LYS:HE2	1.88	0.55
6:7:441:ASP:OD1	6:7:442:LYS:N	2.40	0.55
1:2:484:PHE:CE1	1:2:766:TYR:HD1	2.25	0.55
1:2:560:ALA:HB3	1:2:563:ALA:HB2	1.89	0.55
2:3:678:VAL:HG21	2:3:723:LYS:HG3	1.87	0.55
3:4:188:GLN:C	3:4:190:CYS:N	2.64	0.55
3:4:331:LEU:HA	3:4:431:ASP:O	2.07	0.55
4:5:675:ARG:HG3	4:5:676:HIS:N	2.21	0.55
5:6:158:LEU:HD21	5:6:170:ILE:HD12	1.88	0.55
6:7:165:ASN:HB3	6:7:166:LEU:CA	2.37	0.55
6:7:426:LEU:O	6:7:430:LYS:HB2	2.07	0.55
1:2:601:LYS:NZ	1:2:643:ARG:HH11	2.04	0.55
2:3:389:VAL:HG12	2:3:390:GLU:N	2.14	0.55
5:6:696:ARG:O	5:6:696:ARG:NH1	2.36	0.55
6:7:90:ASN:HD21	6:7:214:ARG:NE	2.03	0.55
1:2:793:LEU:HD21	1:2:842:VAL:HG22	1.89	0.54
2:3:653:ILE:HD12	4:5:402:ASP:HA	1.88	0.54
3:4:234:ARG:HB3	3:4:280:MET:HE1	1.89	0.54
4:5:49:GLN:O	4:5:53:ASN:ND2	2.40	0.54
4:5:90:PHE:CD2	4:5:137:LEU:HD21	2.42	0.54
4:5:376:PRO:HB2	4:5:585:ASN:HD21	1.73	0.54
5:6:283:LYS:O	5:6:286:SER:OG	2.20	0.54
6:7:1:MET:HG2	6:7:2:SER:O	2.06	0.54
6:7:462:PRO:HD3	6:7:573:ARG:HE	1.72	0.54
3:4:267:GLU:O	3:4:270:SER:OG	2.20	0.54
3:4:565:LEU:HB2	3:4:702:PHE:CD2	2.42	0.54
3:4:651:GLN:HE21	5:6:586:LYS:HZ3	1.54	0.54
1:2:264:PRO:HG3	1:2:317:LEU:HB2	1.89	0.54
5:6:601:LYS:HB2	5:6:643:LYS:HB3	1.90	0.54
6:7:90:ASN:HD21	6:7:214:ARG:HE	1.56	0.54
4:5:631:LYS:HE3	4:5:635:ILE:HD11	1.88	0.54
5:6:517:LYS:O	5:6:521:LYS:HG2	2.07	0.54
6:7:398:GLU:O	6:7:402:MET:HG3	2.08	0.54
6:7:421:GLU:HA	6:7:625:GLN:NE2	2.23	0.54
1:2:557:GLU:OE2	1:2:565:PHE:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:332:ARG:O	2:3:333:SER:OG	2.21	0.54
2:3:354:SER:HB3	2:3:717:LEU:HD22	1.89	0.54
5:6:183:LYS:HZ1	5:6:186:ARG:HH12	1.53	0.54
2:3:169:ARG:NH2	2:3:269:GLN:OE1	2.40	0.54
3:4:604:TYR:OH	6:7:554:ASN:OD1	2.23	0.54
6:7:87:GLN:NE2	6:7:214:ARG:NH1	2.54	0.54
6:7:208:SER:CB	6:7:209:GLN:CA	2.85	0.54
1:2:212:LYS:NZ	1:2:275:ALA:HB2	2.23	0.54
2:3:687:ARG:HH12	2:3:698:THR:HA	1.73	0.54
4:5:441:GLY:HA3	4:5:443:GLY:H	1.73	0.54
5:6:781:ARG:NE	5:6:795:ILE:O	2.41	0.54
6:7:443:ARG:NH1	6:7:449:LYS:HZ2	2.06	0.54
1:2:234:LEU:HD12	1:2:234:LEU:O	2.08	0.54
2:3:32:LEU:HD11	2:3:132:LEU:HD22	1.89	0.54
2:3:362:ILE:HG23	2:3:651:VAL:HG21	1.88	0.54
3:4:324:LYS:HZ2	6:7:138:VAL:HG11	1.73	0.54
3:4:408:ASP:OD1	6:7:517:ASP:OD2	2.25	0.54
3:4:545:PHE:CE1	3:4:751:ILE:HG12	2.43	0.54
1:2:429:ILE:HD12	1:2:431:LYS:HE2	1.90	0.54
2:3:440:VAL:HG12	2:3:441:GLY:H	1.73	0.54
2:3:712:HIS:ND1	2:3:725:ASP:OD1	2.38	0.54
3:4:712:VAL:HG22	6:7:672:LYS:HZ2	1.72	0.54
4:5:569:ALA:O	4:5:573:ILE:HD12	2.08	0.54
5:6:112:ARG:HH22	5:6:183:LYS:HB2	1.73	0.54
1:2:230:ARG:O	1:2:233:THR:OG1	2.24	0.53
6:7:421:GLU:C	6:7:625:GLN:HE22	2.16	0.53
1:2:517:CYS:SG	1:2:816:ILE:HG23	2.49	0.53
3:4:572:THR:O	3:4:573:SER:OG	2.18	0.53
2:3:553:ILE:HB	4:5:630:ARG:HH11	1.72	0.53
4:5:685:GLN:O	4:5:688:THR:OG1	2.27	0.53
6:7:459:MET:HG3	6:7:460:GLY:H	1.73	0.53
1:2:297:ILE:HG22	1:2:298:SER:N	2.20	0.53
3:4:821:ASP:C	3:4:821:ASP:OD1	2.51	0.53
4:5:65:MET:HG2	4:5:76:TYR:HE1	1.74	0.53
4:5:621:LYS:HG2	4:5:674:GLU:OE2	2.08	0.53
5:6:663:ILE:HD12	5:6:672:LEU:HD12	1.90	0.53
5:6:778:LYS:C	5:6:782:LYS:NZ	2.67	0.53
6:7:214:ARG:CG	6:7:215:TYR:O	2.54	0.53
6:7:395:SER:C	6:7:397:VAL:H	2.16	0.53
6:7:493:LEU:HD12	6:7:494:THR:N	2.24	0.53
3:4:366:GLN:N	3:4:366:GLN:OE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:603:SER:N	5:6:604:SER:HA	2.24	0.53
6:7:138:VAL:HG21	6:7:303:ARG:NH2	2.23	0.53
6:7:459:MET:HB3	6:7:599:LEU:HA	1.90	0.53
2:3:171:LEU:HD23	2:3:172:THR:N	2.23	0.53
2:3:561:ILE:HG21	4:5:650:ILE:HG21	1.89	0.53
3:4:486:MET:HE2	3:4:498:VAL:HG21	1.90	0.53
4:5:577:THR:OG1	4:5:578:GLY:HA2	2.07	0.53
5:6:136:TYR:O	5:6:140:ILE:HD12	2.09	0.53
5:6:183:LYS:HA	5:6:186:ARG:NE	2.23	0.53
6:7:570:LEU:HD13	6:7:585:ASN:HD21	1.73	0.53
1:2:387:ARG:HD2	1:2:407:GLU:OE2	2.09	0.53
5:6:529:LEU:O	5:6:533:ILE:HG13	2.09	0.53
5:6:776:LYS:NZ	5:6:824:ILE:HG22	2.24	0.53
6:7:223:LYS:O	6:7:225:LEU:HG	2.09	0.53
6:7:404:LEU:HD11	6:7:414:LEU:HD21	1.91	0.53
1:2:809:HIS:HE1	1:2:845:PHE:HB2	1.74	0.53
6:7:133:ASP:CG	6:7:134:TYR:H	2.16	0.53
2:3:25:VAL:HG13	2:3:128:ALA:HB2	1.91	0.53
2:3:690:ASP:O	2:3:694:LYS:N	2.40	0.53
5:6:305:TYR:CD1	5:6:306:LYS:HG2	2.43	0.53
5:6:780:LEU:HD12	5:6:828:TYR:CE1	2.43	0.53
2:3:100:LEU:HB3	2:3:111:TRP:CZ3	2.43	0.53
4:5:409:ASP:OD1	4:5:410:ILE:HG23	2.09	0.53
5:6:117:GLN:HG2	5:6:121:ASP:OD2	2.09	0.53
5:6:611:ALA:N	5:6:624:GLU:OE2	2.41	0.53
6:7:484:THR:O	6:7:488:SER:N	2.26	0.53
6:7:536:ALA:O	6:7:540:VAL:HG23	2.08	0.53
1:2:309:LEU:C	1:2:310:ARG:HH11	2.11	0.52
2:3:221:LEU:HD11	2:3:297:VAL:HG21	1.91	0.52
4:5:543:GLN:HE21	4:5:546:ILE:HD11	1.73	0.52
5:6:448:LEU:HD12	5:6:448:LEU:O	2.09	0.52
6:7:137:ASP:OD1	6:7:138:VAL:N	2.42	0.52
3:4:488:ASN:O	3:4:489:LYS:HB3	2.09	0.52
5:6:151:ILE:HD11	5:6:265:ILE:HG23	1.91	0.52
6:7:538:HIS:HD2	6:7:593:ARG:HE	1.56	0.52
6:7:664:TYR:HB2	6:7:689:LEU:HD13	1.90	0.52
2:3:429:ALA:HB3	2:3:469:VAL:O	2.09	0.52
3:4:408:ASP:HB2	6:7:560:ARG:NH2	2.24	0.52
3:4:568:GLY:N	3:4:574:LYS:HZ3	2.08	0.52
4:5:601:ARG:O	4:5:604:THR:OG1	2.27	0.52
5:6:142:PHE:HA	5:6:145:ILE:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:132:ILE:HD13	6:7:144:ASN:ND2	2.24	0.52
1:2:790:TYR:CG	1:2:810:LEU:HD12	2.45	0.52
3:4:712:VAL:HG22	6:7:672:LYS:HZ3	1.74	0.52
4:5:31:PHE:CE1	4:5:75:ILE:HG21	2.44	0.52
6:7:541:MET:HB2	6:7:593:ARG:HH11	1.75	0.52
1:2:294:HIS:HD2	1:2:296:ARG:HH12	1.58	0.52
1:2:339:PHE:CE1	1:2:375:VAL:HG22	2.45	0.52
1:2:795:ARG:HA	1:2:798:ILE:HD12	1.90	0.52
2:3:443:THR:HB	2:3:457:LEU:HB3	1.90	0.52
3:4:598:ALA:HB1	5:6:601:LYS:HZ1	1.75	0.52
4:5:66:GLU:OE2	4:5:143:ALA:HB2	2.09	0.52
4:5:90:PHE:O	4:5:94:ILE:HD12	2.09	0.52
5:6:116:GLU:OE2	5:6:187:ARG:HD3	2.10	0.52
2:3:199:SER:HB3	2:3:212:ARG:HB3	1.92	0.52
2:3:466:ASP:OD1	2:3:467:ARG:N	2.43	0.52
3:4:417:LEU:HD13	3:4:463:VAL:HG11	1.91	0.52
3:4:437:GLY:HA3	3:4:463:VAL:HA	1.92	0.52
3:4:658:LYS:HB3	5:6:604:SER:N	2.24	0.52
4:5:19:PRO:HG2	4:5:21:ASP:HB2	1.90	0.52
4:5:678:ASP:O	4:5:682:ARG:NH1	2.42	0.52
5:6:335:ASN:N	5:6:339:GLU:HA	2.24	0.52
5:6:558:SER:CB	5:6:559:THR:HA	2.33	0.52
6:7:90:ASN:HD22	6:7:214:ARG:NH1	2.08	0.52
6:7:214:ARG:HG2	6:7:216:ARG:HB2	1.92	0.52
2:3:422:VAL:O	2:3:426:ALA:HB2	2.10	0.52
2:3:476:ASP:OD1	2:3:477:LYS:N	2.43	0.52
4:5:655:ALA:O	4:5:659:ILE:HD12	2.10	0.52
1:2:501:MET:HE3	1:2:516:ALA:HA	1.92	0.52
1:2:805:ILE:H	1:2:805:ILE:HD12	1.74	0.52
4:5:282:LEU:HD22	4:5:333:ILE:HG22	1.92	0.52
5:6:264:GLN:NE2	5:6:383:GLY:HA2	2.25	0.52
5:6:763:PRO:HG3	5:6:812:ARG:HD3	1.92	0.52
5:6:794:ARG:HB2	5:6:795:ILE:C	2.35	0.52
6:7:135:LYS:HA	6:7:136:ASP:HB3	1.91	0.52
2:3:183:GLU:OE1	2:3:183:GLU:N	2.43	0.52
3:4:443:PRO:HB3	3:4:457:TYR:CE1	2.45	0.52
4:5:349:PHE:HZ	4:5:609:LYS:HZ1	1.55	0.52
4:5:396:SER:HB3	4:5:661:GLU:HG2	1.91	0.52
5:6:804:ILE:O	5:6:807:SER:OG	2.21	0.52
2:3:193:ARG:HD2	6:7:371:LEU:HD23	1.91	0.52
2:3:236:THR:HA	2:3:237:GLU:C	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:280:MET:O	3:4:284:ILE:HD12	2.10	0.52
3:4:657:ALA:HA	3:4:662:ILE:HG23	1.91	0.52
5:6:776:LYS:HZ3	5:6:824:ILE:C	2.17	0.52
6:7:244:ILE:HD12	6:7:318:LEU:HA	1.92	0.52
1:2:481:GLU:O	1:2:485:ARG:HG2	2.10	0.51
1:2:527:VAL:O	1:2:530:LYS:N	2.43	0.51
1:2:569:GLN:CD	1:2:613:ASN:HD22	2.18	0.51
2:3:450:ARG:HH12	4:5:460:ARG:HB2	1.75	0.51
3:4:190:CYS:SG	3:4:257:LEU:HD13	2.50	0.51
4:5:379:PHE:H	7:5:2001:ADP:N6	2.06	0.51
4:5:498:GLU:OE1	4:5:498:GLU:N	2.42	0.51
3:4:313:GLY:HA2	3:4:403:PRO:HB3	1.92	0.51
4:5:172:LEU:HD22	4:5:252:ASP:OD2	2.09	0.51
1:2:856:GLN:NE2	1:2:859:ARG:HH21	2.08	0.51
5:6:615:ASP:OD2	5:6:617:GLU:HA	2.10	0.51
1:2:211:LEU:HA	1:2:214:PHE:HB3	1.93	0.51
1:2:343:LYS:HZ3	1:2:371:GLY:HA2	1.76	0.51
2:3:397:SER:HB2	6:7:471:LYS:HD2	1.92	0.51
6:7:90:ASN:ND2	6:7:214:ARG:HE	2.08	0.51
6:7:138:VAL:C	6:7:140:ASP:H	2.18	0.51
6:7:197:THR:O	6:7:198:ARG:HD2	2.11	0.51
6:7:723:SER:OG	6:7:724:LYS:N	2.43	0.51
1:2:335:LYS:HD2	1:2:383:ARG:HH11	1.76	0.51
1:2:434:TYR:CG	1:2:435:ASP:N	2.79	0.51
1:2:446:VAL:HG21	5:6:356:TRP:HZ2	1.75	0.51
3:4:491:ASP:OD1	3:4:492:HIS:N	2.42	0.51
4:5:87:ILE:O	4:5:90:PHE:HB2	2.11	0.51
4:5:608:LEU:HD11	4:5:609:LYS:HZ3	1.72	0.51
5:6:580:SER:HA	7:6:2001:ADP:H5'2	1.91	0.51
1:2:286:TYR:CE2	1:2:293:ILE:HD11	2.45	0.51
1:2:562:ARG:HH22	4:5:265:VAL:HG13	1.74	0.51
1:2:689:GLU:OE1	5:6:782:LYS:HD3	2.09	0.51
4:5:27:ILE:O	4:5:30:SER:OG	2.20	0.51
5:6:400:VAL:O	5:6:455:LEU:HB3	2.11	0.51
2:3:430:ILE:HG12	4:5:510:THR:HG21	1.91	0.51
4:5:44:PHE:CE1	4:5:47:ARG:HD3	2.45	0.51
6:7:208:SER:CB	6:7:209:GLN:CB	2.83	0.51
6:7:667:LEU:O	6:7:670:ASP:OD1	2.29	0.51
1:2:520:PHE:CD1	1:2:767:ILE:HG22	2.46	0.51
1:2:601:LYS:HZ1	1:2:643:ARG:HD2	1.75	0.51
1:2:790:TYR:CD1	1:2:810:LEU:HD12	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:538:SER:O	2:3:541:SER:OG	2.24	0.51
3:4:411:THR:OG1	3:4:412:PRO:HD2	2.11	0.51
6:7:114:THR:HG22	6:7:204:PHE:HE2	1.75	0.51
6:7:318:LEU:O	6:7:319:SER:OG	2.25	0.51
6:7:446:ASP:HB2	6:7:447:GLY:HA2	1.92	0.51
6:7:456:VAL:HB	6:7:564:LEU:HG	1.93	0.51
6:7:619:VAL:HG22	6:7:622:HIS:O	2.11	0.51
2:3:103:LEU:O	2:3:107:ASP:N	2.44	0.51
2:3:403:ILE:HD11	2:3:707:ARG:HB3	1.93	0.51
3:4:458:LYS:HZ1	5:6:413:PRO:HB3	1.75	0.51
1:2:215:LEU:HD21	1:2:231:ILE:HD11	1.92	0.51
4:5:607:ARG:HA	4:5:665:LYS:CE	2.42	0.51
4:5:657:ILE:O	4:5:660:THR:OG1	2.26	0.51
6:7:656:VAL:O	6:7:660:VAL:HG23	2.11	0.51
1:2:215:LEU:HD12	1:2:227:TYR:HB3	1.92	0.50
1:2:846:VAL:O	1:2:853:VAL:HG21	2.12	0.50
3:4:231:ASN:HA	3:4:234:ARG:HG2	1.93	0.50
6:7:90:ASN:HD22	6:7:214:ARG:HH11	1.60	0.50
6:7:127:LEU:HG	6:7:128:PRO:HD3	1.93	0.50
6:7:458:LEU:HD22	6:7:600:MET:HE3	1.93	0.50
1:2:486:LYS:O	1:2:489:ARG:HG2	2.11	0.50
2:3:209:PHE:CE2	6:7:10:LEU:HD12	2.47	0.50
4:5:31:PHE:CZ	4:5:90:PHE:HE1	2.29	0.50
4:5:138:ILE:HG23	4:5:332:GLY:HA3	1.93	0.50
5:6:304:LEU:C	5:6:306:LYS:H	2.18	0.50
5:6:691:ARG:HH11	5:6:716:LEU:CD2	2.17	0.50
6:7:400:ARG:HB3	6:7:637:LYS:NZ	2.26	0.50
2:3:33:ASP:HB2	2:3:39:ARG:NH1	2.26	0.50
2:3:372:TYR:CE2	2:3:561:ILE:HG23	2.46	0.50
2:3:374:HIS:HE1	2:3:549:VAL:HG11	1.76	0.50
2:3:704:THR:HA	2:3:707:ARG:HH11	1.77	0.50
3:4:362:ARG:HH11	6:7:299:PHE:HZ	1.59	0.50
4:5:180:SER:OG	4:5:247:SER:OG	2.18	0.50
4:5:629:ILE:HG23	4:5:633:LEU:HD12	1.93	0.50
6:7:440:VAL:O	6:7:441:ASP:OD1	2.28	0.50
1:2:211:LEU:O	1:2:214:PHE:HB3	2.11	0.50
1:2:212:LYS:HG3	1:2:274:VAL:HG12	1.92	0.50
2:3:171:LEU:HD23	2:3:172:THR:H	1.76	0.50
2:3:652:THR:CB	2:3:654:PRO:HD3	2.40	0.50
4:5:256:LEU:HB2	4:5:276:MET:HB2	1.92	0.50
5:6:130:GLY:HA3	5:6:131:GLU:C	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:393:ASP:OD1	5:6:394:ARG:N	2.45	0.50
5:6:401:GLU:OE2	5:6:452:ILE:HG23	2.10	0.50
6:7:689:LEU:O	6:7:692:ILE:HG22	2.11	0.50
2:3:651:VAL:CG1	2:3:651:VAL:O	2.59	0.50
4:5:208:PRO:HG2	4:5:241:TYR:CD2	2.47	0.50
1:2:335:LYS:HD2	1:2:383:ARG:NH1	2.26	0.50
1:2:815:ARG:O	1:2:818:GLU:HG2	2.11	0.50
2:3:372:TYR:OH	2:3:564:HIS:HB3	2.12	0.50
3:4:403:PRO:O	3:4:404:ASP:OD1	2.29	0.50
4:5:356:GLU:CD	4:5:598:LYS:HZ2	2.20	0.50
5:6:777:TYR:CE1	5:6:800:LEU:HB2	2.47	0.50
6:7:396:ASP:O	6:7:399:GLU:HB3	2.11	0.50
1:2:621:HIS:NE2	4:5:481:GLU:OE2	2.44	0.50
2:3:389:VAL:H	2:3:714:LYS:NZ	2.10	0.50
2:3:669:PRO:HG2	2:3:710:THR:HG23	1.93	0.50
3:4:306:TYR:CD2	3:4:307:ASN:HB2	2.46	0.50
3:4:545:PHE:HE1	3:4:751:ILE:HG23	1.77	0.50
3:4:769:GLU:HA	3:4:772:ARG:HG2	1.93	0.50
4:5:69:ILE:HD12	4:5:73:GLU:HA	1.94	0.50
5:6:183:LYS:CB	5:6:186:ARG:HH11	2.25	0.50
6:7:409:ASP:OD2	6:7:412:ASN:HB3	2.12	0.50
1:2:444:PHE:O	1:2:446:VAL:HG23	2.11	0.50
2:3:163:ALA:HB3	2:3:164:HIS:ND1	2.25	0.50
2:3:189:THR:HG22	2:3:190:SER:N	2.27	0.50
2:3:683:TYR:CZ	2:3:687:ARG:HD2	2.46	0.50
5:6:793:TYR:O	5:6:794:ARG:NH1	2.40	0.50
2:3:451:GLU:O	2:3:452:THR:OG1	2.25	0.50
3:4:428:ARG:HH11	3:4:482:GLU:HA	1.77	0.50
3:4:534:GLU:OE1	3:4:534:GLU:N	2.38	0.50
3:4:677:PRO:HG2	3:4:680:SER:O	2.12	0.50
4:5:254:GLN:HG2	4:5:256:LEU:HD12	1.94	0.50
4:5:340:SER:HB2	4:5:342:ILE:HG13	1.94	0.50
4:5:481:GLU:HB3	4:5:484:LYS:HB2	1.94	0.50
5:6:775:GLU:HA	5:6:778:LYS:HB3	1.93	0.50
6:7:25:LEU:C	6:7:27:THR:H	2.19	0.50
6:7:333:ILE:HG12	6:7:376:LEU:HB3	1.94	0.50
1:2:335:LYS:CD	1:2:383:ARG:HH11	2.25	0.49
2:3:245:TYR:C	2:3:247:TYR:H	2.20	0.49
3:4:299:LYS:NZ	3:4:301:TYR:HE1	2.10	0.49
3:4:354:HIS:HB2	3:4:373:ARG:HB2	1.93	0.49
3:4:732:LYS:HD2	3:4:733:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:45:ILE:HG13	4:5:46:TYR:N	2.27	0.49
4:5:141:SER:H	4:5:295:VAL:HG21	1.77	0.49
5:6:653:HIS:NE2	5:6:704:PRO:HB2	2.27	0.49
6:7:497:VAL:HG12	6:7:506:MET:HE3	1.94	0.49
1:2:332:PRO:HG3	4:5:300:ILE:HD11	1.94	0.49
1:2:811:GLU:CD	1:2:815:ARG:NH1	2.70	0.49
5:6:118:PHE:HD1	5:6:161:ARG:HD3	1.77	0.49
6:7:149:ARG:HH11	6:7:152:ARG:NE	2.10	0.49
1:2:546:GLY:HA3	5:6:796:THR:HG23	1.93	0.49
1:2:585:ILE:HG12	1:2:586:THR:H	1.77	0.49
2:3:126:GLU:O	2:3:130:THR:HG23	2.13	0.49
2:3:414:ALA:O	2:3:418:LEU:N	2.41	0.49
3:4:324:LYS:NZ	6:7:138:VAL:HG11	2.27	0.49
4:5:370:LEU:HG	4:5:599:MET:HE1	1.94	0.49
6:7:458:LEU:HD23	6:7:598:PHE:HB2	1.94	0.49
1:2:338:LYS:HZ3	1:2:376:ASN:HD21	1.60	0.49
3:4:354:HIS:NE2	3:4:356:MET:HG2	2.26	0.49
4:5:407:ARG:O	4:5:658:ARG:HD3	2.13	0.49
4:5:677:VAL:O	4:5:681:ILE:HD12	2.11	0.49
5:6:644:MET:HE3	5:6:649:GLN:OE1	2.13	0.49
7:6:2001:ADP:N3	7:6:2001:ADP:H2'	2.26	0.49
1:2:518:SER:OG	1:2:537:ILE:O	2.23	0.49
1:2:853:VAL:O	1:2:856:GLN:HB3	2.12	0.49
2:3:195:LYS:HA	6:7:371:LEU:HA	1.94	0.49
7:3:2001:ADP:O5'	4:5:651:ARG:NH1	2.45	0.49
3:4:315:ARG:HG2	3:4:410:GLN:NE2	2.28	0.49
3:4:378:GLU:O	3:4:380:ASN:N	2.41	0.49
3:4:455:SER:OG	3:4:456:LEU:N	2.35	0.49
4:5:338:GLU:N	4:5:339:THR:HA	2.28	0.49
4:5:413:LEU:HD11	4:5:550:PHE:CD2	2.47	0.49
5:6:380:ILE:O	5:6:455:LEU:HD12	2.13	0.49
6:7:232:GLY:O	6:7:235:LEU:HD13	2.12	0.49
6:7:636:SER:HA	6:7:639:ARG:HH21	1.77	0.49
1:2:384:ASN:N	1:2:384:ASN:OD1	2.45	0.49
1:2:481:GLU:HA	1:2:484:PHE:HB3	1.93	0.49
3:4:419:VAL:HA	3:4:463:VAL:HG23	1.94	0.49
4:5:606:CYS:C	4:5:665:LYS:HZ2	2.11	0.49
5:6:378:ASP:C	5:6:378:ASP:OD1	2.54	0.49
6:7:240:THR:HG23	6:7:352:THR:HG22	1.93	0.49
1:2:247:ARG:NH2	1:2:299:ASP:OD2	2.45	0.49
1:2:274:VAL:HA	1:2:277:GLU:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:437:ASN:HA	1:2:438:LEU:C	2.37	0.49
2:3:480:ASP:O	2:3:484:VAL:HG23	2.13	0.49
3:4:362:ARG:HH12	6:7:263:ASP:CG	2.19	0.49
3:4:658:LYS:CB	5:6:604:SER:H	2.26	0.49
4:5:4:ASP:OD1	4:5:4:ASP:N	2.43	0.49
6:7:90:ASN:ND2	6:7:214:ARG:NE	2.60	0.49
6:7:235:LEU:HD12	6:7:355:PHE:HE2	1.77	0.49
6:7:436:LEU:HD21	6:7:473:ILE:HG23	1.93	0.49
1:2:693:GLU:CA	5:6:778:LYS:HZ1	2.25	0.49
2:3:187:THR:O	2:3:257:THR:OG1	2.28	0.49
3:4:244:ASP:OD2	3:4:247:ASN:ND2	2.45	0.49
5:6:547:ILE:HD11	5:6:584:PHE:HB3	1.94	0.49
5:6:701:MET:HB2	5:6:705:ILE:HD11	1.94	0.49
6:7:2:SER:C	6:7:4:ALA:H	2.21	0.49
1:2:840:VAL:O	1:2:843:ASP:OD1	2.31	0.49
3:4:184:ASN:HD22	6:7:141:VAL:HG11	1.78	0.49
3:4:408:ASP:OD2	6:7:517:ASP:OD1	2.30	0.49
3:4:585:THR:HG21	3:4:628:VAL:H	1.78	0.49
6:7:28:PHE:HE2	6:7:31:ASP:H	1.60	0.49
1:2:220:ASP:OD1	1:2:221:GLU:N	2.44	0.49
1:2:597:VAL:HG23	1:2:629:ILE:HD12	1.94	0.49
2:3:101:ASP:OD1	2:3:104:ARG:NH2	2.46	0.49
3:4:521:LEU:O	3:4:524:ARG:HG2	2.13	0.49
3:4:635:ASP:OD2	3:4:675:ALA:HB1	2.13	0.49
5:6:735:HIS:O	5:6:736:MET:HE2	2.12	0.49
5:6:780:LEU:HD12	5:6:828:TYR:HE1	1.78	0.49
6:7:397:VAL:HA	6:7:400:ARG:HH21	1.77	0.49
1:2:811:GLU:OE1	1:2:815:ARG:NH1	2.45	0.48
2:3:406:LEU:HB3	2:3:546:LEU:HD23	1.94	0.48
2:3:653:ILE:HD13	4:5:402:ASP:HA	1.83	0.48
3:4:367:GLU:OE1	3:4:367:GLU:N	2.43	0.48
5:6:603:SER:H	5:6:604:SER:HA	1.78	0.48
6:7:89:GLN:NE2	6:7:102:LEU:H	2.11	0.48
6:7:214:ARG:CG	6:7:215:TYR:C	2.58	0.48
6:7:322:VAL:HG12	6:7:323:PRO:O	2.13	0.48
6:7:443:ARG:NH1	6:7:449:LYS:HZ1	2.02	0.48
1:2:230:ARG:NH1	1:2:243:GLU:O	2.46	0.48
1:2:522:GLY:C	1:2:822:LYS:HZ1	2.08	0.48
2:3:566:LEU:HD13	4:5:619:ALA:HB1	1.94	0.48
3:4:693:ASP:CG	3:4:694:LEU:H	2.19	0.48
4:5:464:LEU:HD12	4:5:513:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:568:ASP:CG	5:6:569:ILE:H	2.21	0.48
5:6:601:LYS:HA	5:6:644:MET:HG2	1.96	0.48
6:7:394:THR:HG23	6:7:398:GLU:OE2	2.13	0.48
2:3:435:ARG:NH1	2:3:477:LYS:O	2.45	0.48
6:7:128:PRO:HD2	6:7:129:THR:HA	1.95	0.48
2:3:427:SER:O	2:3:428:LEU:HB2	2.13	0.48
4:5:28:ILE:HG23	4:5:93:ALA:HB2	1.95	0.48
4:5:211:CYS:HB2	4:5:240:PRO:HG3	1.94	0.48
4:5:349:PHE:CZ	4:5:609:LYS:NZ	2.80	0.48
6:7:334:HIS:HD2	6:7:375:TYR:CD1	2.31	0.48
6:7:459:MET:HG3	6:7:569:PRO:HG3	1.95	0.48
1:2:684:ARG:HB3	1:2:685:ASP:CA	2.43	0.48
1:2:767:ILE:HG13	1:2:768:HIS:N	2.29	0.48
3:4:505:ASP:OD1	3:4:505:ASP:N	2.46	0.48
3:4:587:ARG:HD2	3:4:625:ASP:O	2.13	0.48
3:4:828:LEU:O	3:4:831:SER:OG	2.28	0.48
4:5:342:ILE:HG22	4:5:345:SER:HB3	1.95	0.48
5:6:597:TYR:HD1	5:6:637:CYS:SG	2.37	0.48
3:4:306:TYR:HB3	3:4:465:HIS:CD2	2.49	0.48
3:4:309:GLY:O	3:4:327:ASN:ND2	2.46	0.48
6:7:441:ASP:HB3	6:7:452:GLY:HA2	1.95	0.48
1:2:405:HIS:ND1	5:6:621:TYR:HB2	2.29	0.48
2:3:530:HIS:C	2:3:532:ASN:H	2.22	0.48
4:5:331:LEU:HD12	4:5:331:LEU:O	2.14	0.48
6:7:214:ARG:HH21	6:7:214:ARG:CB	2.24	0.48
1:2:343:LYS:HZ1	1:2:370:LYS:C	2.21	0.48
3:4:445:ARG:HG2	3:4:453:LEU:HD23	1.95	0.48
5:6:817:ASP:C	5:6:819:ILE:H	2.22	0.48
6:7:198:ARG:O	6:7:199:ARG:HB3	2.14	0.48
3:4:243:LEU:HD23	3:4:244:ASP:N	2.29	0.48
3:4:340:PRO:HD3	5:6:452:ILE:HD12	1.95	0.48
3:4:497:GLU:HG3	3:4:498:VAL:N	2.28	0.48
3:4:600:GLY:HA2	3:4:604:TYR:HE1	1.77	0.48
3:4:625:ASP:HB3	5:6:370:THR:OG1	2.14	0.48
4:5:489:ASP:O	4:5:493:ILE:HG12	2.14	0.48
6:7:460:GLY:HA3	6:7:600:MET:O	2.13	0.48
6:7:570:LEU:HB2	6:7:585:ASN:HD21	1.79	0.48
6:7:584:ILE:HD12	6:7:681:PHE:CZ	2.48	0.48
1:2:601:LYS:HZ1	1:2:643:ARG:NH1	2.11	0.48
2:3:189:THR:HA	2:3:256:ILE:HG22	1.95	0.48
2:3:198:ARG:O	2:3:248:SER:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:38:PHE:HZ	4:5:67:HIS:NE2	2.11	0.48
4:5:357:PHE:HE1	4:5:598:LYS:HE2	1.78	0.48
1:2:340:ASN:HD21	1:2:374:ARG:NH2	2.12	0.47
1:2:405:HIS:CE1	5:6:621:TYR:HB2	2.48	0.47
2:3:653:ILE:HD13	4:5:402:ASP:HB2	1.74	0.47
3:4:177:LEU:HD12	3:4:178:ARG:O	2.14	0.47
3:4:443:PRO:HB3	3:4:457:TYR:HE1	1.77	0.47
3:4:527:ALA:HB3	3:4:537:LYS:HZ3	1.79	0.47
3:4:563:ASN:HD22	3:4:649:MET:CE	2.27	0.47
2:3:390:GLU:HG2	2:3:509:ARG:NH1	2.29	0.47
3:4:318:ASN:HD22	6:7:341:ARG:HH12	1.63	0.47
3:4:796:ARG:NH1	7:6:2001:ADP:H4'	2.29	0.47
4:5:19:PRO:N	4:5:20:ASN:HA	2.29	0.47
2:3:346:ASP:O	2:3:350:ILE:HD12	2.14	0.47
2:3:372:TYR:H	7:3:2001:ADP:HN62	1.62	0.47
2:3:447:THR:HB	2:3:448:THR:HG22	1.95	0.47
4:5:19:PRO:HB2	4:5:20:ASN:C	2.40	0.47
4:5:299:SER:OG	4:5:300:ILE:N	2.48	0.47
5:6:612:VAL:HG23	5:6:623:ILE:HA	1.96	0.47
1:2:278:ALA:O	1:2:281:LEU:HG	2.15	0.47
1:2:315:SER:N	1:2:430:TYR:O	2.36	0.47
1:2:785:LYS:HG3	1:2:788:ARG:NH2	2.29	0.47
2:3:342:LEU:O	2:3:346:ASP:HB2	2.14	0.47
4:5:626:PHE:HZ	4:5:630:ARG:HH21	1.63	0.47
5:6:124:VAL:HB	5:6:133:GLU:HA	1.95	0.47
5:6:373:MET:HG3	5:6:374:PRO:HD2	1.95	0.47
5:6:609:THR:HG22	5:6:610:ALA:N	2.25	0.47
2:3:201:HIS:CE1	2:3:243:THR:HG22	2.49	0.47
2:3:443:THR:OG1	2:3:457:LEU:HD22	2.15	0.47
3:4:578:LEU:HD22	3:4:630:CYS:HB3	1.96	0.47
3:4:818:GLU:HG3	3:4:820:GLU:H	1.80	0.47
5:6:121:ASP:OD2	5:6:161:ARG:NH2	2.47	0.47
5:6:144:LYS:HZ1	5:6:194:PRO:CG	2.27	0.47
5:6:559:THR:HG23	5:6:565:LEU:HD23	1.95	0.47
5:6:811:ALA:HB2	5:6:819:ILE:HG12	1.96	0.47
6:7:628:LEU:N	6:7:629:ASP:HA	2.29	0.47
1:2:201:PRO:HG2	1:2:203:VAL:HG23	1.96	0.47
2:3:252:ASP:CG	6:7:231:LYS:HZ3	2.22	0.47
3:4:191:THR:OG1	3:4:275:THR:HG22	2.15	0.47
3:4:809:ALA:HB2	3:4:817:VAL:HG23	1.94	0.47
5:6:112:ARG:HH22	5:6:183:LYS:CB	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:769:TYR:CZ	1:2:773:LYS:HD3	2.50	0.47
1:2:805:ILE:HD11	1:2:845:PHE:CZ	2.50	0.47
1:2:861:PHE:O	1:2:864:TYR:HB3	2.15	0.47
2:3:176:LEU:HD23	2:3:177:ASN:N	2.30	0.47
2:3:444:ALA:O	2:3:499:LYS:NZ	2.37	0.47
2:3:670:GLN:HE22	2:3:719:LYS:NZ	2.12	0.47
3:4:184:ASN:ND2	6:7:141:VAL:HG11	2.30	0.47
3:4:249:LEU:HA	3:4:250:ALA:HA	1.60	0.47
3:4:265:PRO:HB3	3:4:325:LEU:HG	1.97	0.47
3:4:367:GLU:OE2	5:6:421:LEU:HB3	2.15	0.47
3:4:455:SER:HB3	6:7:276:ARG:O	2.14	0.47
3:4:651:GLN:NE2	5:6:586:LYS:NZ	2.62	0.47
3:4:656:ILE:HG23	3:4:658:LYS:HG2	1.97	0.47
3:4:823:GLN:OE1	3:4:823:GLN:N	2.44	0.47
5:6:568:ASP:OD1	5:6:677:SER:HB3	2.14	0.47
5:6:579:THR:HG23	5:6:717:ASP:OD2	2.15	0.47
5:6:767:LYS:HG2	5:6:769:ALA:H	1.79	0.47
5:6:768:GLU:OE1	5:6:768:GLU:N	2.47	0.47
6:7:88:TYR:CZ	6:7:92:LYS:HG3	2.49	0.47
6:7:414:LEU:O	6:7:418:ILE:HD12	2.15	0.47
6:7:441:ASP:OD1	6:7:441:ASP:C	2.57	0.47
1:2:549:LYS:NZ	1:2:651:ASN:OD1	2.47	0.47
3:4:557:ARG:NH1	3:4:668:ARG:HH21	2.10	0.47
5:6:819:ILE:HG22	5:6:820:THR:N	2.27	0.47
6:7:484:THR:HG23	6:7:487:GLY:CA	2.44	0.47
2:3:484:VAL:HG22	6:7:528:LYS:HG2	1.97	0.47
2:3:655:PHE:HA	2:3:658:LYS:HZ3	1.80	0.47
3:4:263:ASN:HD21	6:7:135:LYS:HD3	1.80	0.47
3:4:796:ARG:HH11	7:6:2001:ADP:H4'	1.79	0.47
4:5:455:ARG:HH12	4:5:460:ARG:HD2	1.78	0.47
6:7:670:ASP:HA	6:7:673:ARG:HG2	1.97	0.47
2:3:152:PRO:HB2	2:3:154:LYS:HE3	1.95	0.47
3:4:334:ARG:NH1	3:4:398:LYS:HD2	2.30	0.47
4:5:239:ASP:HA	4:5:240:PRO:HD2	1.82	0.47
4:5:294:ILE:HG21	4:5:330:ILE:HG12	1.97	0.47
4:5:412:VAL:HB	4:5:520:LEU:HG	1.96	0.47
6:7:451:ARG:HA	6:7:452:GLY:HA3	1.62	0.47
6:7:570:LEU:HB2	6:7:585:ASN:ND2	2.30	0.47
1:2:342:LEU:N	1:2:371:GLY:O	2.47	0.46
1:2:660:THR:O	1:2:850:LYS:HG3	2.15	0.46
2:3:411:PRO:O	2:3:412:SER:OG	2.20	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:422:VAL:HG11	2:3:513:ILE:HD12	1.96	0.46
3:4:281:VAL:HG22	3:4:297:GLU:HG2	1.97	0.46
3:4:435:VAL:HG22	3:4:466:VAL:HG22	1.98	0.46
3:4:688:VAL:HG12	3:4:692:ILE:HD11	1.96	0.46
4:5:673:GLN:OE1	4:5:675:ARG:NH2	2.47	0.46
5:6:282:GLU:OE1	5:6:282:GLU:N	2.48	0.46
5:6:600:GLY:HA2	5:6:601:LYS:C	2.40	0.46
5:6:710:ASP:HA	5:6:711:LEU:HA	1.60	0.46
5:6:777:TYR:CD1	5:6:800:LEU:HB2	2.50	0.46
6:7:83:ASP:OD1	6:7:207:LEU:HB3	2.16	0.46
6:7:257:VAL:HG22	6:7:306:LYS:HB3	1.98	0.46
1:2:435:ASP:N	1:2:436:GLY:HA3	2.30	0.46
1:2:656:ARG:NH1	5:6:794:ARG:HD3	2.29	0.46
3:4:211:GLU:CD	3:4:212:ARG:NH1	2.74	0.46
3:4:530:ILE:HA	7:4:2001:ADP:C2	2.50	0.46
4:5:2:SER:OG	4:5:3:PHE:N	2.43	0.46
5:6:426:ILE:HG22	5:6:427:SER:N	2.26	0.46
5:6:769:ALA:O	5:6:772:TYR:HB3	2.16	0.46
2:3:247:TYR:OH	6:7:12:VAL:HG21	2.16	0.46
2:3:347:ILE:HG12	2:3:351:ASN:HD21	1.79	0.46
2:3:524:ASP:O	2:3:532:ASN:ND2	2.47	0.46
3:4:308:VAL:HG21	3:4:325:LEU:HB3	1.97	0.46
3:4:762:ILE:HG12	5:6:736:MET:CE	2.46	0.46
4:5:25:THR:C	4:5:27:ILE:H	2.23	0.46
4:5:549:ARG:HG2	4:5:651:ARG:NH2	2.31	0.46
4:5:568:ILE:HD11	7:5:2001:ADP:C6	2.51	0.46
6:7:25:LEU:HD11	6:7:117:PHE:CE1	2.50	0.46
6:7:158:THR:HB	6:7:185:VAL:HG21	1.97	0.46
1:2:674:LEU:HD21	1:2:680:LEU:HD21	1.97	0.46
2:3:488:GLU:OE2	2:3:492:GLN:HG2	2.16	0.46
3:4:408:ASP:C	3:4:410:GLN:N	2.73	0.46
3:4:428:ARG:HD3	5:6:370:THR:O	2.15	0.46
4:5:50:LEU:HD22	4:5:101:ILE:HD12	1.97	0.46
4:5:184:ARG:NH1	4:5:240:PRO:HA	2.30	0.46
4:5:438:TYR:OH	4:5:480:ASP:OD2	2.20	0.46
4:5:535:SER:OG	4:5:538:ASP:OD2	2.21	0.46
5:6:182:GLN:O	5:6:186:ARG:HG3	2.15	0.46
5:6:533:ILE:HD13	5:6:548:LEU:HD13	1.98	0.46
5:6:699:LEU:HD23	5:6:701:MET:HE3	1.97	0.46
1:2:543:GLY:HA3	1:2:549:LYS:CD	2.37	0.46
2:3:33:ASP:CA	2:3:39:ARG:HH11	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:467:ARG:NH2	2:3:509:ARG:NH1	2.64	0.46
2:3:569:HIS:CD2	4:5:657:ILE:HD13	2.50	0.46
3:4:318:ASN:ND2	6:7:341:ARG:HH12	2.13	0.46
3:4:404:ASP:OD1	3:4:405:PHE:N	2.49	0.46
3:4:688:VAL:O	3:4:692:ILE:HD12	2.16	0.46
3:4:743:PRO:HG2	3:4:747:LEU:HD23	1.96	0.46
4:5:276:MET:HE1	4:5:328:ILE:HD12	1.98	0.46
6:7:154:LEU:O	6:7:158:THR:HG22	2.16	0.46
1:2:584:PRO:HD2	4:5:270:MET:HE1	1.97	0.46
1:2:843:ASP:OD1	1:2:843:ASP:C	2.59	0.46
2:3:31:PHE:CD1	2:3:32:LEU:HA	2.50	0.46
4:5:286:VAL:HG13	4:5:290:THR:OG1	2.16	0.46
5:6:162:GLU:O	5:6:163:ASN:HB2	2.15	0.46
5:6:606:ALA:HA	5:6:607:GLY:C	2.39	0.46
1:2:583:ASP:OD2	1:2:590:THR:HG23	2.16	0.46
2:3:437:SER:CB	2:3:438:SER:HA	2.40	0.46
3:4:377:ASN:CB	3:4:378:GLU:HA	2.46	0.46
4:5:486:ARG:O	4:5:490:ARG:HB2	2.16	0.46
6:7:245:ILE:HG12	6:7:315:ILE:HD11	1.98	0.46
6:7:322:VAL:HG21	6:7:328:PRO:HG3	1.97	0.46
2:3:555:GLU:O	2:3:558:ASP:HB3	2.15	0.46
3:4:206:ARG:HA	3:4:209:LEU:HB3	1.97	0.46
3:4:462:ASP:OD1	3:4:462:ASP:O	2.33	0.46
3:4:662:ILE:HD13	5:6:627:ALA:N	2.30	0.46
4:5:588:GLU:HB3	4:5:593:GLU:HB2	1.97	0.46
5:6:109:GLU:OE2	5:6:112:ARG:HD3	2.15	0.46
5:6:303:GLU:O	5:6:353:PHE:HA	2.16	0.46
5:6:422:ASP:OD1	5:6:424:ARG:HG3	2.15	0.46
5:6:603:SER:OG	5:6:644:MET:SD	2.74	0.46
5:6:752:ARG:C	5:6:756:LYS:NZ	2.74	0.46
1:2:233:THR:C	1:2:235:GLY:HA3	2.41	0.46
1:2:305:SER:OG	1:2:306:LEU:N	2.46	0.46
1:2:557:GLU:CD	1:2:565:PHE:HB2	2.40	0.46
1:2:785:LYS:HG3	1:2:788:ARG:HH21	1.80	0.46
2:3:653:ILE:N	2:3:654:PRO:CD	2.61	0.46
2:3:700:ARG:O	2:3:704:THR:HG23	2.15	0.46
3:4:333:LEU:HD12	3:4:398:LYS:NZ	2.27	0.46
3:4:509:ILE:HG13	3:4:746:PHE:CZ	2.51	0.46
6:7:356:LEU:HA	6:7:357:PRO:HD3	1.59	0.46
2:3:235:ASP:HB2	2:3:241:LEU:HD11	1.98	0.46
3:4:234:ARG:HG3	3:4:291:TYR:OH	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:633:LEU:HB2	4:5:648:ILE:HD11	1.98	0.46
5:6:399:GLY:HA2	5:6:454:PHE:CE1	2.50	0.46
5:6:420:THR:HG22	5:6:445:VAL:HG12	1.98	0.46
5:6:644:MET:HB3	5:6:648:ASP:OD2	2.16	0.46
1:2:271:PHE:HE2	1:2:295:VAL:HG11	1.81	0.45
2:3:252:ASP:OD2	6:7:231:LYS:NZ	2.45	0.45
2:3:330:HIS:HB2	2:3:337:ALA:HB3	1.97	0.45
4:5:549:ARG:HG2	4:5:651:ARG:HH22	1.80	0.45
5:6:730:HIS:O	5:6:733:ASP:HB2	2.16	0.45
1:2:589:TRP:CH2	4:5:457:PRO:HG3	2.50	0.45
1:2:703:HIS:CD2	5:6:565:LEU:HD22	2.51	0.45
2:3:57:ASN:O	2:3:61:ASP:HB2	2.16	0.45
3:4:471:ASP:HB3	3:4:474:LEU:HG	1.97	0.45
4:5:349:PHE:HZ	4:5:609:LYS:NZ	2.13	0.45
4:5:413:LEU:HD23	4:5:415:LEU:HD23	1.98	0.45
4:5:605:TYR:HE2	4:5:668:LEU:HD11	1.81	0.45
1:2:314:LEU:O	1:2:315:SER:OG	2.28	0.45
1:2:601:LYS:HZ2	1:2:643:ARG:HD2	1.81	0.45
1:2:794:ARG:O	1:2:797:SER:OG	2.30	0.45
2:3:220:THR:HG21	2:3:224:ARG:HH12	1.82	0.45
3:4:758:ILE:HD13	3:4:813:LEU:HA	1.98	0.45
4:5:266:PRO:C	4:5:268:GLY:H	2.24	0.45
5:6:355:ASP:OD2	5:6:383:GLY:CA	2.62	0.45
5:6:537:VAL:HG11	5:6:584:PHE:CE1	2.51	0.45
1:2:505:ILE:C	1:2:507:GLY:H	2.23	0.45
1:2:576:LEU:HD23	1:2:595:ALA:HB3	1.97	0.45
4:5:261:ILE:HG22	4:5:263:GLU:H	1.81	0.45
5:6:356:TRP:HB2	5:6:381:LEU:O	2.17	0.45
6:7:149:ARG:CZ	6:7:152:ARG:HH11	2.25	0.45
6:7:399:GLU:OE2	6:7:403:GLU:OE2	2.35	0.45
6:7:685:THR:HB	6:7:686:PRO:HD2	1.97	0.45
1:2:401:ARG:N	5:6:390:LYS:NZ	2.64	0.45
2:3:656:LEU:O	2:3:660:VAL:HG23	2.16	0.45
2:3:673:GLN:HA	2:3:676:ILE:HD12	1.98	0.45
3:4:419:VAL:O	3:4:420:TYR:CD2	2.70	0.45
3:4:447:ASN:O	3:4:448:SER:OG	2.22	0.45
3:4:641:THR:O	3:4:642:ARG:HB2	2.16	0.45
4:5:152:ASP:H	4:5:155:HIS:CD2	2.35	0.45
4:5:179:LEU:HD12	4:5:179:LEU:O	2.16	0.45
5:6:134:LYS:HG2	5:6:137:ARG:HD3	1.99	0.45
6:7:209:GLN:HB3	6:7:210:ASN:H	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:258:ILE:O	6:7:270:PHE:HA	2.15	0.45
6:7:480:GLY:HA2	6:7:520:ILE:O	2.16	0.45
1:2:537:ILE:HG23	1:2:678:ASP:OD2	2.17	0.45
2:3:345:PHE:HE1	2:3:348:ARG:HH21	1.64	0.45
3:4:731:ASP:OD1	3:4:732:LYS:N	2.44	0.45
4:5:66:GLU:HA	4:5:69:ILE:HG22	1.98	0.45
4:5:363:ASN:HB2	4:5:366:LEU:HB2	1.99	0.45
5:6:173:GLN:O	5:6:176:ARG:HB3	2.17	0.45
5:6:288:LEU:N	5:6:399:GLY:HA3	2.28	0.45
5:6:566:ARG:HA	5:6:567:GLY:HA3	1.72	0.45
6:7:213:ARG:O	6:7:215:TYR:CD1	2.69	0.45
6:7:290:SER:C	6:7:292:ASN:H	2.24	0.45
6:7:659:TYR:OH	6:7:714:GLU:OE1	2.27	0.45
1:2:397:VAL:HG12	1:2:398:PRO:O	2.17	0.45
1:2:767:ILE:HG13	1:2:768:HIS:H	1.81	0.45
3:4:209:LEU:O	3:4:210:ASP:HB2	2.17	0.45
3:4:211:GLU:HG3	3:4:212:ARG:HG2	1.99	0.45
3:4:267:GLU:O	3:4:271:ILE:HD12	2.15	0.45
4:5:426:LEU:HA	4:5:426:LEU:HD23	1.59	0.45
6:7:19:ASN:O	6:7:22:THR:OG1	2.27	0.45
6:7:466:LYS:HG2	7:7:2001:ADP:O2B	2.17	0.45
6:7:466:LYS:N	7:7:2001:ADP:O2B	2.50	0.45
6:7:516:ALA:O	6:7:561:THR:HG22	2.16	0.45
6:7:581:LEU:HB2	6:7:681:PHE:CE1	2.52	0.45
6:7:668:ARG:HH22	6:7:686:PRO:HD3	1.81	0.45
1:2:410:LEU:C	1:2:411:LEU:HD12	2.42	0.45
2:3:40:ASP:O	2:3:43:ARG:HB3	2.17	0.45
2:3:176:LEU:HA	2:3:298:PHE:HD2	1.82	0.45
3:4:271:ILE:O	3:4:275:THR:HG23	2.17	0.45
5:6:134:LYS:NZ	5:6:137:ARG:HD2	2.32	0.45
5:6:532:SER:HB3	5:6:745:PRO:HG2	1.99	0.45
5:6:560:VAL:HB	5:6:561:GLU:HA	1.99	0.45
5:6:802:SER:O	5:6:805:ARG:HG2	2.16	0.45
6:7:606:ARG:O	6:7:610:GLU:HG2	2.17	0.45
3:4:337:PRO:HB3	5:6:375:ARG:HD3	1.98	0.45
3:4:662:ILE:HD13	5:6:627:ALA:H	1.82	0.45
4:5:343:TRP:CG	4:5:344:ASN:N	2.85	0.45
6:7:138:VAL:HG22	6:7:139:LEU:N	2.32	0.45
6:7:709:ASP:O	6:7:712:ASP:HB3	2.16	0.45
1:2:245:ASN:HA	1:2:298:SER:HB2	1.98	0.45
4:5:65:MET:HG2	4:5:76:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:154:ASP:OD1	5:6:155:TYR:N	2.49	0.45
5:6:313:MET:HA	5:6:314:CYS:HA	1.47	0.45
6:7:400:ARG:HB3	6:7:637:LYS:HZ2	1.82	0.45
6:7:670:ASP:OD1	6:7:670:ASP:C	2.59	0.45
1:2:290:HIS:C	1:2:292:GLU:H	2.24	0.44
1:2:343:LYS:NZ	1:2:371:GLY:N	2.66	0.44
1:2:520:PHE:HD1	1:2:767:ILE:HG22	1.83	0.44
3:4:284:ILE:HA	3:4:290:ASP:OD2	2.17	0.44
3:4:343:LYS:NZ	3:4:392:ALA:HB3	2.32	0.44
3:4:416:SER:O	3:4:460:TYR:HB2	2.17	0.44
3:4:799:GLU:OE1	5:6:735:HIS:NE2	2.50	0.44
5:6:390:LYS:HD2	5:6:391:PRO:HD2	1.97	0.44
5:6:732:VAL:O	5:6:736:MET:HG2	2.16	0.44
6:7:235:LEU:HD12	6:7:355:PHE:CE2	2.52	0.44
6:7:444:VAL:CG2	6:7:448:MET:H	2.29	0.44
1:2:839:LYS:HD2	1:2:839:LYS:HA	1.80	0.44
2:3:444:ALA:C	2:3:499:LYS:HZ2	2.22	0.44
2:3:488:GLU:O	2:3:492:GLN:HB3	2.17	0.44
2:3:730:ALA:O	2:3:734:ARG:HG2	2.17	0.44
3:4:329:LYS:HA	3:4:433:ILE:O	2.17	0.44
3:4:417:LEU:HD22	3:4:463:VAL:HG11	1.99	0.44
3:4:519:TYR:CZ	3:4:538:LYS:HD3	2.51	0.44
4:5:34:PHE:CE1	4:5:68:LEU:HD23	2.52	0.44
5:6:537:VAL:HG11	5:6:584:PHE:CZ	2.51	0.44
6:7:136:ASP:CG	6:7:137:ASP:H	2.26	0.44
3:4:696:PRO:N	3:4:697:PRO:HD2	2.31	0.44
4:5:31:PHE:HE1	4:5:75:ILE:HG21	1.83	0.44
5:6:537:VAL:HA	7:6:2001:ADP:N1	2.33	0.44
1:2:299:ASP:OD1	1:2:301:PRO:HD3	2.17	0.44
2:3:345:PHE:O	2:3:349:ASN:ND2	2.51	0.44
2:3:409:GLY:H	2:3:415:LYS:HZ3	1.65	0.44
3:4:315:ARG:NH1	6:7:250:ASP:HA	2.33	0.44
3:4:770:LEU:HD21	3:4:802:ILE:HG22	2.00	0.44
4:5:663:LEU:HA	4:5:666:LEU:HD12	1.99	0.44
5:6:625:ALA:CB	5:6:626:GLY:HA2	2.46	0.44
5:6:689:TYR:HA	5:6:690:ASN:CB	2.41	0.44
6:7:160:GLU:O	6:7:163:SER:OG	2.24	0.44
6:7:214:ARG:HD3	6:7:214:ARG:C	2.42	0.44
1:2:493:ILE:HG13	1:2:494:ILE:N	2.32	0.44
1:2:505:ILE:CD1	1:2:552:ILE:HG13	2.48	0.44
4:5:239:ASP:N	4:5:239:ASP:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:387:ALA:HA	4:5:390:CYS:SG	2.58	0.44
6:7:258:ILE:HD12	6:7:271:GLN:HE21	1.83	0.44
6:7:440:VAL:O	6:7:440:VAL:HG12	2.17	0.44
6:7:495:ALA:HA	6:7:510:GLY:HA2	1.99	0.44
1:2:325:THR:HG22	1:2:326:ARG:N	2.28	0.44
3:4:422:GLU:HG3	3:4:492:HIS:HE1	1.82	0.44
3:4:428:ARG:HH12	3:4:482:GLU:CG	2.19	0.44
4:5:343:TRP:O	4:5:344:ASN:HB2	2.18	0.44
5:6:749:GLU:HA	5:6:752:ARG:NH2	2.32	0.44
6:7:28:PHE:CG	6:7:29:LYS:N	2.84	0.44
6:7:544:GLN:NE2	6:7:560:ARG:HG2	2.32	0.44
1:2:401:ARG:N	5:6:390:LYS:HZ2	2.16	0.44
1:2:855:ARG:HG3	1:2:858:ARG:NH2	2.32	0.44
2:3:152:PRO:CB	2:3:154:LYS:HE3	2.48	0.44
3:4:235:GLU:HG3	3:4:291:TYR:OH	2.17	0.44
3:4:562:ILE:HB	3:4:703:ASP:OD2	2.18	0.44
5:6:577:PRO:O	5:6:578:SER:HB2	2.18	0.44
6:7:432:LEU:HD13	6:7:473:ILE:HD11	1.99	0.44
6:7:718:ARG:O	6:7:722:VAL:HG23	2.17	0.44
2:3:216:ASP:OD1	2:3:216:ASP:C	2.60	0.44
4:5:664:ALA:N	4:5:676:HIS:HE1	2.15	0.44
6:7:31:ASP:C	6:7:62:LYS:HB2	2.43	0.44
6:7:538:HIS:HD2	6:7:593:ARG:NE	2.16	0.44
6:7:541:MET:C	6:7:543:GLN:H	2.24	0.44
2:3:381:ILE:HD11	2:3:418:LEU:HD21	1.99	0.44
3:4:178:ARG:O	3:4:179:ILE:HB	2.16	0.44
3:4:315:ARG:HG2	3:4:410:GLN:HE21	1.81	0.44
3:4:649:MET:HB3	3:4:701:ARG:HD3	1.99	0.44
3:4:799:GLU:O	3:4:802:ILE:HG12	2.18	0.44
4:5:152:ASP:N	4:5:155:HIS:HD2	2.16	0.44
5:6:397:PHE:HE1	5:6:459:VAL:HG13	1.82	0.44
2:3:138:ASP:OD1	2:3:138:ASP:N	2.51	0.43
2:3:672:THR:O	2:3:676:ILE:HD12	2.17	0.43
3:4:532:GLU:HG2	3:4:533:LEU:N	2.32	0.43
4:5:15:GLN:HA	4:5:16:GLY:HA3	1.61	0.43
4:5:421:ALA:HB2	7:5:2001:ADP:C8	2.53	0.43
5:6:420:THR:HG22	5:6:445:VAL:CG1	2.48	0.43
5:6:814:ASN:C	5:6:816:VAL:H	2.25	0.43
6:7:354:ILE:O	6:7:377:GLU:HB3	2.17	0.43
6:7:393:LEU:HB2	6:7:395:SER:N	2.33	0.43
6:7:470:LEU:CD2	6:7:564:LEU:HD22	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:499:LYS:NZ	6:7:504:ASP:OD1	2.50	0.43
6:7:619:VAL:HA	6:7:620:HIS:C	2.43	0.43
3:4:203:TYR:HE1	3:4:222:GLU:HA	1.83	0.43
3:4:318:ASN:ND2	6:7:341:ARG:NH1	2.66	0.43
3:4:573:SER:HA	7:4:2001:ADP:H5'1	2.00	0.43
4:5:546:ILE:HD12	4:5:546:ILE:H	1.84	0.43
4:5:584:GLN:O	4:5:588:GLU:HG2	2.18	0.43
6:7:131:GLU:OE1	6:7:131:GLU:N	2.50	0.43
6:7:421:GLU:CA	6:7:625:GLN:HE22	2.31	0.43
6:7:595:ASP:OD1	6:7:595:ASP:N	2.51	0.43
1:2:484:PHE:CZ	1:2:766:TYR:HD1	2.36	0.43
2:3:428:LEU:HB3	2:3:429:ALA:HB2	2.00	0.43
2:3:652:THR:CA	2:3:654:PRO:HD3	2.38	0.43
2:3:683:TYR:OH	2:3:687:ARG:HD2	2.18	0.43
3:4:346:PHE:CD2	3:4:388:ARG:HB2	2.54	0.43
3:4:473:ARG:NH2	6:7:446:ASP:O	2.51	0.43
4:5:198:ASN:OD1	4:5:201:THR:N	2.51	0.43
4:5:635:ILE:HA	4:5:638:LEU:HG	2.00	0.43
5:6:119:LEU:HD11	5:6:188:VAL:HG21	1.99	0.43
5:6:304:LEU:HG	5:6:353:PHE:HE1	1.83	0.43
2:3:194:PRO:HG2	6:7:372:THR:HG1	1.82	0.43
4:5:149:ARG:HD3	4:5:260:GLU:OE1	2.19	0.43
6:7:208:SER:HB3	6:7:209:GLN:CA	2.49	0.43
1:2:484:PHE:CZ	1:2:766:TYR:CD1	3.06	0.43
1:2:566:ALA:HB1	1:2:576:LEU:HG	2.00	0.43
2:3:389:VAL:CG1	2:3:390:GLU:H	2.13	0.43
3:4:354:HIS:CD2	3:4:372:GLU:HG3	2.46	0.43
3:4:721:ALA:HB3	6:7:661:VAL:HG13	2.00	0.43
5:6:279:ILE:HD11	5:6:290:ILE:HG12	2.01	0.43
5:6:579:THR:N	7:6:2001:ADP:O1A	2.51	0.43
1:2:227:TYR:OH	1:2:248:HIS:ND1	2.34	0.43
1:2:394:PRO:HB2	5:6:673:ASN:ND2	2.34	0.43
1:2:481:GLU:O	1:2:484:PHE:HB3	2.18	0.43
2:3:391:LYS:HE2	6:7:620:HIS:O	2.19	0.43
2:3:492:GLN:HE22	6:7:471:LYS:HE3	1.84	0.43
3:4:404:ASP:OD1	3:4:404:ASP:C	2.61	0.43
3:4:463:VAL:HG23	3:4:463:VAL:O	2.17	0.43
3:4:737:SER:HB2	3:4:742:LEU:HD11	1.99	0.43
4:5:602:TYR:O	4:5:605:TYR:HB3	2.18	0.43
2:3:377:ILE:O	2:3:380:ALA:HB3	2.19	0.43
2:3:536:PRO:HA	2:3:537:ASP:HA	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:529:SER:O	3:4:723:HIS:NE2	2.31	0.43
4:5:678:ASP:HB3	4:5:682:ARG:HH12	1.83	0.43
5:6:560:VAL:C	5:6:562:GLY:HA3	2.43	0.43
5:6:575:GLY:C	5:6:581:LYS:NZ	2.71	0.43
6:7:18:PHE:CE1	6:7:119:ARG:NH1	2.87	0.43
6:7:128:PRO:CD	6:7:129:THR:HA	2.49	0.43
6:7:225:LEU:H	6:7:241:VAL:HA	1.84	0.43
6:7:385:LYS:HG2	6:7:639:ARG:HH12	1.83	0.43
1:2:656:ARG:HH11	5:6:794:ARG:CA	2.15	0.43
2:3:130:THR:HG22	2:3:153:TRP:HB2	2.00	0.43
2:3:172:THR:HB	2:3:173:ALA:HA	2.00	0.43
2:3:687:ARG:NH1	2:3:698:THR:HA	2.34	0.43
2:3:696:PRO:HB3	6:7:573:ARG:NH1	2.32	0.43
3:4:402:THR:HA	3:4:403:PRO:HD2	1.86	0.43
3:4:563:ASN:HD22	3:4:649:MET:HE1	1.83	0.43
4:5:27:ILE:HG22	4:5:31:PHE:CE2	2.54	0.43
5:6:386:VAL:C	5:6:388:ARG:H	2.27	0.43
5:6:576:ASP:O	5:6:579:THR:OG1	2.22	0.43
6:7:367:LYS:HE3	6:7:367:LYS:HB2	1.87	0.43
6:7:469:LEU:O	6:7:472:ALA:HB3	2.19	0.43
6:7:485:GLY:C	6:7:487:GLY:HA3	2.44	0.43
6:7:564:LEU:HD23	6:7:565:ALA:N	2.34	0.43
2:3:500:ALA:H	2:3:501:GLY:HA3	1.83	0.43
2:3:542:ARG:NH1	2:3:700:ARG:CZ	2.82	0.43
2:3:654:PRO:C	2:3:658:LYS:NZ	2.77	0.43
3:4:370:ARG:HH12	5:6:426:ILE:HG13	1.82	0.43
3:4:489:LYS:HG3	3:4:494:GLU:HG3	2.01	0.43
3:4:531:TYR:CE2	3:4:532:GLU:HB2	2.54	0.43
3:4:682:TYR:HB2	3:4:691:ASN:ND2	2.34	0.43
4:5:408:GLY:HA2	4:5:409:ASP:HA	1.72	0.43
4:5:664:ALA:N	4:5:676:HIS:CE1	2.87	0.43
5:6:288:LEU:O	5:6:399:GLY:N	2.51	0.43
5:6:776:LYS:NZ	5:6:824:ILE:C	2.77	0.43
6:7:360:TYR:CD2	6:7:373:GLU:HG3	2.54	0.43
6:7:546:ILE:HD12	6:7:557:LEU:HD11	1.99	0.43
1:2:208:ALA:O	1:2:212:LYS:HG2	2.18	0.43
1:2:857:LEU:O	1:2:860:SER:OG	2.27	0.43
2:3:414:ALA:HB2	7:3:2001:ADP:C8	2.54	0.43
2:3:480:ASP:OD1	2:3:481:VAL:N	2.52	0.43
3:4:769:GLU:O	3:4:772:ARG:HG2	2.19	0.43
3:4:811:MET:O	3:4:812:LYS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:65:MET:O	4:5:68:LEU:HB2	2.19	0.43
4:5:319:SER:OG	4:5:320:GLY:N	2.52	0.43
4:5:663:LEU:O	4:5:666:LEU:HB2	2.19	0.43
6:7:394:THR:O	6:7:394:THR:HG22	2.18	0.43
1:2:212:LYS:O	1:2:215:LEU:HB3	2.19	0.42
1:2:233:THR:O	1:2:235:GLY:HA3	2.19	0.42
2:3:100:LEU:HB2	2:3:159:GLY:HA2	2.01	0.42
2:3:487:HIS:NE2	2:3:539:LEU:HG	2.34	0.42
2:3:656:LEU:O	2:3:659:TYR:HB3	2.19	0.42
2:3:698:THR:HG21	6:7:462:PRO:HG2	2.01	0.42
2:3:727:LYS:O	2:3:730:ALA:HB3	2.19	0.42
4:5:62:THR:HA	4:5:138:ILE:O	2.18	0.42
5:6:275:ARG:HD2	5:6:367:GLU:CD	2.44	0.42
5:6:653:HIS:HB2	5:6:705:ILE:HG22	2.01	0.42
6:7:559:ALA:HB1	6:7:561:THR:HG23	2.01	0.42
6:7:671:SER:O	6:7:674:GLU:HB3	2.19	0.42
1:2:856:GLN:NE2	1:2:859:ARG:HD3	2.33	0.42
2:3:287:LYS:HB3	6:7:326:HIS:ND1	2.34	0.42
5:6:550:GLN:HA	5:6:569:ILE:CG2	2.49	0.42
2:3:429:ALA:HB3	2:3:469:VAL:C	2.45	0.42
2:3:519:VAL:HG23	2:3:532:ASN:O	2.19	0.42
2:3:703:GLU:HB3	2:3:707:ARG:NH2	2.34	0.42
3:4:312:LYS:HZ2	3:4:405:PHE:HD2	1.65	0.42
3:4:419:VAL:O	3:4:420:TYR:CG	2.72	0.42
4:5:614:LEU:HA	4:5:672:ALA:HB3	2.00	0.42
6:7:284:CYS:HB2	6:7:296:GLY:O	2.19	0.42
6:7:465:ALA:HA	7:7:2001:ADP:O2A	2.19	0.42
1:2:314:LEU:C	1:2:316:SER:H	2.28	0.42
2:3:467:ARG:CZ	2:3:509:ARG:NH1	2.82	0.42
2:3:558:ASP:OD1	4:5:626:PHE:CD2	2.73	0.42
4:5:264:LEU:HB2	4:5:265:VAL:CG2	2.43	0.42
4:5:374:ILE:HG23	4:5:428:PHE:CE2	2.55	0.42
6:7:68:GLN:O	6:7:71:ALA:N	2.53	0.42
6:7:385:LYS:HE2	6:7:478:PRO:HA	2.01	0.42
6:7:459:MET:HG3	6:7:460:GLY:N	2.34	0.42
2:3:201:HIS:ND1	2:3:243:THR:HG22	2.35	0.42
2:3:530:HIS:O	2:3:531:GLN:HB2	2.19	0.42
3:4:400:GLN:NE2	6:7:555:THR:HG22	2.34	0.42
3:4:567:CYS:HB3	3:4:675:ALA:HB3	2.00	0.42
3:4:794:THR:HG23	3:4:796:ARG:H	1.85	0.42
4:5:379:PHE:N	7:5:2001:ADP:HN62	2.11	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:413:LEU:HA	4:5:521:ALA:O	2.20	0.42
5:6:123:SER:HB2	5:6:135:VAL:N	2.30	0.42
5:6:664:ALA:HB2	5:6:669:HIS:CD2	2.54	0.42
5:6:786:GLN:HA	5:6:787:GLY:HA2	1.80	0.42
1:2:803:PHE:HB2	1:2:804:PRO:HA	2.01	0.42
2:3:372:TYR:CE1	2:3:564:HIS:HB3	2.55	0.42
3:4:593:GLY:C	3:4:595:GLY:H	2.28	0.42
3:4:728:TYR:CG	3:4:729:LEU:N	2.86	0.42
3:4:774:TYR:HE1	3:4:795:THR:HA	1.85	0.42
5:6:765:LEU:CD2	5:6:770:ARG:HB3	2.49	0.42
6:7:664:TYR:CD1	6:7:689:LEU:HB2	2.54	0.42
1:2:210:GLU:O	1:2:213:SER:HB3	2.19	0.42
1:2:405:HIS:HB2	5:6:621:TYR:CD1	2.54	0.42
2:3:97:ILE:HG21	2:3:158:LYS:HE3	2.02	0.42
2:3:259:GLN:HB2	4:5:461:GLU:OE2	2.19	0.42
3:4:419:VAL:HA	3:4:463:VAL:CG2	2.49	0.42
3:4:557:ARG:HE	3:4:668:ARG:HH21	1.67	0.42
5:6:379:VAL:HG11	5:6:397:PHE:HE2	1.85	0.42
6:7:82:LEU:HD12	6:7:206:PRO:HA	2.02	0.42
6:7:83:ASP:O	6:7:86:LEU:HB3	2.20	0.42
6:7:627:ASP:OD1	6:7:628:LEU:N	2.53	0.42
1:2:341:CYS:O	1:2:342:LEU:HD12	2.20	0.42
2:3:388:GLY:HA2	2:3:710:THR:HB	2.01	0.42
3:4:571:SER:H	7:4:2001:ADP:PB	2.43	0.42
4:5:181:ILE:HG21	4:5:241:TYR:HB3	2.02	0.42
4:5:194:ILE:O	4:5:194:ILE:HG13	2.20	0.42
4:5:407:ARG:HD3	4:5:498:GLU:O	2.20	0.42
4:5:440:SER:OG	4:5:480:ASP:HB2	2.19	0.42
4:5:607:ARG:HA	4:5:665:LYS:NZ	2.35	0.42
4:5:652:GLN:O	4:5:655:ALA:HB3	2.19	0.42
6:7:349:VAL:HG23	6:7:383:GLN:HA	2.02	0.42
6:7:680:SER:CB	6:7:681:PHE:HA	2.50	0.42
1:2:208:ALA:HB1	1:2:274:VAL:HG21	2.01	0.42
1:2:338:LYS:HZ1	1:2:376:ASN:HD21	1.66	0.42
1:2:544:ASP:OD2	1:2:656:ARG:HB2	2.20	0.42
2:3:476:ASP:CA	2:3:483:ARG:HH12	2.29	0.42
2:3:716:ARG:C	2:3:718:SER:H	2.27	0.42
2:3:737:LEU:C	2:3:738:LEU:HD12	2.44	0.42
3:4:284:ILE:HG23	3:4:290:ASP:OD2	2.20	0.42
3:4:484:GLU:OE1	5:6:275:ARG:NH2	2.53	0.42
3:4:545:PHE:CE1	3:4:751:ILE:HG23	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:758:ILE:CD1	3:4:813:LEU:HA	2.50	0.42
4:5:663:LEU:HB3	4:5:676:HIS:CE1	2.55	0.42
5:6:177:PHE:O	5:6:181:LEU:HD13	2.20	0.42
5:6:640:GLU:N	5:6:681:ALA:O	2.47	0.42
5:6:689:TYR:HD2	5:6:716:LEU:HD12	1.85	0.42
5:6:777:TYR:CZ	5:6:781:ARG:HD2	2.55	0.42
5:6:790:ARG:NH1	5:6:839:ASP:CG	2.77	0.42
1:2:656:ARG:HG3	1:2:657:TYR:N	2.35	0.42
1:2:804:PRO:HD2	1:2:845:PHE:HE1	1.85	0.42
2:3:433:THR:HG22	2:3:473:ASP:HB2	2.02	0.42
2:3:443:THR:C	2:3:445:ALA:H	2.28	0.42
2:3:558:ASP:OD1	2:3:558:ASP:C	2.61	0.42
3:4:233:MET:SD	3:4:241:LEU:HB2	2.59	0.42
3:4:568:GLY:O	3:4:574:LYS:NZ	2.52	0.42
4:5:275:THR:C	4:5:276:MET:HE2	2.45	0.42
4:5:577:THR:HA	4:5:579:ASN:N	2.35	0.42
6:7:73:ARG:NH1	6:7:136:ASP:CG	2.75	0.42
6:7:208:SER:CB	6:7:209:GLN:HG3	2.50	0.42
6:7:247:ARG:O	6:7:248:VAL:HG12	2.20	0.42
6:7:481:VAL:CG2	6:7:516:ALA:HB2	2.50	0.42
1:2:400:GLY:C	5:6:390:LYS:NZ	2.78	0.41
1:2:621:HIS:CE1	4:5:481:GLU:OE2	2.73	0.41
1:2:690:GLU:CD	1:2:694:ARG:HE	2.22	0.41
3:4:179:ILE:HG12	3:4:180:ILE:O	2.20	0.41
3:4:604:TYR:HD2	3:4:617:GLU:OE1	2.03	0.41
3:4:679:GLY:HA3	3:4:681:ARG:O	2.20	0.41
3:4:763:THR:O	3:4:767:LYS:NZ	2.53	0.41
4:5:585:ASN:O	4:5:589:GLU:HG2	2.20	0.41
5:6:358:LYS:HD2	5:6:378:ASP:OD2	2.20	0.41
5:6:370:THR:HA	5:6:371:GLY:HA2	1.73	0.41
5:6:759:ARG:CA	5:6:812:ARG:HH21	2.30	0.41
6:7:479:ARG:HG3	6:7:479:ARG:O	2.20	0.41
1:2:201:PRO:HB2	1:2:202:ASN:H	1.63	0.41
1:2:311:GLU:O	1:2:314:LEU:HG	2.21	0.41
1:2:693:GLU:HG3	5:6:778:LYS:NZ	2.34	0.41
1:2:794:ARG:HD3	4:5:565:ASP:OD2	2.20	0.41
2:3:666:ARG:HA	2:3:667:VAL:HA	1.69	0.41
3:4:303:VAL:HG12	3:4:305:PRO:HD3	2.03	0.41
3:4:352:CYS:N	3:4:353:ASP:HA	2.35	0.41
3:4:415:ILE:HG22	3:4:416:SER:N	2.36	0.41
3:4:641:THR:HG22	3:4:642:ARG:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:166:ILE:HD11	4:5:256:LEU:HD23	2.02	0.41
4:5:453:VAL:CG1	4:5:509:ILE:HD11	2.50	0.41
6:7:13:ASP:O	6:7:17:LEU:HD13	2.20	0.41
1:2:534:ARG:HG2	1:2:536:ASP:H	1.85	0.41
1:2:596:LEU:HD13	1:2:623:ALA:HB2	2.02	0.41
1:2:693:GLU:HA	5:6:778:LYS:HZ1	1.84	0.41
1:2:760:GLN:O	1:2:763:LEU:HG	2.19	0.41
2:3:27:ARG:NH1	2:3:106:PHE:CE2	2.88	0.41
2:3:300:SER:HA	2:3:319:THR:HG22	2.01	0.41
3:4:245:ALA:HA	3:4:246:ARG:HA	1.61	0.41
3:4:502:THR:HG22	3:4:503:ASP:N	2.35	0.41
3:4:774:TYR:CE1	3:4:795:THR:HA	2.55	0.41
4:5:264:LEU:HA	4:5:265:VAL:HA	1.81	0.41
4:5:677:VAL:HG12	4:5:681:ILE:HD11	2.01	0.41
5:6:642:ASP:OD2	5:6:683:ASN:O	2.37	0.41
5:6:685:VAL:HG23	5:6:698:ASN:O	2.20	0.41
5:6:786:GLN:OE1	5:6:787:GLY:HA2	2.19	0.41
1:2:770:ALA:O	1:2:774:ILE:HG22	2.20	0.41
1:2:780:GLN:HE21	4:5:577:THR:C	2.27	0.41
2:3:413:THR:O	2:3:413:THR:HG22	2.21	0.41
3:4:260:GLN:O	3:4:268:VAL:HG21	2.20	0.41
3:4:370:ARG:NH2	5:6:426:ILE:HG13	2.35	0.41
3:4:455:SER:O	3:4:456:LEU:C	2.63	0.41
3:4:557:ARG:HH11	3:4:668:ARG:CZ	2.30	0.41
4:5:165:ILE:HD12	4:5:262:PRO:HD2	2.01	0.41
4:5:571:HIS:O	4:5:575:ILE:HG13	2.20	0.41
5:6:577:PRO:HA	7:6:2001:ADP:O1B	2.21	0.41
1:2:446:VAL:HG21	5:6:356:TRP:CZ2	2.56	0.41
1:2:447:PHE:CE2	5:6:304:LEU:HD11	2.55	0.41
1:2:826:SER:C	1:2:828:PHE:H	2.28	0.41
2:3:447:THR:HA	2:3:448:THR:HA	1.71	0.41
2:3:468:GLY:O	2:3:511:SER:OG	2.27	0.41
3:4:246:ARG:HG3	3:4:246:ARG:O	2.20	0.41
4:5:530:TYR:HD1	4:5:533:LEU:HD12	1.85	0.41
4:5:543:GLN:HG3	4:5:546:ILE:CD1	2.51	0.41
5:6:116:GLU:CD	5:6:187:ARG:HD3	2.44	0.41
5:6:304:LEU:O	5:6:305:TYR:CD2	2.73	0.41
5:6:569:ILE:HG13	5:6:570:ASN:N	2.36	0.41
6:7:517:ASP:OD1	6:7:517:ASP:N	2.52	0.41
1:2:260:LEU:HD23	1:2:267:MET:HG2	2.02	0.41
1:2:406:ARG:HH11	1:2:430:TYR:HE1	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:313:GLY:CA	3:4:403:PRO:HB3	2.51	0.41
3:4:572:THR:O	3:4:572:THR:HG22	2.21	0.41
3:4:650:GLU:OE2	3:4:796:ARG:NH1	2.50	0.41
4:5:278:CYS:SG	4:5:330:ILE:HD12	2.60	0.41
4:5:305:ASN:HB2	4:5:319:SER:HB3	2.01	0.41
5:6:426:ILE:CG2	5:6:427:SER:H	2.24	0.41
5:6:537:VAL:HG21	5:6:584:PHE:CE1	2.55	0.41
6:7:242:ARG:HA	6:7:349:VAL:O	2.20	0.41
6:7:318:LEU:O	6:7:318:LEU:HD23	2.21	0.41
6:7:570:LEU:HD13	6:7:585:ASN:ND2	2.34	0.41
6:7:573:ARG:O	6:7:574:TYR:C	2.63	0.41
1:2:309:LEU:N	1:2:310:ARG:NH1	2.65	0.41
1:2:811:GLU:HG2	4:5:576:HIS:NE2	2.35	0.41
2:3:261:MET:HB3	2:3:264:MET:HB3	2.03	0.41
2:3:442:LEU:O	2:3:460:GLY:N	2.53	0.41
3:4:230:LEU:HD21	3:4:280:MET:SD	2.60	0.41
3:4:347:PHE:CZ	3:4:384:LEU:HD12	2.56	0.41
3:4:649:MET:CB	3:4:701:ARG:HD3	2.51	0.41
4:5:493:ILE:HG22	4:5:497:MET:HE2	2.02	0.41
5:6:143:MET:CE	5:6:148:LEU:HB2	2.51	0.41
5:6:290:ILE:HD13	5:6:454:PHE:CE1	2.56	0.41
5:6:689:TYR:HB3	5:6:691:ARG:N	2.35	0.41
5:6:772:TYR:CE2	5:6:776:LYS:HE3	2.55	0.41
1:2:609:PHE:HB3	1:2:669:LEU:HD21	2.02	0.41
2:3:435:ARG:HA	2:3:436:GLY:HA3	1.65	0.41
2:3:450:ARG:N	2:3:451:GLU:HA	2.36	0.41
2:3:686:LEU:HD21	2:3:734:ARG:NH2	2.36	0.41
3:4:276:ILE:O	3:4:280:MET:HG2	2.21	0.41
3:4:561:ASP:OD1	3:4:670:SER:HA	2.21	0.41
3:4:777:MET:SD	3:4:830:ARG:NE	2.93	0.41
5:6:767:LYS:NZ	5:6:820:THR:HA	2.35	0.41
6:7:262:CYS:C	6:7:264:GLN:H	2.29	0.41
6:7:476:ILE:O	6:7:639:ARG:HD3	2.20	0.41
6:7:523:ILE:HG21	6:7:526:PHE:HD1	1.84	0.41
1:2:440:ALA:O	1:2:442:ASN:ND2	2.53	0.41
1:2:533:ILE:HG22	1:2:534:ARG:H	1.85	0.41
1:2:547:THR:HG22	1:2:548:ALA:N	2.36	0.41
1:2:661:LEU:HB3	1:2:662:PRO:HD2	2.02	0.41
2:3:101:ASP:HA	2:3:104:ARG:NH2	2.29	0.41
2:3:440:VAL:HG12	2:3:441:GLY:N	2.36	0.41
2:3:703:GLU:C	2:3:707:ARG:NH1	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:454:LYS:O	3:4:454:LYS:HG2	2.21	0.41
3:4:569:ASP:OD1	3:4:681:ARG:HA	2.21	0.41
3:4:646:HIS:HE1	3:4:698:LEU:HB2	1.85	0.41
3:4:713:ASP:CB	3:4:716:ASN:HB2	2.44	0.41
4:5:356:GLU:CD	4:5:598:LYS:NZ	2.78	0.41
4:5:414:LEU:HD23	4:5:414:LEU:HA	1.90	0.41
4:5:541:ASP:CG	4:5:542:PHE:H	2.29	0.41
5:6:575:GLY:H	5:6:581:LYS:HZ3	1.67	0.41
5:6:645:ASP:HB3	5:6:646:ILE:H	1.68	0.41
6:7:149:ARG:NH1	6:7:152:ARG:NE	2.65	0.41
1:2:307:ARG:HG3	1:2:308:GLU:HG2	2.03	0.41
2:3:464:LEU:HD23	4:5:510:THR:HG21	2.02	0.41
2:3:671:LEU:HD22	6:7:621:MET:HB2	2.03	0.41
3:4:497:GLU:HG3	3:4:498:VAL:HG23	2.03	0.41
3:4:636:LYS:HE2	3:4:636:LYS:HB2	1.78	0.41
3:4:832:ALA:HB1	3:4:836:TYR:CZ	2.55	0.41
4:5:3:PHE:HB3	4:5:4:ASP:H	1.45	0.41
4:5:464:LEU:HD23	4:5:466:GLY:N	2.36	0.41
5:6:326:LYS:H	5:6:327:TYR:HA	1.85	0.41
5:6:363:GLU:OE2	5:6:367:GLU:HB3	2.21	0.41
5:6:373:MET:CG	5:6:374:PRO:HD2	2.50	0.41
6:7:421:GLU:HA	6:7:625:GLN:CD	2.46	0.41
6:7:529:MET:HE2	6:7:534:ARG:N	2.36	0.41
1:2:544:ASP:H	1:2:549:LYS:HD3	1.85	0.40
2:3:414:ALA:O	2:3:417:GLN:N	2.54	0.40
4:5:473:ASP:OD1	4:5:474:GLY:N	2.54	0.40
4:5:620:GLU:O	4:5:623:SER:OG	2.22	0.40
4:5:675:ARG:HA	4:5:678:ASP:OD2	2.21	0.40
6:7:465:ALA:CA	7:7:2001:ADP:H5'1	2.50	0.40
1:2:528:ASN:HA	1:2:529:GLY:HA2	1.50	0.40
2:3:252:ASP:OD2	6:7:231:LYS:HD2	2.22	0.40
3:4:284:ILE:HG23	3:4:290:ASP:HB2	2.03	0.40
3:4:325:LEU:HD23	3:4:325:LEU:HA	1.94	0.40
3:4:354:HIS:HB3	3:4:372:GLU:HG2	2.03	0.40
3:4:820:GLU:O	3:4:821:ASP:CG	2.63	0.40
4:5:69:ILE:HB	4:5:76:TYR:CG	2.56	0.40
5:6:559:THR:O	5:6:560:VAL:HG22	2.21	0.40
5:6:570:ASN:OD1	5:6:656:MET:HE2	2.21	0.40
6:7:106:ILE:O	6:7:110:ALA:HB2	2.20	0.40
6:7:214:ARG:CD	6:7:215:TYR:O	2.69	0.40
6:7:654:GLU:O	6:7:657:ASN:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:342:LEU:HD11	1:2:374:ARG:NH1	2.36	0.40
2:3:237:GLU:O	2:3:239:ASN:N	2.54	0.40
3:4:718:ARG:HA	6:7:665:ILE:HD11	2.03	0.40
3:4:727:LEU:HA	3:4:728:TYR:C	2.47	0.40
4:5:337:VAL:HA	4:5:338:GLU:HA	1.74	0.40
4:5:545:THR:O	4:5:548:SER:OG	2.19	0.40
5:6:284:ILE:HD11	5:6:403:VAL:CG2	2.51	0.40
5:6:777:TYR:CE1	5:6:781:ARG:HD2	2.57	0.40
6:7:339:LEU:HD11	6:7:381:VAL:HG23	2.02	0.40
6:7:452:GLY:H	6:7:694:ARG:HD2	1.86	0.40
1:2:429:ILE:HG13	1:2:429:ILE:O	2.19	0.40
2:3:44:SER:O	2:3:47:VAL:HB	2.22	0.40
2:3:330:HIS:CD2	2:3:337:ALA:H	2.39	0.40
3:4:366:GLN:O	3:4:366:GLN:HG2	2.21	0.40
3:4:422:GLU:HG3	3:4:492:HIS:CE1	2.56	0.40
3:4:563:ASN:O	3:4:703:ASP:HB3	2.20	0.40
4:5:442:LYS:HD3	4:5:486:ARG:HG3	2.04	0.40
4:5:453:VAL:HG11	4:5:509:ILE:HD11	2.03	0.40
5:6:599:SER:O	5:6:600:GLY:C	2.64	0.40
6:7:89:GLN:NE2	6:7:101:ASP:HA	2.37	0.40
6:7:238:LEU:HA	6:7:354:ILE:HA	2.04	0.40
6:7:472:ALA:O	6:7:476:ILE:HD12	2.22	0.40
6:7:540:VAL:O	6:7:540:VAL:HG12	2.22	0.40
1:2:338:LYS:HZ2	1:2:347:ILE:HG22	1.86	0.40
1:2:402:LEU:HD21	5:6:629:MET:HE3	2.02	0.40
1:2:777:LYS:H	1:2:828:PHE:HA	1.86	0.40
2:3:421:PHE:CD1	4:5:402:ASP:OD2	2.74	0.40
2:3:490:MET:HE1	2:3:543:PHE:CD1	2.55	0.40
3:4:258:TYR:CZ	3:4:262:LEU:HD11	2.57	0.40
3:4:366:GLN:H	3:4:366:GLN:CD	2.30	0.40
3:4:411:THR:HG21	6:7:508:LEU:O	2.20	0.40
4:5:338:GLU:HB2	4:5:339:THR:C	2.45	0.40
4:5:578:GLY:O	4:5:579:ASN:CG	2.65	0.40
5:6:153:ILE:HD11	5:6:267:PHE:CE1	2.57	0.40
5:6:153:ILE:O	5:6:267:PHE:HA	2.20	0.40
5:6:574:VAL:HB	5:6:714:VAL:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	2	597/868 (69%)	544 (91%)	47 (8%)	6 (1%)	12	43
2	3	595/971 (61%)	548 (92%)	40 (7%)	7 (1%)	10	40
3	4	632/933 (68%)	554 (88%)	71 (11%)	7 (1%)	11	41
4	5	621/775 (80%)	586 (94%)	32 (5%)	3 (0%)	24	57
5	6	608/1017 (60%)	547 (90%)	52 (9%)	9 (2%)	8	36
6	7	681/845 (81%)	619 (91%)	52 (8%)	10 (2%)	8	36
All	All	3734/5409 (69%)	3398 (91%)	294 (8%)	42 (1%)	14	41

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	4	189	GLU
3	4	609	VAL
4	5	596	ILE
5	6	317	ILE
6	7	26	VAL
6	7	209	GLN
6	7	464	VAL
6	7	544	GLN
1	2	297	ILE
2	3	230	ILE
2	3	389	VAL
3	4	179	ILE
3	4	419	VAL
3	4	494	GLU
4	5	267	VAL
4	5	410	ILE
5	6	321	VAL
5	6	402	ILE
5	6	426	ILE
5	6	541	GLU

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Mol	Chain	Res	Type
5	6	560	VAL
5	6	819	ILE
6	7	371	LEU
6	7	374	THR
1	2	305	SER
2	3	336	VAL
5	6	305	TYR
1	2	291	SER
1	2	533	ILE
1	2	585	ILE
3	4	493	ASN
6	7	375	TYR
6	7	502	VAL
2	3	440	VAL
5	6	569	ILE
6	7	678	LYS
1	2	372	PRO
2	3	238	GLY
3	4	463	VAL
2	3	519	VAL
6	7	248	VAL
2	3	326	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	2	509/770 (66%)	507 (100%)	2 (0%)	84	83
2	3	523/835 (63%)	522 (100%)	1 (0%)	87	87
3	4	573/848 (68%)	570 (100%)	3 (0%)	81	81
4	5	566/688 (82%)	565 (100%)	1 (0%)	87	87
5	6	497/886 (56%)	495 (100%)	2 (0%)	84	83
6	7	609/753 (81%)	606 (100%)	3 (0%)	81	81
All	All	3277/4780 (69%)	3265 (100%)	12 (0%)	81	83

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	498	ILE
1	2	838	ILE
2	3	676	ILE
3	4	284	ILE
3	4	360	ILE
3	4	442	ILE
4	5	294	ILE
5	6	290	ILE
5	6	571	ILE
6	7	214	ARG
6	7	315	ILE
6	7	476	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	333	GLN
1	2	376	ASN
1	2	391	GLN
1	2	437	ASN
1	2	551	GLN
1	2	561	HIS
1	2	613	ASN
1	2	703	HIS
1	2	779	HIS
1	2	780	GLN
1	2	809	HIS
1	2	849	GLN
1	2	856	GLN
2	3	330	HIS
2	3	349	ASN
2	3	351	ASN
2	3	374	HIS
2	3	492	GLN
2	3	493	GLN
2	3	554	ASN
2	3	569	HIS
2	3	670	GLN
2	3	688	ASN
3	4	193	ASN
3	4	247	ASN

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Mol	Chain	Res	Type
3	4	263	ASN
3	4	266	GLN
3	4	318	ASN
3	4	354	HIS
3	4	400	GLN
3	4	465	HIS
3	4	579	GLN
3	4	582	HIS
3	4	646	HIS
3	4	651	GLN
3	4	757	HIS
3	4	759	HIS
3	4	808	HIS
4	5	49	GLN
4	5	155	HIS
4	5	254	GLN
4	5	411	ASN
4	5	424	GLN
4	5	494	HIS
4	5	543	GLN
4	5	585	ASN
4	5	590	ASN
4	5	676	HIS
5	6	125	GLN
5	6	139	GLN
5	6	149	ASN
5	6	458	HIS
5	6	540	HIS
5	6	659	GLN
5	6	690	ASN
5	6	698	ASN
6	7	87	GLN
6	7	89	GLN
6	7	90	ASN
6	7	98	GLN
6	7	124	ASN
6	7	144	ASN
6	7	334	HIS
6	7	379	GLN
6	7	384	HIS
6	7	538	HIS
6	7	543	GLN

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Mol	Chain	Res	Type
6	7	544	GLN
6	7	554	ASN
6	7	585	ASN
6	7	620	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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
7	ADP	4	2001	-	28,29,29	1.39	5 (17%)	43,45,45	1.83	9 (20%)
7	ADP	7	2001	-	28,29,29	1.38	4 (14%)	43,45,45	1.89	8 (18%)
7	ADP	3	2001	-	28,29,29	1.41	6 (21%)	43,45,45	1.74	7 (16%)
7	ADP	5	2001	-	28,29,29	1.36	4 (14%)	43,45,45	1.90	8 (18%)
7	ADP	6	2001	-	28,29,29	1.40	4 (14%)	43,45,45	1.96	7 (16%)
7	ADP	2	2001	-	28,29,29	1.37	4 (14%)	43,45,45	1.88	11 (25%)

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
7	ADP	4	2001	-	-	5/16/32/32	0/3/3/3
7	ADP	7	2001	-	-	1/16/32/32	0/3/3/3
7	ADP	3	2001	-	-	2/16/32/32	0/3/3/3
7	ADP	5	2001	-	-	4/16/32/32	0/3/3/3
7	ADP	6	2001	-	-	4/16/32/32	0/3/3/3
7	ADP	2	2001	-	-	0/16/32/32	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	6	2001	ADP	C5-C4	4.88	1.47	1.39
7	3	2001	ADP	C5-C4	4.48	1.47	1.39
7	2	2001	ADP	C5-C4	4.47	1.47	1.39
7	7	2001	ADP	C5-C4	4.44	1.47	1.39
7	4	2001	ADP	C5-C4	4.39	1.46	1.39
7	5	2001	ADP	C5-C4	4.35	1.46	1.39
7	3	2001	ADP	C5-N7	-2.72	1.34	1.39
7	5	2001	ADP	C5-N7	-2.71	1.34	1.39
7	6	2001	ADP	C5-C6	2.63	1.48	1.41
7	4	2001	ADP	C5-N7	-2.56	1.34	1.39
7	7	2001	ADP	C5-C6	2.55	1.48	1.41
7	4	2001	ADP	C5-C6	2.54	1.48	1.41
7	2	2001	ADP	C5-N7	-2.54	1.34	1.39
7	7	2001	ADP	C5-N7	-2.50	1.34	1.39
7	2	2001	ADP	C5-C6	2.47	1.47	1.41
7	6	2001	ADP	C5-N7	-2.42	1.34	1.39
7	5	2001	ADP	C5-C6	2.39	1.47	1.41
7	2	2001	ADP	C8-N7	2.36	1.36	1.31
7	3	2001	ADP	C5-C6	2.35	1.47	1.41
7	4	2001	ADP	C8-N7	2.26	1.36	1.31
7	6	2001	ADP	C8-N7	2.24	1.36	1.31
7	4	2001	ADP	C4-N9	-2.23	1.33	1.37
7	3	2001	ADP	C4-N9	-2.16	1.33	1.37
7	3	2001	ADP	C8-N7	2.09	1.35	1.31
7	5	2001	ADP	C8-N7	2.09	1.35	1.31
7	3	2001	ADP	C8-N9	-2.08	1.34	1.37
7	7	2001	ADP	C8-N7	2.08	1.35	1.31

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	6	2001	ADP	C5-C4-N3	-6.65	117.56	126.72
7	5	2001	ADP	C5-C4-N3	-6.48	117.79	126.72
7	7	2001	ADP	C5-C4-N3	-6.10	118.31	126.72
7	4	2001	ADP	C5-C4-N3	-5.85	118.66	126.72
7	3	2001	ADP	C5-C4-N3	-5.71	118.86	126.72
7	2	2001	ADP	C5-C4-N3	-5.64	118.96	126.72
7	6	2001	ADP	N3-C4-N9	5.28	136.15	127.17
7	5	2001	ADP	N3-C4-N9	5.10	135.84	127.17
7	7	2001	ADP	N3-C4-N9	5.03	135.71	127.17
7	3	2001	ADP	N3-C4-N9	4.56	134.93	127.17
7	2	2001	ADP	N3-C4-N9	4.52	134.85	127.17
7	4	2001	ADP	N3-C4-N9	4.30	134.47	127.17
7	6	2001	ADP	C2-N3-C4	4.07	121.76	111.83
7	5	2001	ADP	C2-N3-C4	3.89	121.34	111.83
7	2	2001	ADP	C2-N3-C4	3.77	121.03	111.83
7	7	2001	ADP	C2-N3-C4	3.72	120.93	111.83
7	4	2001	ADP	C4-C5-N7	-3.63	106.43	110.58
7	4	2001	ADP	C2-N3-C4	3.63	120.69	111.83
7	2	2001	ADP	N3-C2-N1	-3.62	123.10	128.58
7	3	2001	ADP	C2-N3-C4	3.46	120.27	111.83
7	6	2001	ADP	N3-C2-N1	-3.34	123.52	128.58
7	6	2001	ADP	C4-C5-N7	-3.30	106.81	110.58
7	5	2001	ADP	C4-C5-N7	-3.27	106.84	110.58
7	7	2001	ADP	C4-C5-N7	-3.21	106.91	110.58
7	3	2001	ADP	C4-C5-N7	-3.16	106.96	110.58
7	3	2001	ADP	N3-C2-N1	-3.10	123.88	128.58
7	2	2001	ADP	C4-C5-N7	-3.10	107.04	110.58
7	5	2001	ADP	N3-C2-N1	-3.09	123.91	128.58
7	7	2001	ADP	N3-C2-N1	-3.08	123.92	128.58
7	6	2001	ADP	C3'-C2'-C1'	2.94	107.02	101.46
7	4	2001	ADP	N3-C2-N1	-2.91	124.18	128.58
7	2	2001	ADP	C3'-C2'-C1'	2.80	106.77	101.46
7	7	2001	ADP	C4-N9-C8	2.72	108.59	105.74
7	7	2001	ADP	C3'-C2'-C1'	2.59	106.35	101.46
7	2	2001	ADP	C2'-C1'-N9	-2.56	106.94	113.30
7	2	2001	ADP	C4-N9-C8	2.49	108.35	105.74
7	6	2001	ADP	C5-N7-C8	2.45	107.30	103.45
7	4	2001	ADP	C2'-C1'-N9	-2.43	107.27	113.30
7	4	2001	ADP	C5-N7-C8	2.42	107.26	103.45
7	5	2001	ADP	C3'-C2'-C1'	2.42	106.04	101.46
7	7	2001	ADP	C5-N7-C8	2.35	107.15	103.45
7	5	2001	ADP	C5-N7-C8	2.35	107.15	103.45
7	3	2001	ADP	C4-N9-C8	2.33	108.19	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	2	2001	ADP	C5-N7-C8	2.25	106.99	103.45
7	4	2001	ADP	C6-C5-N7	2.21	136.36	132.09
7	4	2001	ADP	C4-N9-C8	2.21	108.06	105.74
7	5	2001	ADP	C4-N9-C8	2.18	108.03	105.74
7	3	2001	ADP	C5-N7-C8	2.10	106.75	103.45
7	2	2001	ADP	C2-N1-C6	2.05	122.09	118.73
7	2	2001	ADP	C6-C5-N7	2.03	136.01	132.09

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	3	2001	ADP	C5'-O5'-PA-O3A
7	4	2001	ADP	C5'-O5'-PA-O1A
7	4	2001	ADP	C5'-O5'-PA-O2A
7	4	2001	ADP	C5'-O5'-PA-O3A
7	5	2001	ADP	C5'-O5'-PA-O3A
7	6	2001	ADP	C5'-O5'-PA-O3A
7	4	2001	ADP	C3'-C4'-C5'-O5'
7	4	2001	ADP	O4'-C4'-C5'-O5'
7	6	2001	ADP	C2'-C1'-N9-C4
7	6	2001	ADP	C2'-C1'-N9-C8
7	3	2001	ADP	C5'-O5'-PA-O1A
7	5	2001	ADP	C5'-O5'-PA-O1A
7	6	2001	ADP	C5'-O5'-PA-O1A
7	7	2001	ADP	O4'-C4'-C5'-O5'
7	5	2001	ADP	C3'-C4'-C5'-O5'
7	5	2001	ADP	C2'-C1'-N9-C8

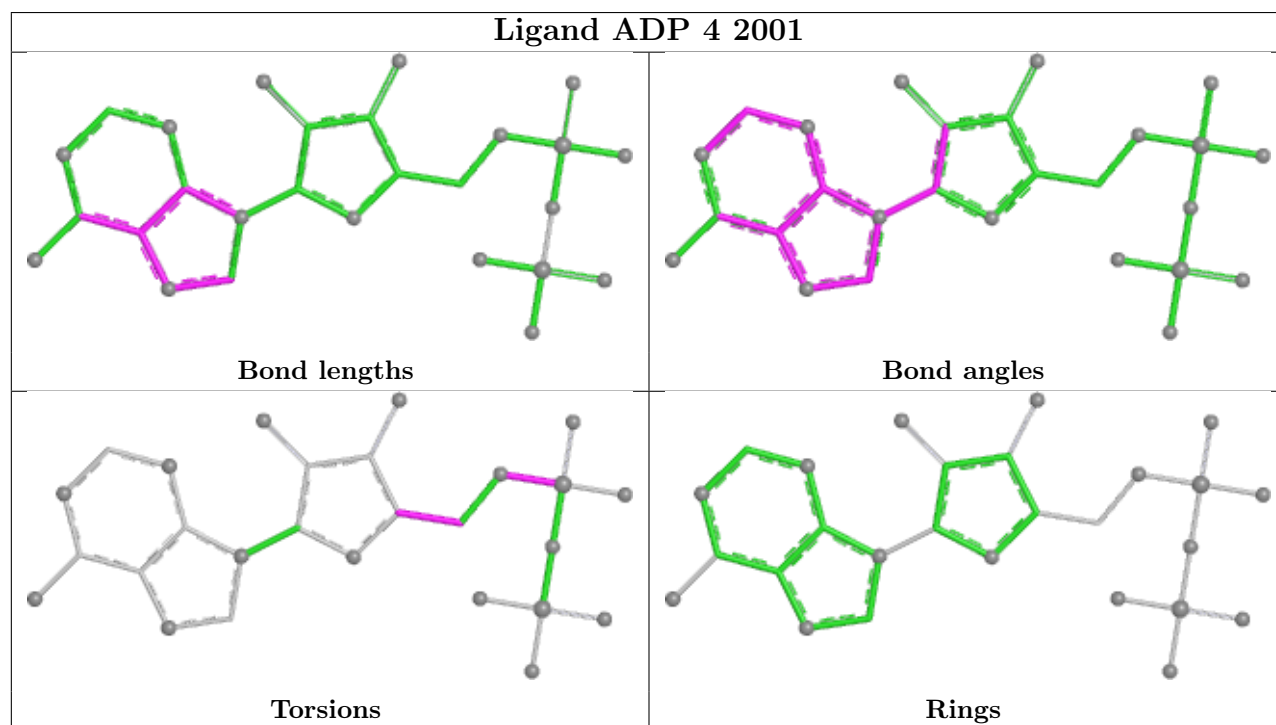
There are no ring outliers.

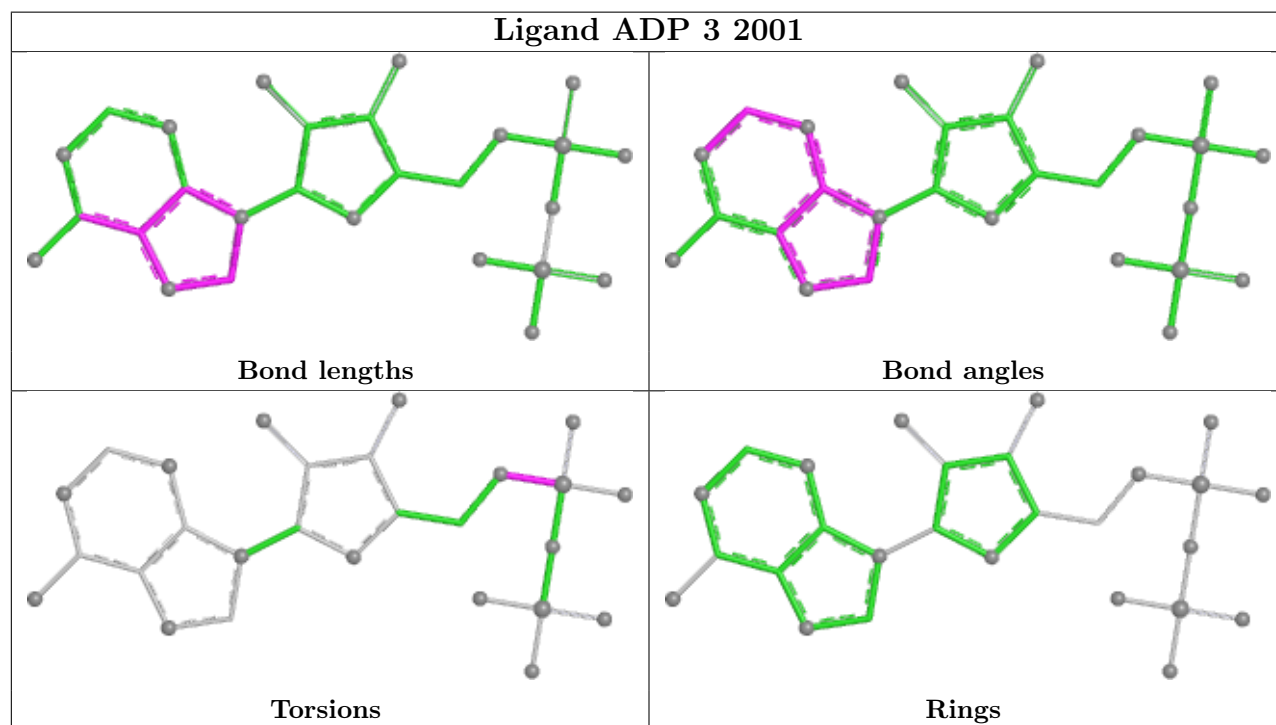
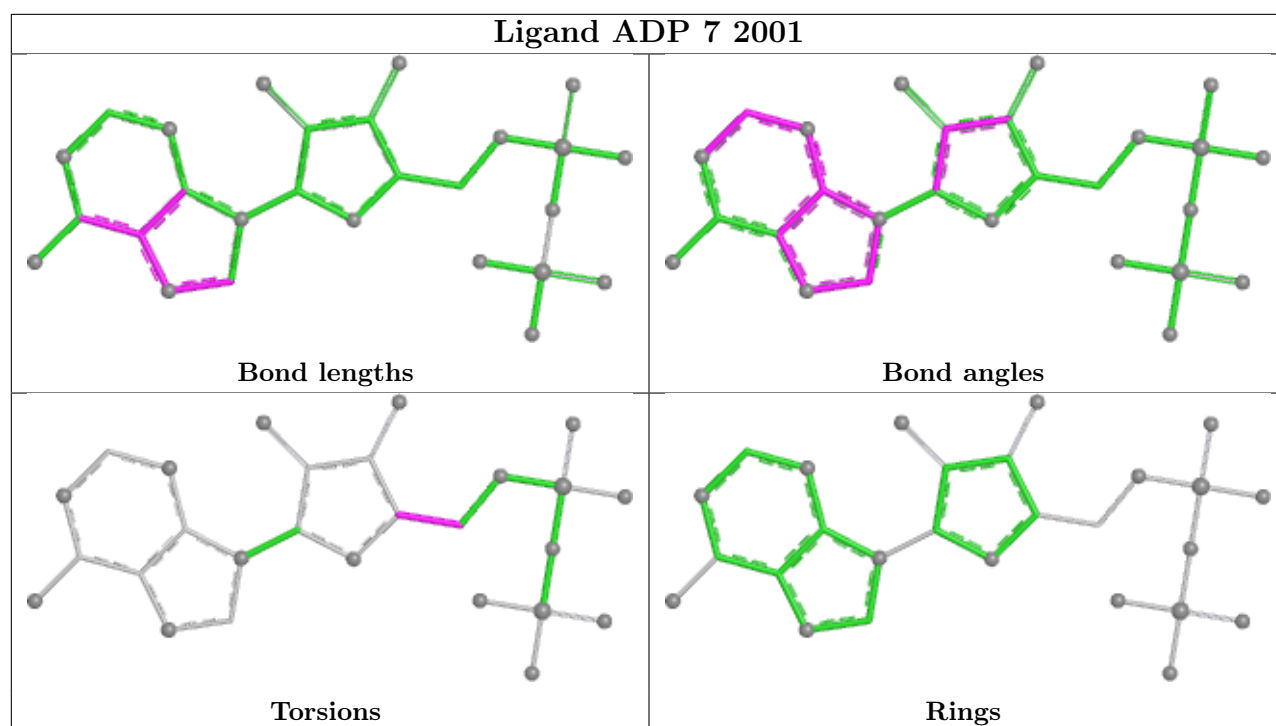
6 monomers are involved in 34 short contacts:

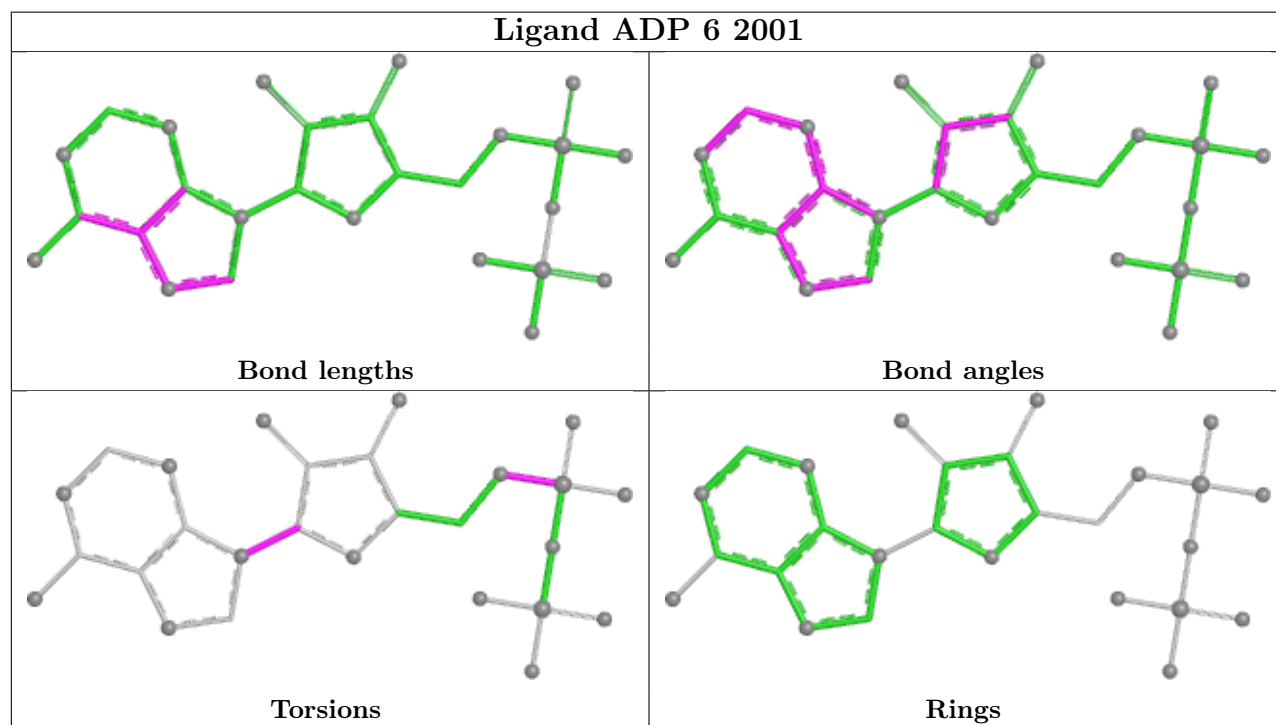
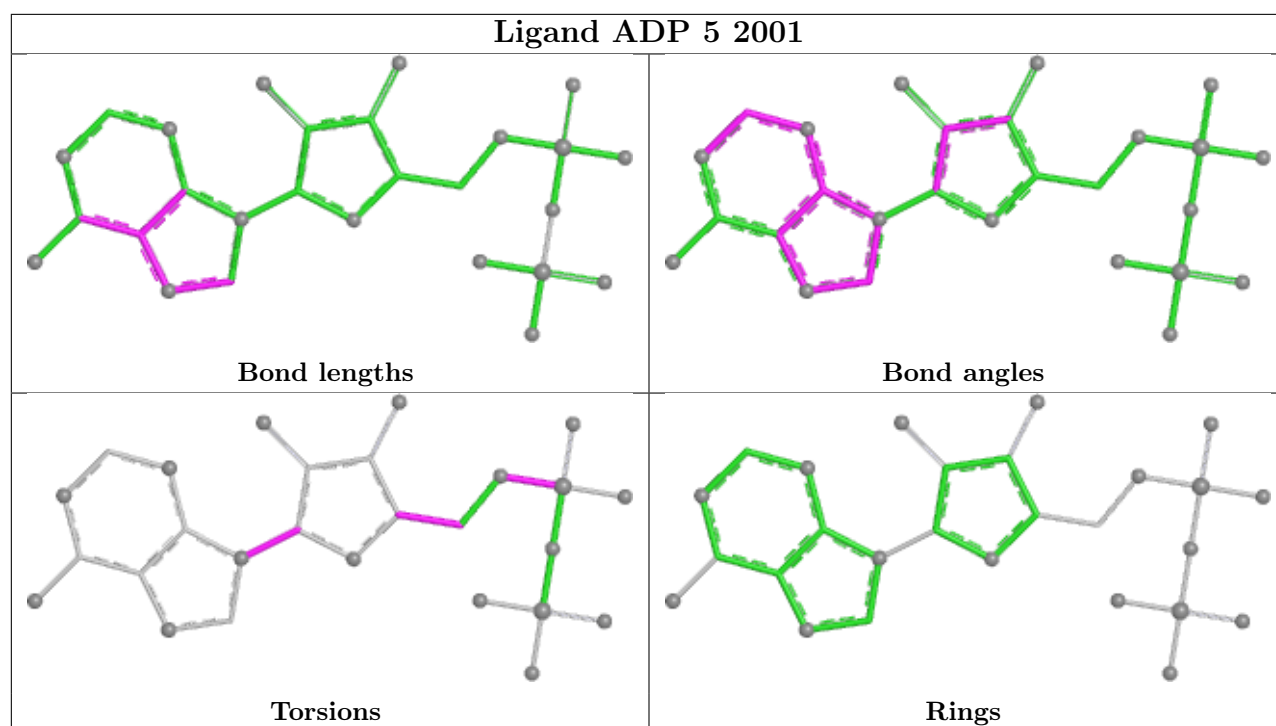
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	4	2001	ADP	6	0
7	7	2001	ADP	6	0
7	3	2001	ADP	4	0
7	5	2001	ADP	7	0
7	6	2001	ADP	10	0
7	2	2001	ADP	1	0

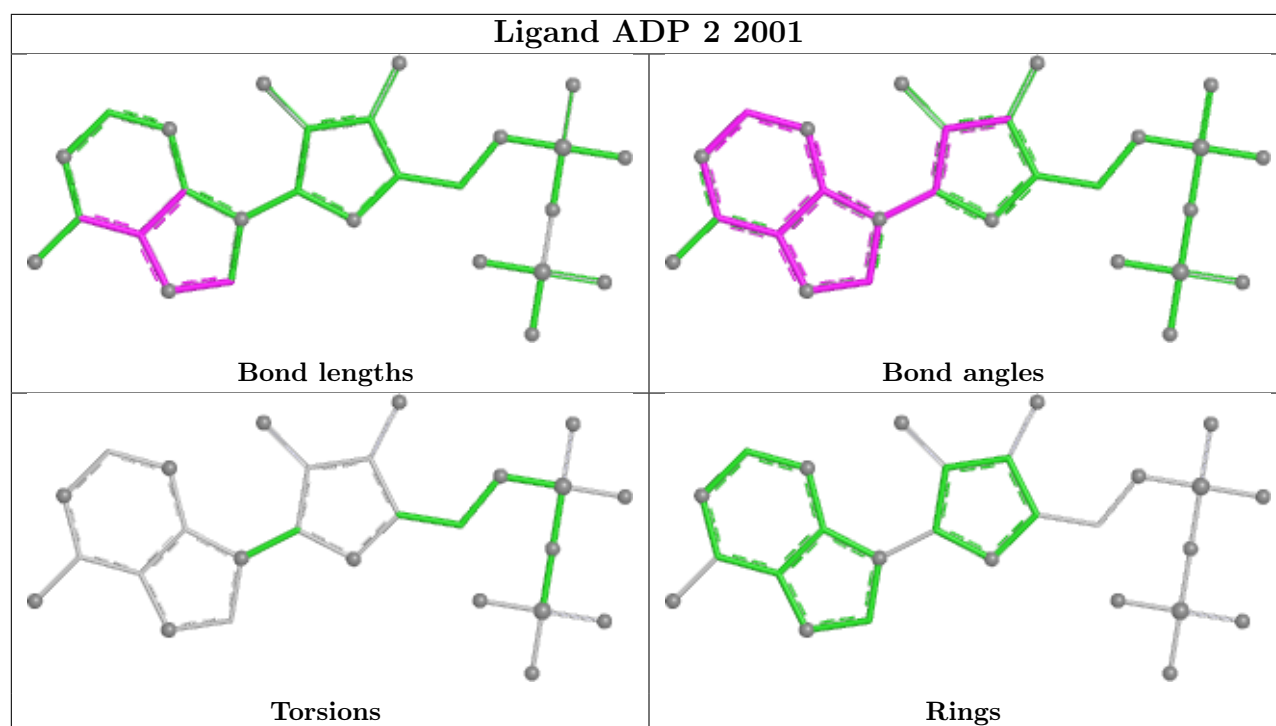
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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









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.

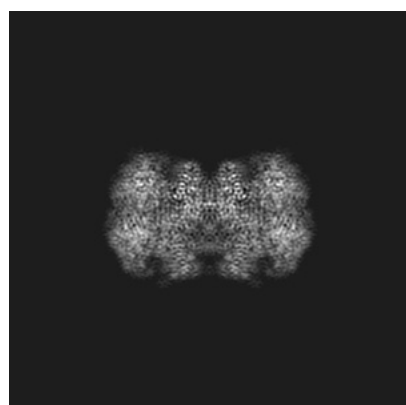
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6338. These allow visual inspection of the internal detail of the map and identification of artifacts.

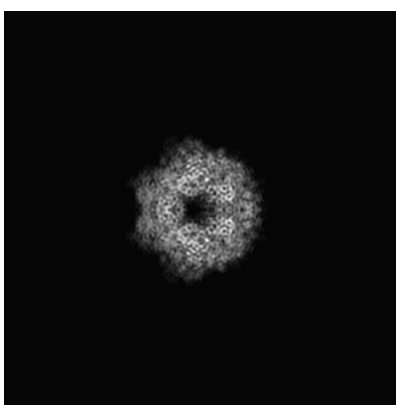
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

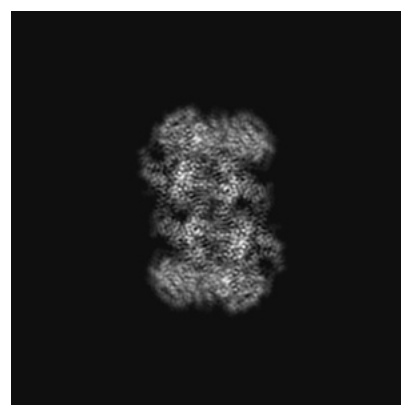
6.1.1 Primary map



X



Y



Z

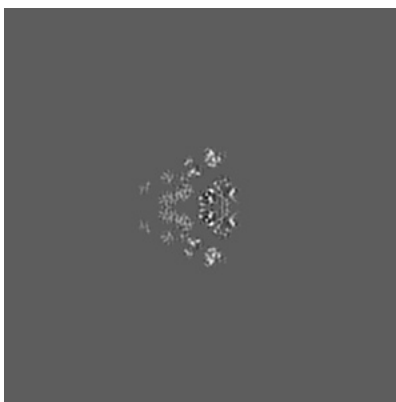
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

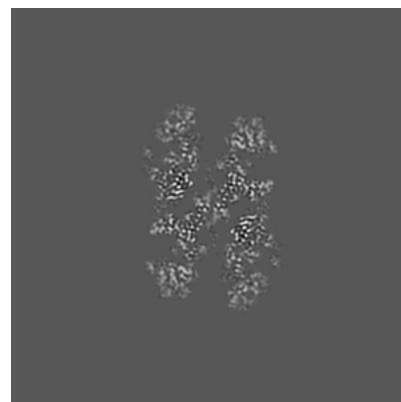
6.2.1 Primary map



X Index: 150



Y Index: 150

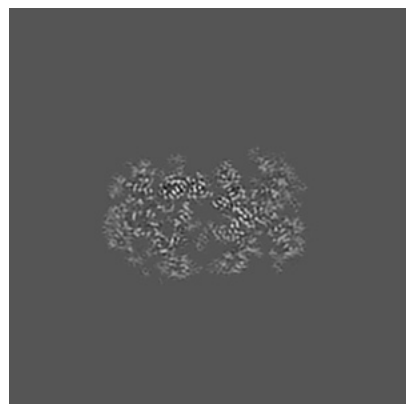


Z Index: 150

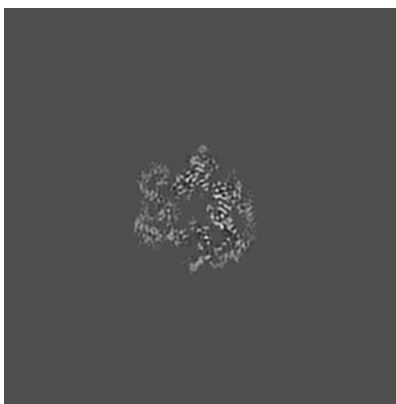
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

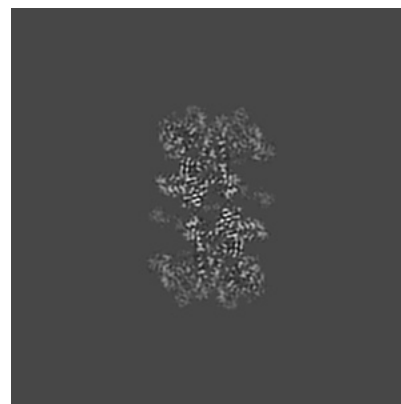
6.3.1 Primary map



X Index: 166



Y Index: 169

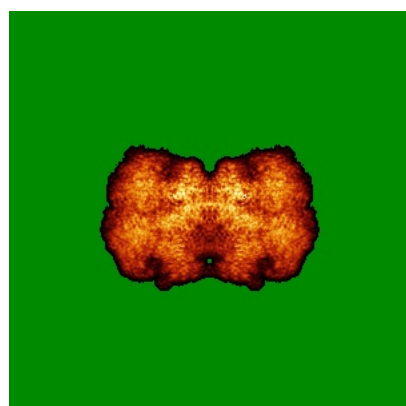


Z Index: 166

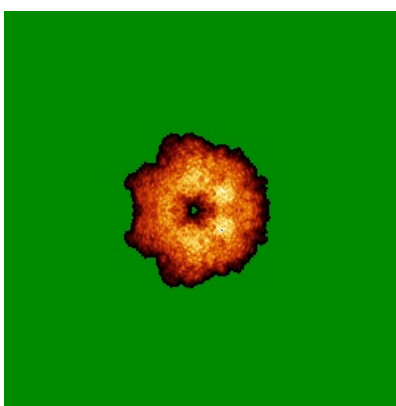
The images above show the largest variance slices of the map in three orthogonal directions.

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

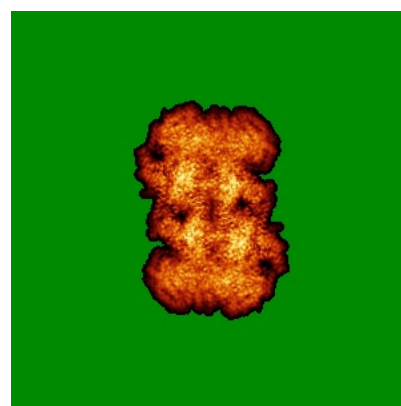
6.4.1 Primary map



X



Y

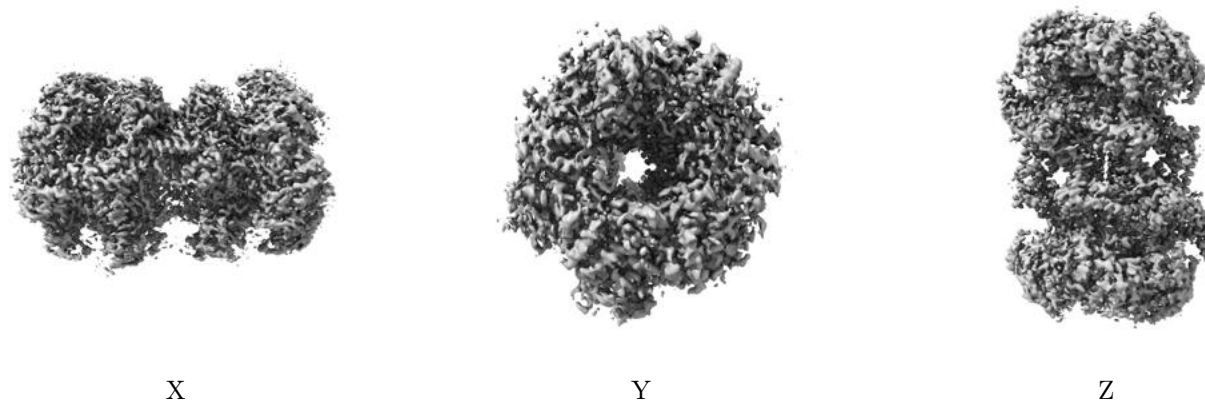


Z

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

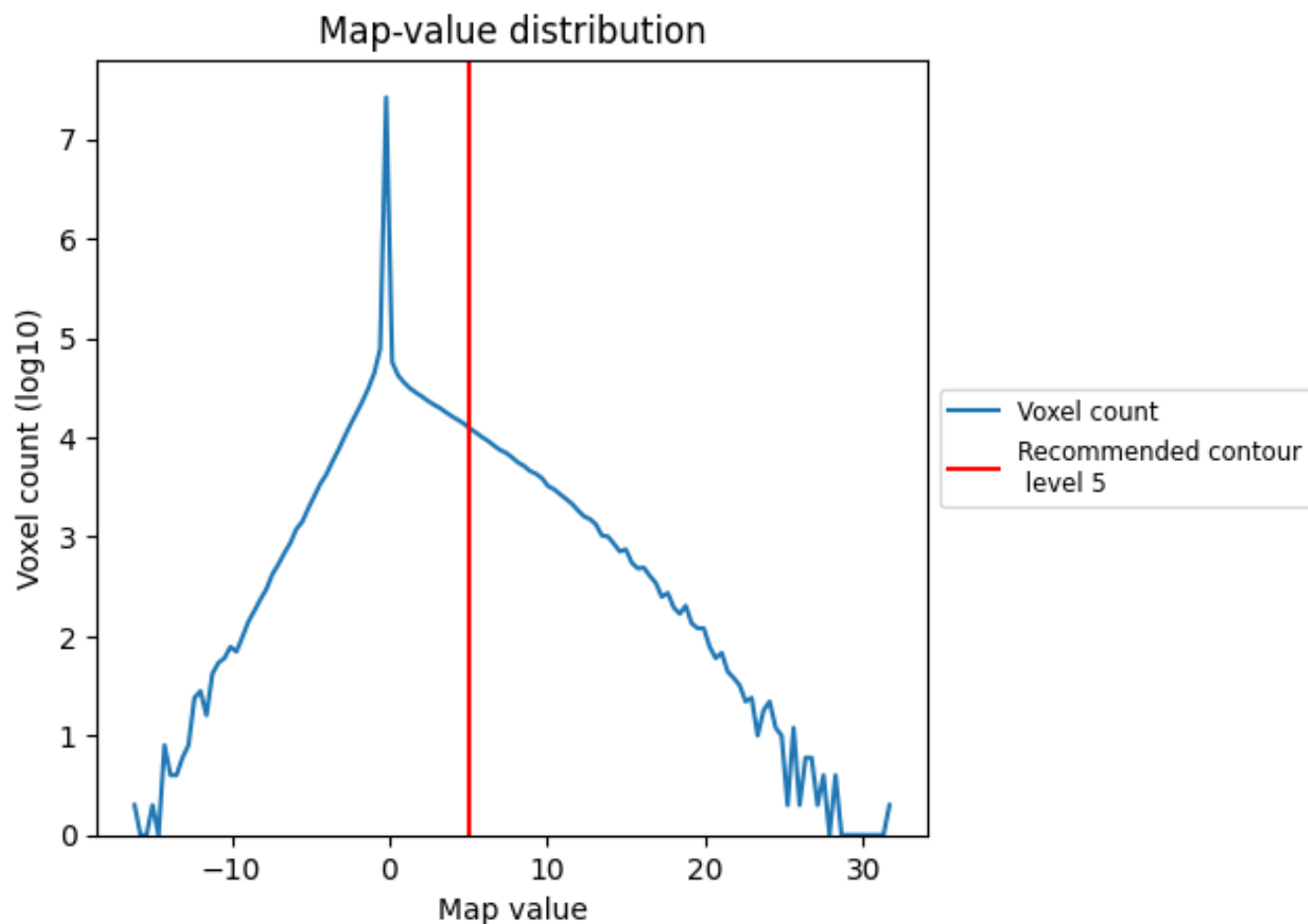
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

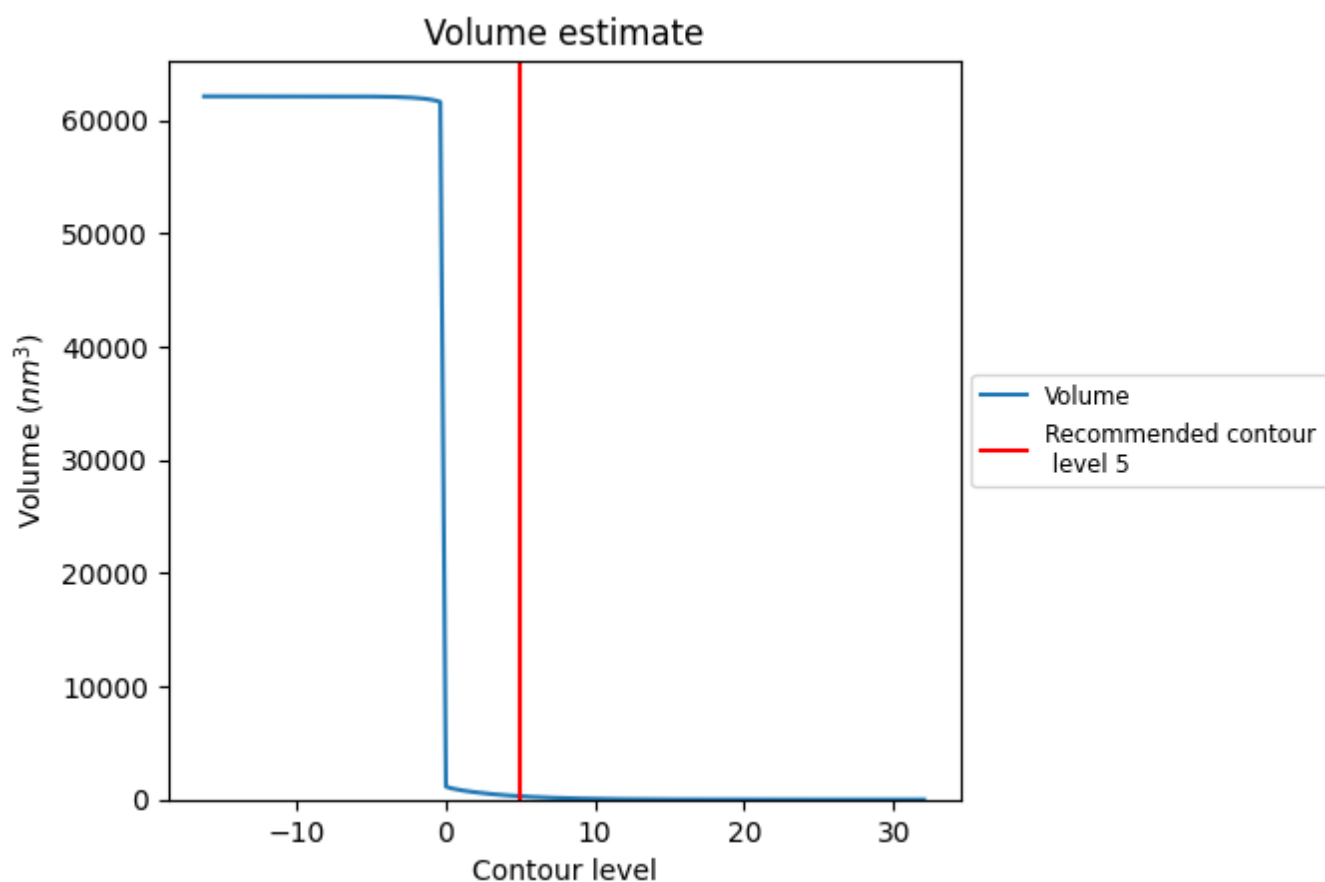
This section contains the results of statistical analysis of the map.

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.

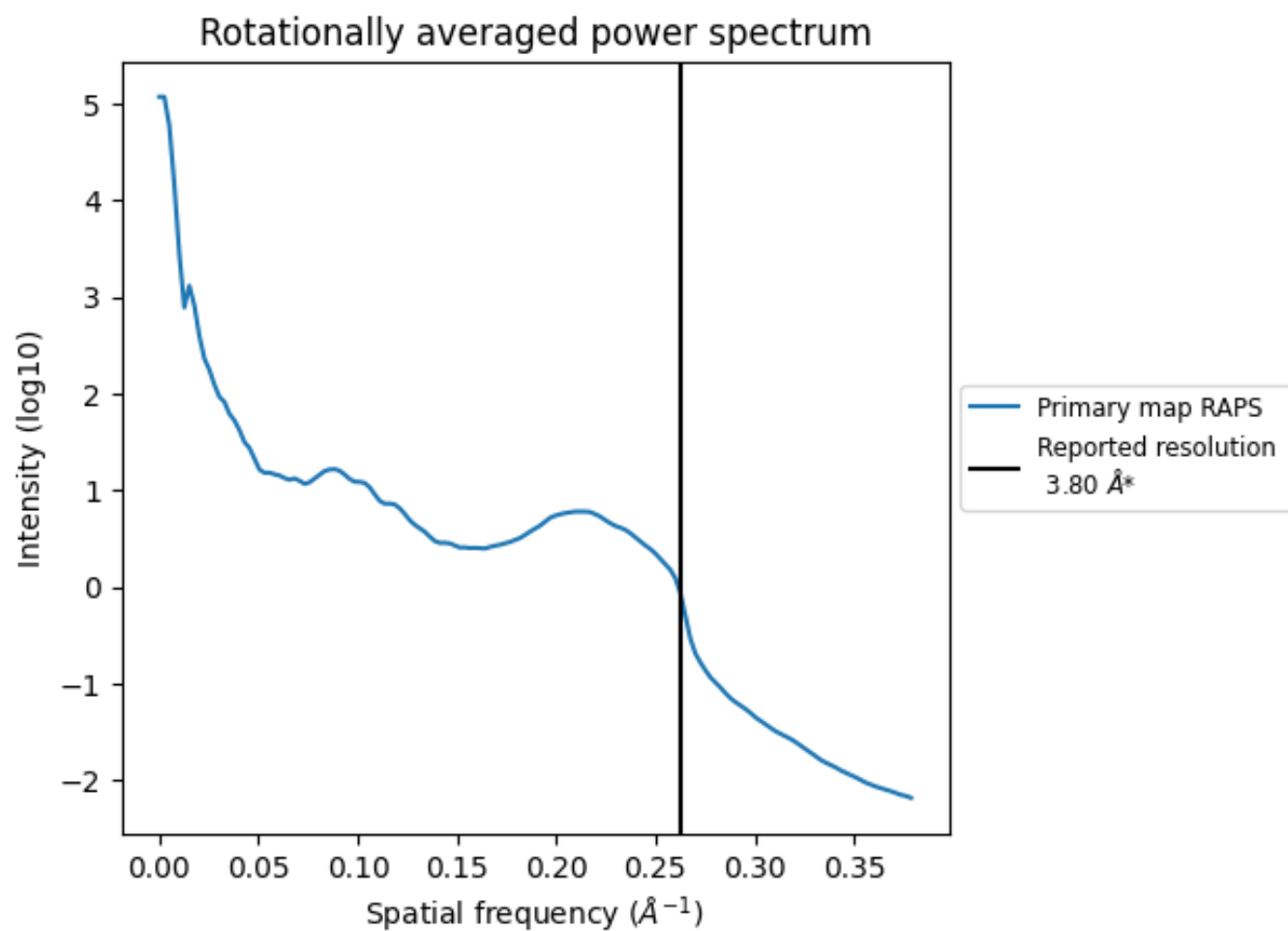
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 292 nm³; this corresponds to an approximate mass of 264 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

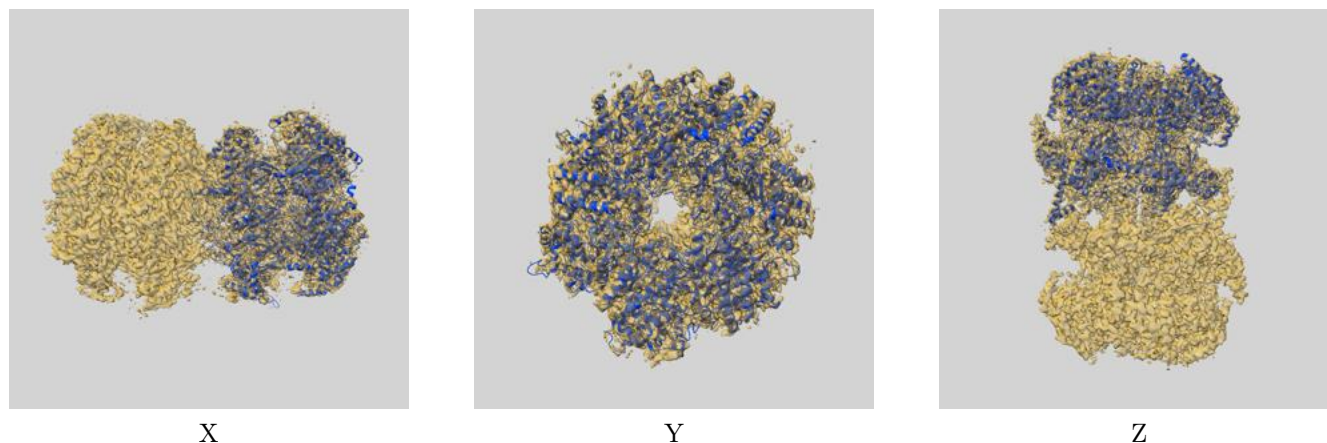
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

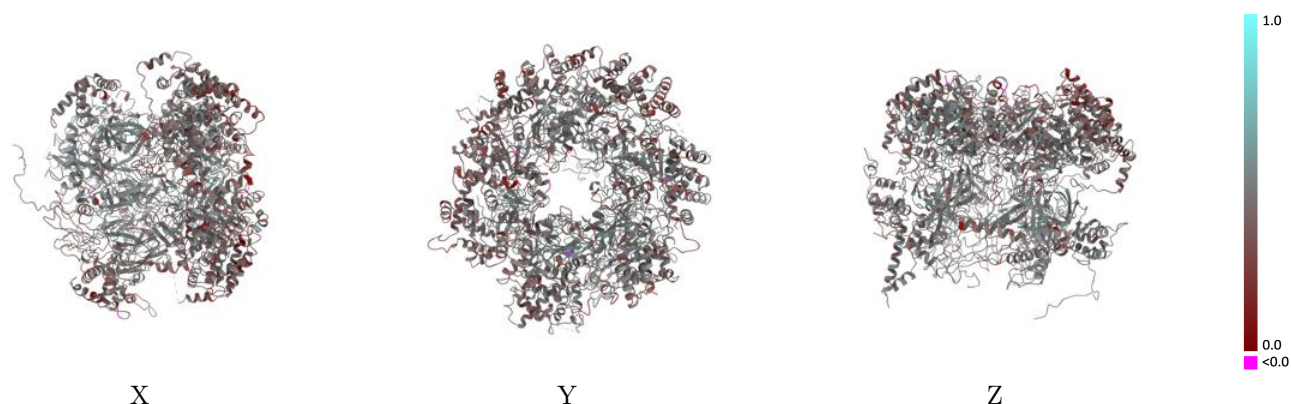
This section contains information regarding the fit between EMDB map EMD-6338 and PDB model 3JA8. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



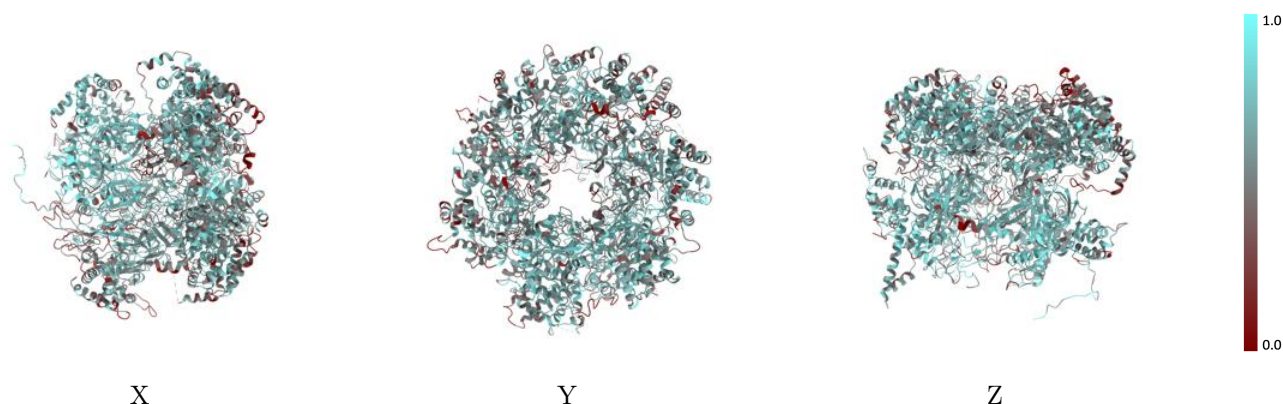
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



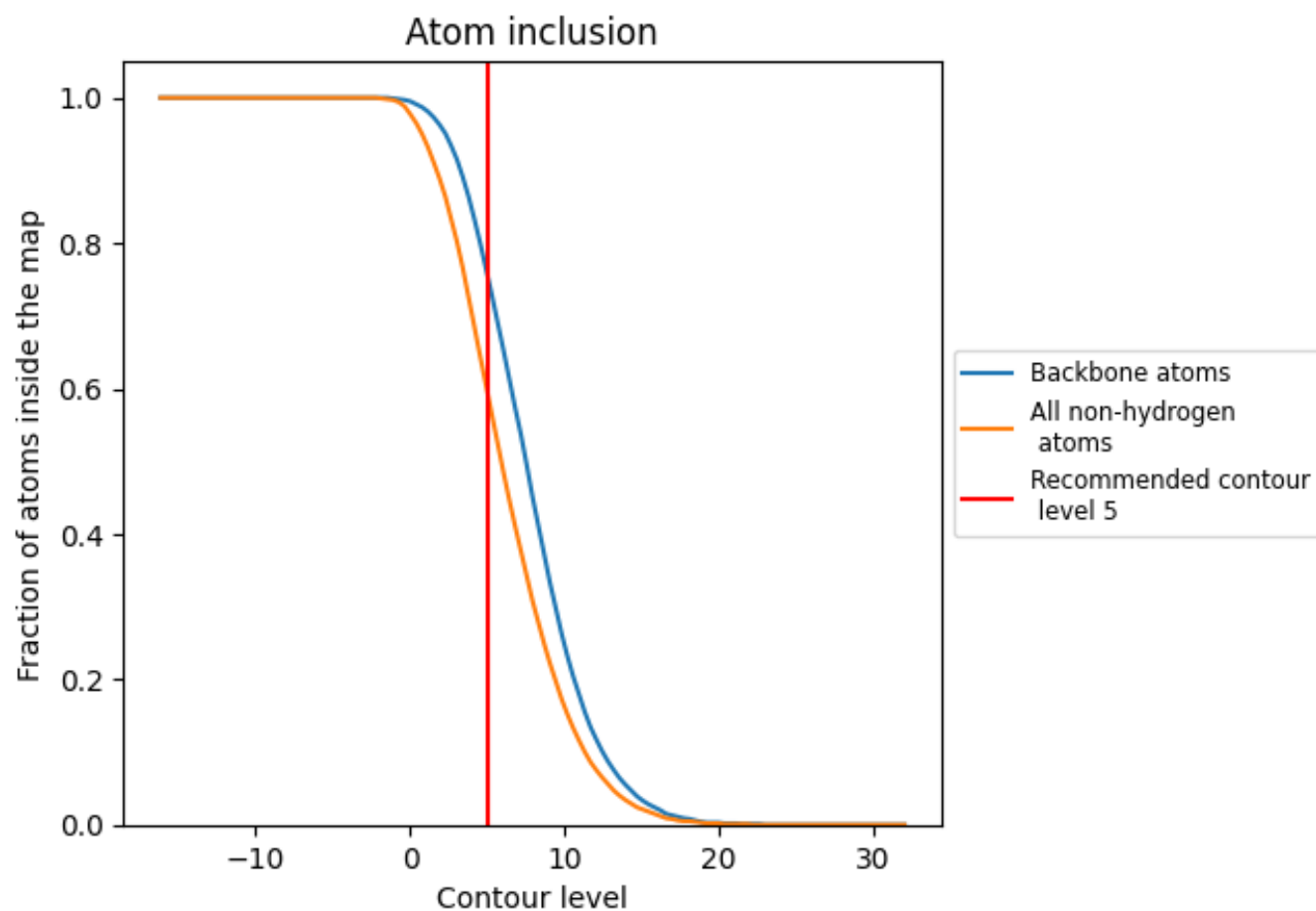
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 60% 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 (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5980	0.4280
2	0.5590	0.4130
3	0.6210	0.4300
4	0.6210	0.4320
5	0.5890	0.4360
6	0.5320	0.4040
7	0.6540	0.4510

1.0

0.0

<0.0