



Full wwPDB EM Validation Report ⓘ

Aug 18, 2026 – 01:54 pm BST

PDB ID : 9TGM / pdb_00009tgm
EMDB ID : EMD-55904
Title : Cryo-EM structure of MCM2-7 DH bound to Sld3-Sld7
Authors : Saleh, A.; Noguchi, Y.; Ivanova, M.E.; Aramayo, R.; Speck, C.
Deposited on : 2025-12-02
Resolution : 3.60 Å(reported)
Based on initial models : 7P30, 3WI3, 3X38, 5BK4, 7PT6

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.dev133
Mogul : 1.8.4, CSD as541be (2020)
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 EMD 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) : 2.50

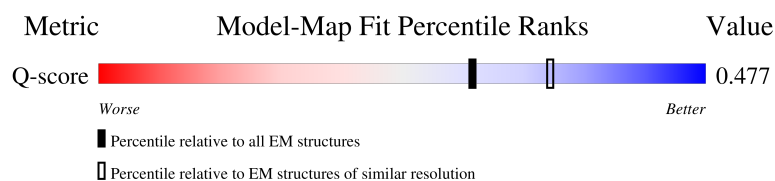
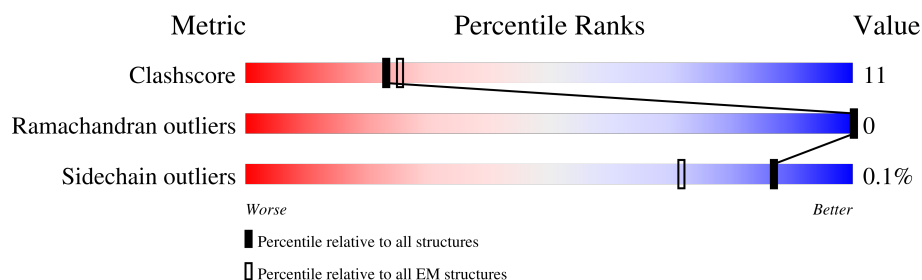
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	2	868	7% 50% 22% 28%
1	B	868	50% 22% 28%
2	3	971	50% 15% 35%
2	C	971	54% 11% 35%

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Mol	Chain	Length	Quality of chain
3	4	933	
3	D	933	
4	5	775	
4	E	775	
5	6	1017	
5	F	1017	
6	7	845	
6	G	845	
7	8	668	
7	X	668	
8	Y	257	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 63086 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 DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	624	Total	C	N	O	S	0	0
			4947	3116	876	936	19		
1	B	624	Total	C	N	O	S	0	0
			4947	3116	876	936	19		

- Molecule 2 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	631	Total	C	N	O	S	0	0
			4947	3130	880	924	13		
2	C	631	Total	C	N	O	S	0	0
			4947	3130	880	924	13		

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	668	Total	C	N	O	S	0	0
			5326	3343	919	1035	29		
3	D	668	Total	C	N	O	S	0	0
			5326	3343	919	1035	29		

- Molecule 4 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	643	Total	C	N	O	S	0	0
			5033	3160	863	986	24		
4	E	643	Total	C	N	O	S	0	0
			5033	3160	863	986	24		

- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	647	Total	C	N	O	S	0	0
			5127	3226	895	980	26		
5	F	647	Total	C	N	O	S	0	0
			5127	3226	895	980	26		

- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	690	Total	C	N	O	S	0	0
			5438	3424	942	1042	30		
6	G	690	Total	C	N	O	S	0	0
			5438	3424	942	1042	30		

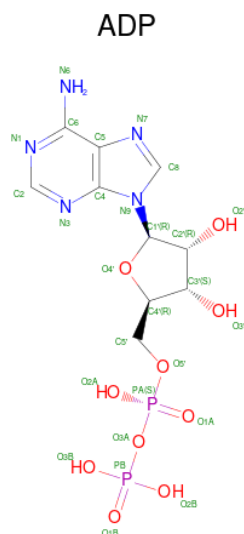
- Molecule 7 is a protein called DNA replication regulator SLD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	29	Total	C	N	O	S	0	0
			236	144	40	51	1		
7	X	29	Total	C	N	O	S	0	0
			236	144	40	51	1		

- Molecule 8 is a protein called Mitochondrial morphogenesis protein SLD7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Y	94	Total	C	N	O	S	0	0
			752	466	137	148	1		

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	2	1	Total 27	C 10	N 5	O 10	P 2	0
9	3	1	Total 27	C 10	N 5	O 10	P 2	0
9	5	1	Total 27	C 10	N 5	O 10	P 2	0
9	7	1	Total 27	C 10	N 5	O 10	P 2	0
9	B	1	Total 27	C 10	N 5	O 10	P 2	0
9	C	1	Total 27	C 10	N 5	O 10	P 2	0
9	E	1	Total 27	C 10	N 5	O 10	P 2	0
9	G	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

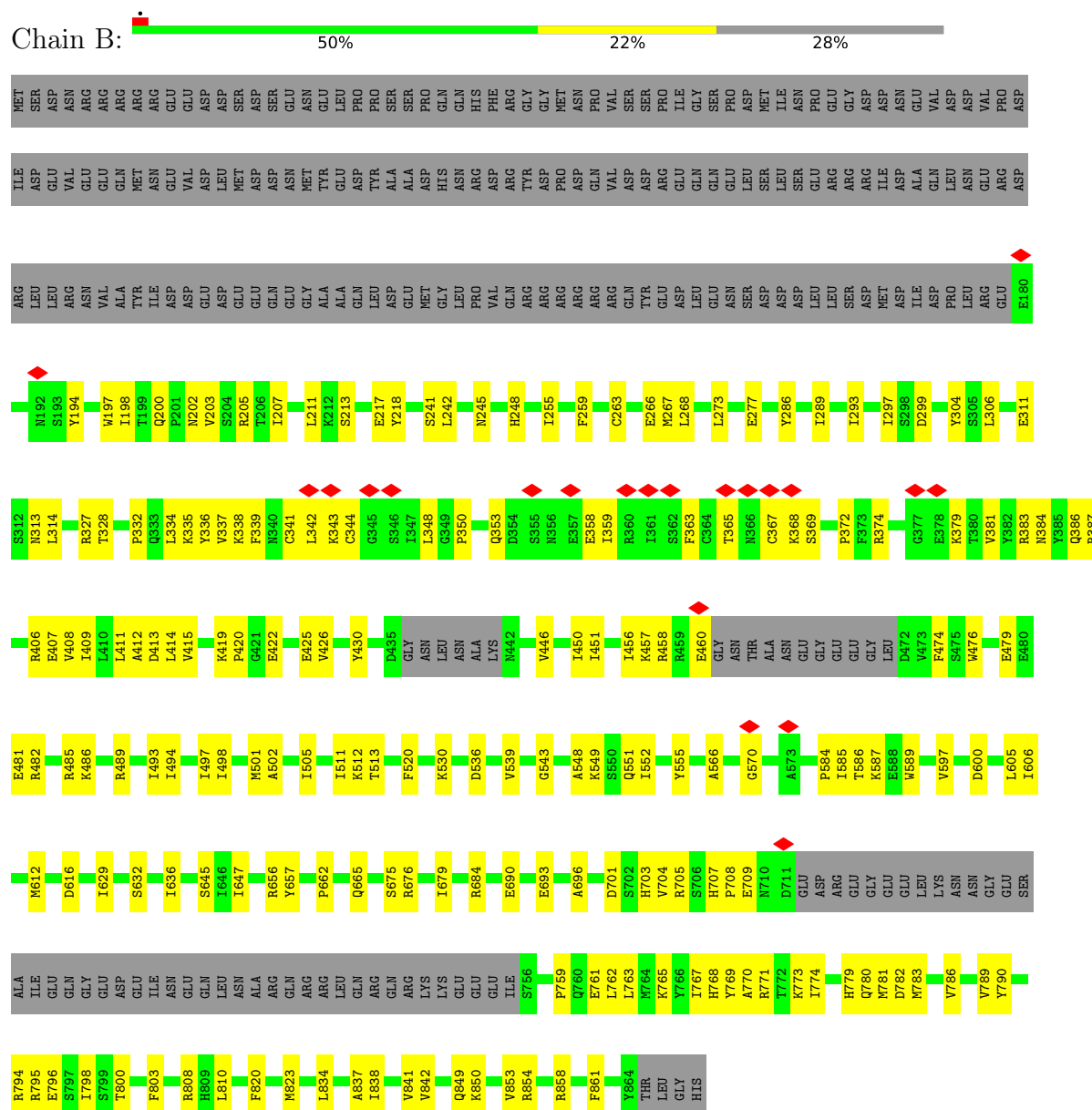
Mol	Chain	Residues	Atoms	AltConf
10	2	1	Total Zn 1 1	0
10	4	1	Total Zn 1 1	0
10	5	1	Total Zn 1 1	0

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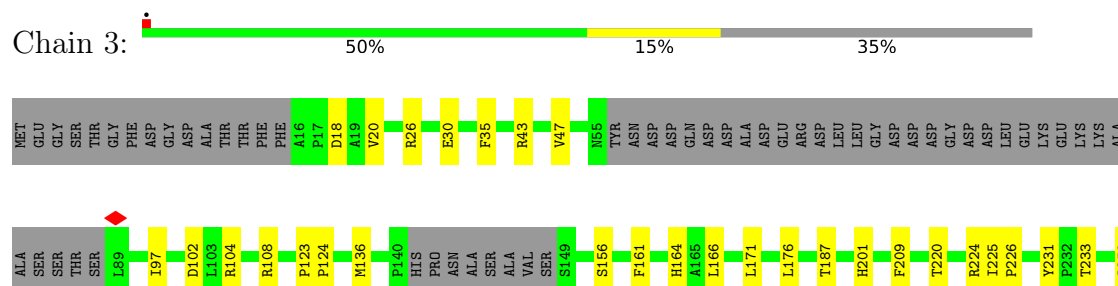
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Mol	Chain	Residues	Atoms		AltConf
10	6	1	Total 1	Zn 1	0
10	7	1	Total 1	Zn 1	0
10	B	1	Total 1	Zn 1	0
10	D	1	Total 1	Zn 1	0
10	E	1	Total 1	Zn 1	0
10	F	1	Total 1	Zn 1	0
10	G	1	Total 1	Zn 1	0

- Molecule 1: DNA replication licensing factor MCM2

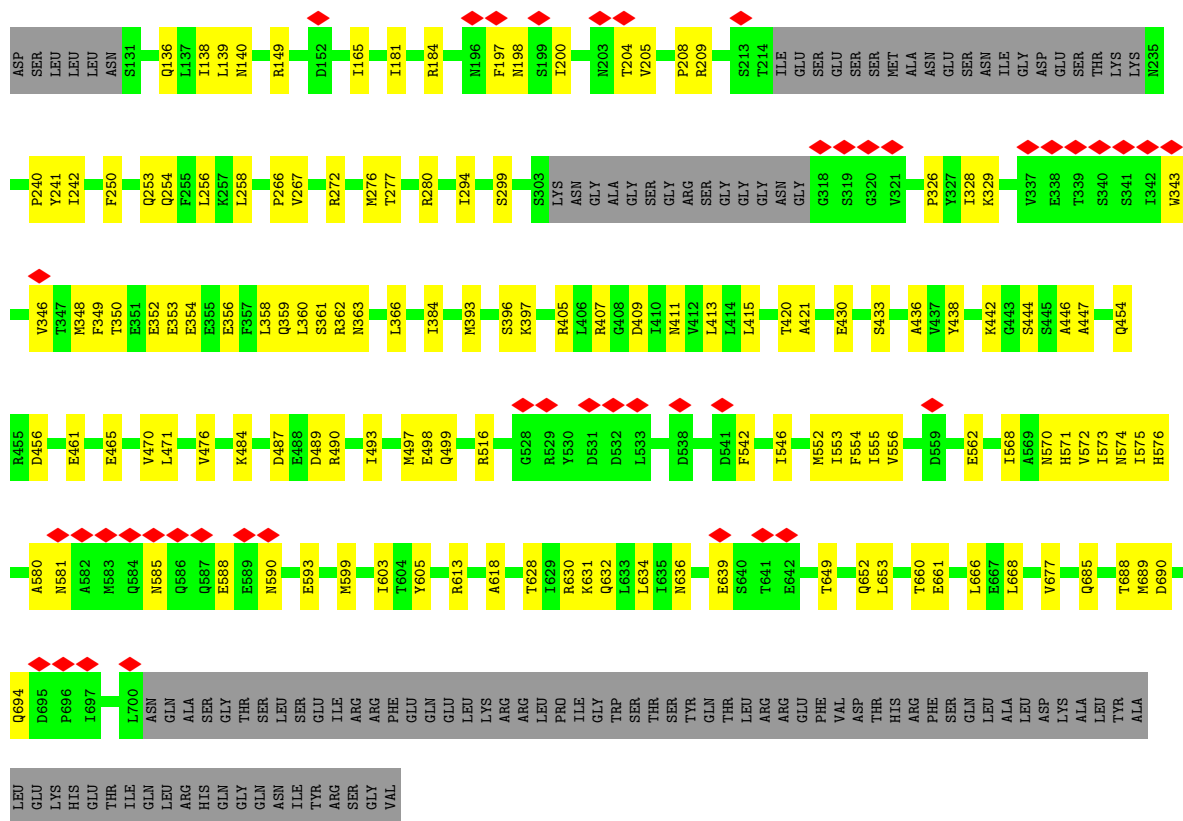


- Molecule 2: DNA replication licensing factor MCM3

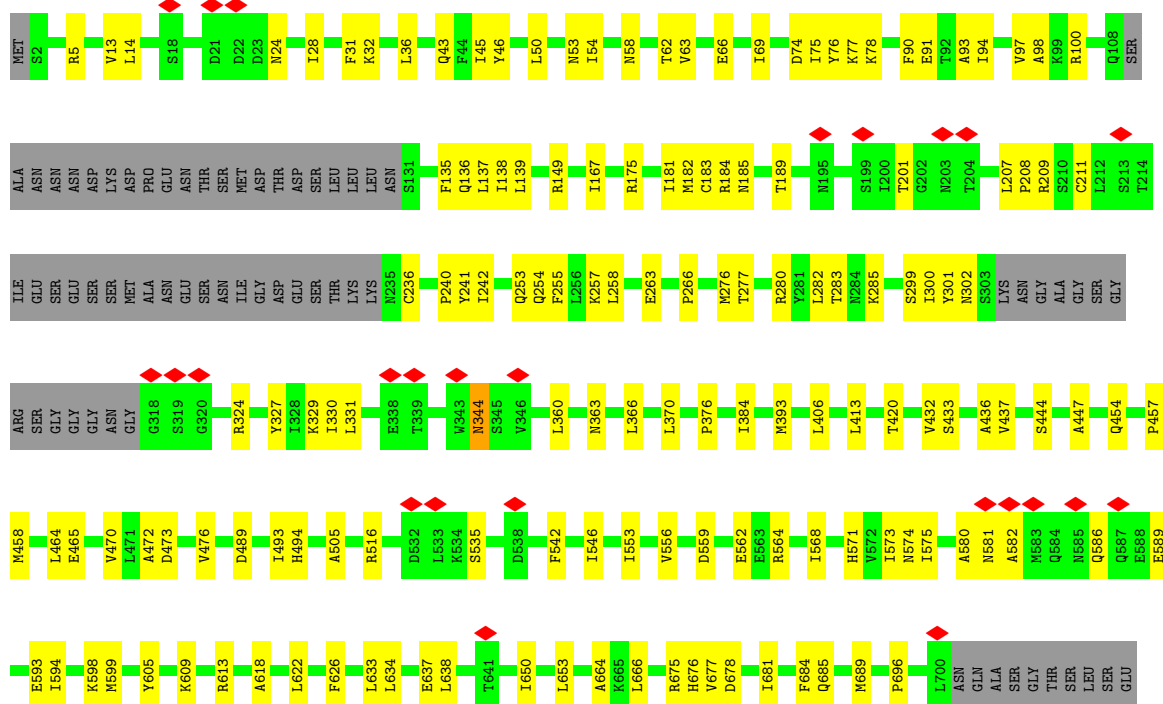


Frequency	Percentage
Daily	50%
Weekly	21%
Monthly	28%





• Molecule 4: Minichromosome maintenance protein 5

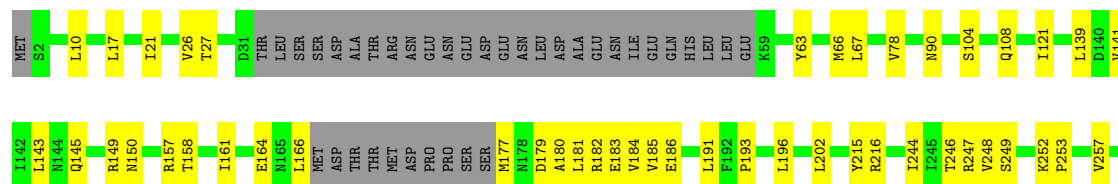
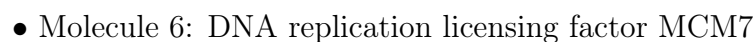


- Molecule 5: DNA replication licensing factor MCM6



PHE	LYS	VAL	THR	ASP	K737	V613	M484	L412	R315	ASN	MET	Q139	PHE
ILE	VAL	VAL	VAL	GLU	R738	R614	M484	P413	R316	GLY	GLY	I140	VAL
LYS	THR	THR	THR	MET	E740	D615	M487	C414	A316	SER	SER	E141	ASN
ARG	ASP	GLU	TYR	ASP	A741	E616	L488	V415	I317	LEU	LEU	K144	ASP
LEU	LEU	GLU	LYS	GLU	I742	E617	L488	V416	V318	PRO	PRO	I145	THR
VAL	VAL	TYR	LYS	PHE	F745	D618	Q489	L421	F326	ARG	ARG	Y146	GLN
LYS	LYS	VAL	VAL	ASP	A748	D619	A490	D422	F327	ASP	ASP	T150	PHE
ARG	ASP	ASP	VAL	ASN	A749	D620	M491	T423	T328	SER	SER	T151	SER
ILE	ILE	GLU	MET	ILE	V493	T622	M492	R424	P330	GLY	GLY	I151	GLN
LEU	LEU	ASN	ASN	SER	V494	G626	V494	G426	T331	SER	SER	L158	LEU
GLN	GLN	MET	MET	GLN	Q495	G627	Q495	ASN	F332	ALA	ALA	R161	GLN
THR	THR	THR	ILE	SER	D496	R629	D496	THR	C333	PRO	PRO	L166	THR
ARG	ARG	ARG	LYS	ALA	R759	L630	M497	THR	P334	GLY	GLY	A167	ASP
THR	THR	ILE	ILE	SER	C637	C637	R499	GLU	R336	ASN	ASN	M168	SER
ARG	ARG	ALA	ALA	GLY	F641	F641	D500	LEU	S337	GLY	GLY	A169	ALA
HIS	HIS	VAL	VAL	ASN	E648	E648	E501	ASN	R341	SER	MET	I170	THR
ASN	ASN	ASP	ASP	ASP	H653	H653	V503	GLY	A342	ALA	ALA	E172	ASN
LEU	LEU	ASP	GLY	ASN	E657	E657	F504	THR	F343	ARG	ARG	R176	GLU
GLU	GLU	ASP	GLY	ASP	Q658	Q658	L505	GLY	W344	SER	SER	F177	GLY
GLU	GLU	THR	GLU	THR	R780	R780	L506	LEU	R350	ILE	ILE	G184	ASN
ASN	ASN	THR	GLY	GLY	Q659	Q659	R509	ARG	R351	GLY	GLY	L185	GLY
ASN	ASN	ALA	ALA	GLY	D763	D763	D511	SER	R352	THR	THR	R187	ARG
ASN	ASN	VAL	VAL	VAL	A670	A670	E512	ARG	D355	THR	THR	I188	SER
LYS	LYS	ILE	ILE	ILE	T671	T671	L516	LEU	W356	SER	SER	K191	PHE
THR	THR	VAL	VAL	SER	L672	L672	K521	D447	V359	PRO	PRO	Y192	LYS
VAL	VAL	ASP	ASP	GLU	PHE	PHE	R521	R448	E363	GLU	GLU	A196	ARG
VAL	VAL	PRO	TRP	PRO	SER	A674	L529	L449	E364	ASN	ASN	L198	ALA
THR	THR	TYR	TYR	ALA	R790	R790	L529	THR	T259	ASP	ASP	S200	LEU
ILE	ILE	LEU	LEU	ALA	G791	G791	G686	GLY	Q264	SER	SER	V100	GLY
HIS	HIS	LEU	LEU	ASP	E792	E792	S632	A453	I265	LEU	LEU	K101	ARG
PRO	PRO	GLN	GLN	ILE	R793	R793	I533	F454	P369	LYS	LYS	K102	LEU
ASN	ASN	LYS	LYS	GLU	R794	R794	P535	T462	T370	ARG	ARG	V103	HIS
CYS	CYS	GLU	GLU	GLU	G686	G686	A534	GLY	G371	SER	SER	D104	PHE
GLU	GLU	ASN	ASN	GLY	A703	A703	A536	SER	S372	GLY	GLY	K110	SER
VAL	VAL	GLN	ASP	GLN	R798	R798	V537	GLY	R373	ASP	ASP	E113	SER
LEU	LEU	SER	LEU	SER	L800	L800	F538	ASN	P374	GLU	GLU	F118	GLN
ASP	ASP	GLY	GLY	ALA	E801	E801	R544	ILE	R277	GLY	GLY	E113	HIS
GLN	GLN	LEU	LEU	ALA	R806	R806	R708	GLY	R280	GLU	GLU	F118	VAL
LEU	LEU	THR	LEU	THR	L806	L806	R709	ALA	T284	GLY	GLY	F118	SER
GLU	GLU	ALA	ALA	ALA	R810	R810	L548	SER	V294	GLN	GLN	F118	THR
PRO	PRO	GLU	GLU	ARG	T810	T810	L549	SER	T295	GLN	GLN	F118	VAL
GLN	GLN	TYR	TYR	PRO	D711	D711	M549	PRO	R296	ASP	ASP	T127	SER
ASP	ASP	GLY	GLY	GLY	R812	R812	N570	ASP	T297	GLU	GLU	D128	SER
SER	SER	THR	THR	THR	F712	F712	C572	ALA	R301	GLN	GLN	T129	THR
SER	SER	GLU	GLU	SER	T725	T725	I571	ASN	G392	GLU	GLU	E131	GLY
ARG	ARG	ARG	ARG	GLU	E726	E726	C572	ASN	S308	ASP	ASP	V132	GLY
LYS	LYS	LEU	LEU	LYS	V838	V838	F584	ASN	E401	ASP	ASP	R137	ASP
VAL	VAL	VAL	ALA	LYS	D732	D732	L585	ASN	V407	GLY	GLY	A138	ASP
ASP	ASP	ASP	ALA	LYS	V733	V733	V589	ARG	T408	ASP	ASP	R137	ASP
					W736	W736	F591	ARG	Q409	ASP	ASP	A138	ASP
							V696	ARG	L410	ASP	ASP		
									Q411				

- Molecule 5: DNA replication licensing factor MCM6

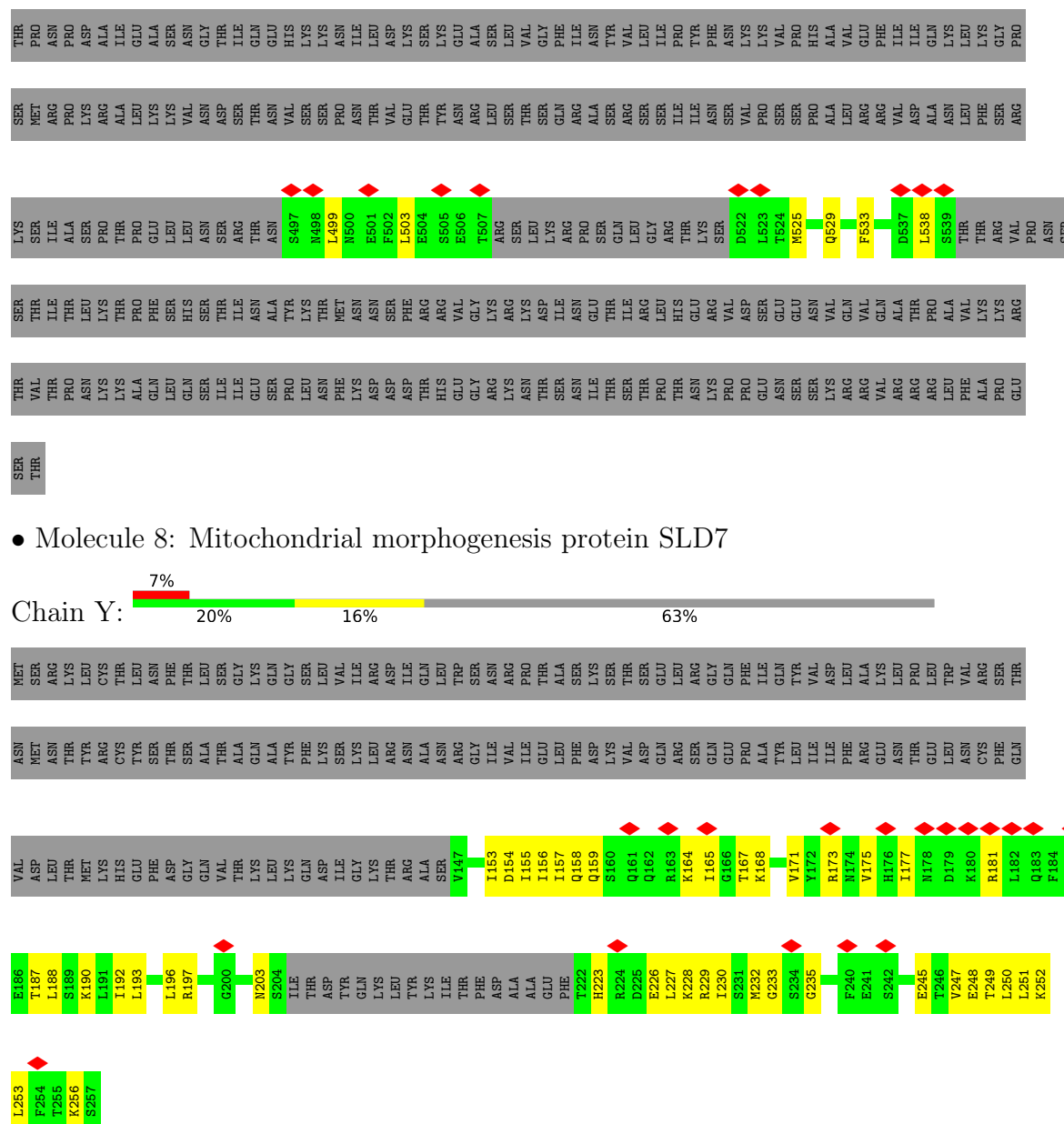


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- Molecule 7: DNA replication regulator SLD3

96%

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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	344362	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.4	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	39.670	Depositor
Minimum map value	-19.985	Depositor
Average map value	0.010	Depositor
Map value standard deviation	1.022	Depositor
Recommended contour level	4	Depositor
Map size ($\text{\AA}$)	542.7184, 542.7184, 542.7184	wwPDB
Map dimensions	376, 376, 376	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.4433999, 1.4433999, 1.4433999	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, ZN

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	0.16	0/5033	0.40	0/6800
1	B	0.16	0/5033	0.40	0/6800
2	3	0.18	0/5033	0.35	0/6823
2	C	0.19	0/5033	0.34	0/6823
3	4	0.16	0/5405	0.37	0/7310
3	D	0.18	0/5405	0.38	0/7310
4	5	0.17	0/5107	0.39	0/6910
4	E	0.18	0/5107	0.40	0/6910
5	6	0.15	0/5207	0.36	0/7026
5	F	0.17	0/5207	0.39	0/7026
6	7	0.18	0/5521	0.37	0/7460
6	G	0.18	0/5521	0.38	0/7460
7	8	0.13	0/237	0.36	0/316
7	X	0.15	0/237	0.48	0/316
8	Y	0.16	0/756	0.48	0/1006
All	All	0.17	0/63842	0.38	0/86296

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
3	4	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	4	420	TYR	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	4947	0	4984	148	0
1	B	4947	0	4984	138	0
2	3	4947	0	5032	106	0
2	C	4947	0	5032	68	0
3	4	5326	0	5385	131	0
3	D	5326	0	5385	150	0
4	5	5033	0	5083	115	0
4	E	5033	0	5083	115	0
5	6	5127	0	5148	125	0
5	F	5127	0	5148	136	0
6	7	5438	0	5507	135	0
6	G	5438	0	5507	123	0
7	8	236	0	221	5	0
7	X	236	0	221	7	0
8	Y	752	0	780	38	0
9	2	27	0	12	0	0
9	3	27	0	12	1	0
9	5	27	0	12	1	0
9	7	27	0	12	1	0
9	B	27	0	12	0	0
9	C	27	0	12	1	0
9	E	27	0	12	0	0
9	G	27	0	12	1	0
10	2	1	0	0	0	0
10	4	1	0	0	0	0
10	5	1	0	0	0	0
10	6	1	0	0	0	0
10	7	1	0	0	0	0
10	B	1	0	0	0	0
10	D	1	0	0	0	0
10	E	1	0	0	0	0
10	F	1	0	0	0	0
10	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	63086	0	63596	1405	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 11.

All (1405) 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)
4:E:211:CYS:HB2	4:E:236:CYS:SG	2.03	0.98
2:3:259:GLN:HE21	2:3:271:PRO:HG2	1.31	0.95
1:2:338:LYS:HD3	1:2:379:LYS:HZ1	1.32	0.92
2:3:585:ARG:HD2	2:3:586:LEU:H	1.37	0.87
5:6:535:PRO:HB2	5:6:742:ILE:HD11	1.57	0.86
1:2:341:CYS:HB3	1:2:344:CYS:SG	2.19	0.83
6:7:67:LEU:HD11	6:7:121:ILE:HG23	1.63	0.81
2:3:577:LEU:HD12	2:3:579:GLY:H	1.45	0.80
6:G:284:CYS:HB3	6:G:289:CYS:SG	2.22	0.79
6:7:90:ASN:HD21	6:7:215:TYR:HE1	1.30	0.79
3:4:692:ILE:HG21	3:4:699:LEU:HD21	1.66	0.78
4:E:31:PHE:HB3	4:E:90:PHE:HD1	1.48	0.77
5:F:767:LYS:HG2	5:F:770:ARG:HH21	1.49	0.77
2:3:502:ILE:HG21	6:7:246:THR:HG23	1.67	0.76
2:3:585:ARG:HD2	2:3:586:LEU:N	2.01	0.76
1:B:770:ALA:HA	1:B:774:ILE:HD13	1.68	0.75
3:D:712:VAL:HG22	6:G:668:ARG:HH21	1.51	0.75
5:6:711:LEU:HD11	5:6:806:LEU:HD21	1.68	0.75
4:E:575:ILE:HA	4:E:581:ASN:HD22	1.50	0.74
3:D:197:PHE:HB2	3:D:254:THR:HG21	1.69	0.74
1:B:505:ILE:HD11	1:B:551:GLN:HB2	1.68	0.74
1:2:265:GLU:HG2	1:2:266:GLU:HG3	1.69	0.74
2:3:416:SER:HB3	4:5:499:GLN:HE22	1.52	0.74
3:4:591:THR:HG22	3:4:593:GLY:H	1.51	0.73
6:7:244:ILE:HG22	6:7:348:ILE:HG12	1.69	0.73
5:6:308:SER:HA	5:6:318:VAL:O	1.89	0.73
1:2:758:ILE:HD12	1:2:759:PRO:HD2	1.70	0.73
1:B:384:ASN:HB2	1:B:412:ALA:HA	1.71	0.73
5:6:296:ARG:HH21	5:6:622:THR:HG21	1.54	0.72
4:E:302:ASN:HB3	4:E:324:ARG:HH21	1.55	0.72
3:D:530:ILE:HD11	3:D:573:SER:HB3	1.69	0.72
6:G:527:ASP:HA	6:G:586:LEU:HD21	1.71	0.72
3:D:591:THR:HG22	3:D:593:GLY:H	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:678:ILE:HD11	3:D:693:ASP:HB2	1.72	0.72
4:E:184:ARG:HH21	4:E:240:PRO:HA	1.54	0.72
1:B:372:PRO:HB2	1:B:374:ARG:HH12	1.54	0.71
6:7:26:VAL:HG23	6:7:27:THR:HG23	1.71	0.71
5:F:742:ILE:HG22	5:F:744:PRO:HD3	1.73	0.71
3:D:704:LEU:HD23	3:D:706:TYR:HE2	1.56	0.70
4:E:675:ARG:HG3	4:E:676:HIS:HD2	1.55	0.70
4:E:344:ASN:C	4:E:344:ASN:HD22	1.99	0.69
5:F:696:ARG:HH12	5:F:703:ALA:HA	1.55	0.69
1:B:520:PHE:HE2	1:B:767:ILE:HG12	1.57	0.69
8:Y:226:GLU:HG2	8:Y:229:ARG:HH21	1.58	0.69
4:E:276:MET:HB3	4:E:330:ILE:HD11	1.75	0.69
3:4:621:LEU:HD13	3:4:648:VAL:HG21	1.75	0.68
4:5:397:LYS:HZ3	4:5:405:ARG:HH21	1.38	0.68
5:F:791:SER:HA	5:F:837:ARG:HH21	1.57	0.68
6:G:26:VAL:HG23	6:G:27:THR:HG23	1.76	0.68
1:B:584:PRO:HA	1:B:587:LYS:HE2	1.76	0.68
8:Y:192:ILE:HA	8:Y:251:LEU:HD11	1.76	0.68
1:2:344:CYS:HB3	1:2:367:CYS:SG	2.33	0.67
6:7:534:ARG:HH21	6:7:586:LEU:HD13	1.58	0.67
5:F:689:TYR:HD2	5:F:716:LEU:HD21	1.60	0.67
6:G:227:VAL:HG22	6:G:317:GLU:HG3	1.76	0.67
1:B:520:PHE:CD1	1:B:823:MET:HG2	2.29	0.67
6:G:182:ARG:HA	6:G:185:VAL:HG22	1.75	0.67
8:Y:188:LEU:O	8:Y:192:ILE:HG12	1.95	0.67
3:4:797:GLN:O	3:4:801:MET:HG3	1.95	0.67
1:2:339:PHE:HB2	1:2:348:LEU:HD22	1.77	0.67
3:4:720:LEU:HD21	6:7:686:PRO:HB3	1.76	0.67
5:6:144:LYS:HA	5:6:196:LEU:HD13	1.74	0.67
3:D:704:LEU:HD11	3:D:804:LEU:HD11	1.74	0.67
4:E:211:CYS:CB	4:E:236:CYS:SG	2.72	0.67
6:G:358:ALA:HB3	6:G:373:GLU:HB2	1.77	0.67
1:B:505:ILE:HD12	1:B:548:ALA:HB1	1.74	0.66
1:B:520:PHE:HD1	1:B:823:MET:HG2	1.58	0.66
4:E:432:VAL:HG21	4:E:599:MET:HE3	1.76	0.66
5:6:275:ARG:HD2	5:6:367:GLU:HG3	1.78	0.66
2:3:123:PRO:HG2	2:3:124:PRO:HD3	1.78	0.66
3:4:548:THR:HB	3:4:760:PRO:HD2	1.76	0.66
2:C:469:VAL:HG12	2:C:511:SER:HB2	1.78	0.66
1:2:624:MET:HB3	1:2:676:ARG:HG2	1.76	0.66
3:4:240:ASN:HD22	3:4:304:ARG:HE	1.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:149:ARG:HH21	4:E:266:PRO:HD2	1.59	0.66
5:F:364:ASN:HB2	5:F:367:GLU:HG3	1.78	0.66
1:2:384:ASN:HB2	1:2:412:ALA:HA	1.78	0.66
5:F:529:LEU:HB3	5:F:548:LEU:HD11	1.77	0.66
1:B:338:LYS:HE2	1:B:379:LYS:HB3	1.77	0.66
1:B:426:VAL:HG22	1:B:456:ILE:HG12	1.76	0.66
1:2:693:GLU:HA	5:6:778:LYS:HZ1	1.60	0.66
1:2:338:LYS:HD3	1:2:379:LYS:NZ	2.07	0.65
2:3:563:GLU:HG3	2:3:567:ARG:HH12	1.61	0.65
3:D:406:VAL:HG13	3:D:410:GLN:HE21	1.60	0.65
3:D:435:VAL:HG12	3:D:466:VAL:HG22	1.77	0.65
3:D:443:PRO:HB2	3:D:453:LEU:HD13	1.76	0.65
2:C:315:ILE:HG22	4:E:175:ARG:HH12	1.60	0.65
2:3:696:PRO:HG3	6:7:573:ARG:HH21	1.60	0.65
4:5:361:SER:HA	4:5:366:LEU:HD11	1.79	0.65
3:D:321:ASP:HA	3:D:324:LYS:HD3	1.78	0.65
3:D:575:SER:HB3	6:G:543:GLN:HE21	1.62	0.65
3:4:333:LEU:HD12	3:4:398:LYS:HG2	1.77	0.65
6:7:182:ARG:HA	6:7:185:VAL:HG22	1.78	0.65
1:2:814:LEU:HD21	4:5:573:ILE:HD12	1.77	0.65
8:Y:165:ILE:HD13	8:Y:168:LYS:HZ1	1.61	0.65
1:2:770:ALA:HA	1:2:774:ILE:HD13	1.77	0.65
5:6:316:ALA:HB3	5:6:334:PRO:HB2	1.79	0.65
5:6:392:GLY:HA3	5:6:630:LEU:HD22	1.79	0.65
1:B:854:ARG:O	1:B:858:ARG:HG2	1.95	0.65
4:E:31:PHE:HB3	4:E:90:PHE:CD1	2.32	0.65
1:B:701:ASP:HB3	1:B:705:ARG:HH12	1.63	0.64
8:Y:192:ILE:HD13	8:Y:247:VAL:HG13	1.78	0.64
3:4:197:PHE:HB2	3:4:254:THR:HG21	1.80	0.64
6:7:527:ASP:HA	6:7:586:LEU:HD21	1.80	0.64
1:B:498:ILE:HD12	1:B:513:THR:HA	1.78	0.64
1:2:336:TYR:HB2	1:2:381:VAL:HB	1.80	0.63
3:D:284:ILE:HG23	3:D:289:LEU:HB2	1.79	0.63
5:F:614:ARG:NH1	5:F:614:ARG:HA	2.13	0.63
6:G:456:VAL:HG12	6:G:596:ILE:HG22	1.81	0.63
4:5:254:GLN:HE21	4:5:256:LEU:HD21	1.63	0.63
2:3:529:PRO:O	2:3:533:ILE:HG13	1.99	0.63
1:2:231:ILE:HG23	1:2:279:THR:HG22	1.81	0.63
1:2:423:GLU:HG3	1:2:459:ARG:HG3	1.80	0.62
4:5:397:LYS:HZ2	4:5:405:ARG:HE	1.47	0.62
3:D:814:LYS:HZ1	3:D:818:GLU:HG2	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:202:ASN:HA	1:2:205:ARG:HE	1.63	0.62
4:5:588:GLU:HG3	4:5:593:GLU:HG2	1.79	0.62
5:F:505:LEU:HA	5:F:508:LEU:HD13	1.81	0.62
3:D:342:MET:HE1	3:D:384:LEU:HD21	1.81	0.62
1:2:353:GLN:HE21	1:2:358:GLU:HA	1.65	0.62
5:6:509:SER:HB3	5:6:512:GLU:HG3	1.81	0.62
1:B:339:PHE:HB2	1:B:348:LEU:HD22	1.81	0.62
2:3:97:ILE:HD13	2:3:156:SER:HB2	1.80	0.62
1:B:311:GLU:HA	1:B:314:LEU:HD23	1.81	0.62
3:D:333:LEU:HD11	3:D:400:GLN:HB2	1.81	0.62
4:E:589:GLU:HA	4:E:593:GLU:HB2	1.81	0.62
6:7:179:ASP:HA	6:7:182:ARG:HG2	1.80	0.62
2:C:184:GLY:HA2	2:C:261:MET:HG3	1.81	0.62
4:E:393:MET:HG3	4:E:666:LEU:HB3	1.80	0.62
5:F:653:HIS:CE1	5:F:704:PRO:HB2	2.34	0.62
5:6:146:TYR:HE2	5:6:488:LEU:HD11	1.64	0.62
2:3:502:ILE:HD13	6:7:246:THR:HG23	1.81	0.61
4:5:599:MET:HE3	4:5:603:ILE:HD11	1.82	0.61
5:6:653:HIS:NE2	5:6:704:PRO:HB2	2.15	0.61
1:B:597:VAL:HG23	1:B:629:ILE:HD12	1.82	0.61
1:B:656:ARG:HH12	5:F:794:ARG:HD3	1.65	0.61
5:F:751:LEU:O	5:F:755:ILE:HG12	2.00	0.61
5:6:260:GLU:HG2	5:6:352:ARG:HH22	1.65	0.61
3:4:802:ILE:O	3:4:806:GLU:HG3	2.01	0.61
3:4:513:ALA:HB2	3:4:813:LEU:HD12	1.83	0.61
1:B:800:THR:HG21	1:B:853:VAL:HG13	1.82	0.61
1:2:676:ARG:HH12	1:2:808:ARG:HH22	1.49	0.61
8:Y:187:THR:HA	8:Y:190:LYS:HG2	1.82	0.61
5:F:661:ILE:HB	5:F:672:LEU:HB2	1.83	0.61
3:D:388:ARG:CZ	5:F:176:ARG:HD3	2.31	0.61
3:D:650:GLU:HB2	3:D:701:ARG:HH22	1.66	0.61
5:F:368:ILE:HD11	5:F:374:PRO:HB3	1.82	0.61
2:3:295:VAL:HB	2:3:325:THR:HB	1.83	0.60
5:6:284:ILE:HA	5:6:401:GLU:HG2	1.82	0.60
6:7:180:ALA:O	6:7:184:VAL:HG23	2.00	0.60
6:7:262:CYS:HB2	6:7:298:LEU:HD23	1.83	0.60
6:7:414:LEU:HD22	6:7:638:MET:HE3	1.83	0.60
3:D:312:LYS:HG3	3:D:316:GLU:OE1	2.02	0.60
2:3:341:MET:HE2	2:3:341:MET:HA	1.83	0.60
3:4:806:GLU:O	3:4:810:LYS:HG3	1.99	0.60
5:6:334:PRO:HD3	5:6:344:TRP:HH2	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:348:LEU:HD23	1:2:361:ILE:HD11	1.83	0.60
6:7:575:ASN:OD1	6:7:577:ARG:HG2	2.01	0.60
5:F:113:GLU:HA	5:F:116:GLU:OE1	2.02	0.60
6:G:538:HIS:CD2	6:G:593:ARG:HH12	2.19	0.60
6:G:638:MET:O	6:G:642:ILE:HG12	2.01	0.60
6:7:657:ASN:O	6:7:661:VAL:HG23	2.01	0.60
3:D:483:GLN:HA	3:D:486:MET:HE2	1.84	0.60
2:3:166:LEU:HD12	2:3:171:LEU:HD23	1.84	0.59
5:6:141:GLU:O	5:6:145:ILE:HG12	2.02	0.59
5:6:529:LEU:HB3	5:6:548:LEU:HD11	1.81	0.59
1:2:481:GLU:O	1:2:485:ARG:HG2	2.01	0.59
4:E:413:LEU:HD23	4:E:553:ILE:HG23	1.83	0.59
2:3:469:VAL:HG12	2:3:511:SER:HB2	1.83	0.59
3:4:336:THR:HG22	3:4:396:VAL:H	1.67	0.59
1:2:327:ARG:HE	1:2:420:PRO:HD3	1.67	0.59
1:2:633:LYS:HE2	4:5:446:ALA:HB1	1.85	0.59
3:4:321:ASP:HA	3:4:324:LYS:HD3	1.85	0.59
5:6:368:ILE:HD11	5:6:374:PRO:HB3	1.83	0.59
1:B:803:PHE:HD2	1:B:849:GLN:HE22	1.50	0.59
2:C:367:LEU:HD23	2:C:656:LEU:HD21	1.83	0.59
5:6:696:ARG:HH12	5:6:703:ALA:HA	1.68	0.59
1:B:383:ARG:HE	1:B:411:LEU:HD12	1.68	0.59
3:D:802:ILE:O	3:D:806:GLU:HG3	2.03	0.59
5:F:540:HIS:HD2	5:F:715:ILE:HD12	1.67	0.59
4:5:136:GLN:HB2	4:5:280:ARG:HE	1.67	0.59
3:D:575:SER:HB3	6:G:543:GLN:NE2	2.17	0.59
3:D:692:ILE:HG21	3:D:699:LEU:HD11	1.83	0.59
6:G:656:VAL:HG12	6:G:710:ILE:HG13	1.83	0.59
7:X:533:PHE:HE2	7:X:538:LEU:HB2	1.68	0.59
1:2:458:ARG:HD3	1:2:460:GLU:H	1.68	0.59
2:3:446:VAL:HG11	2:3:499:LYS:HG2	1.83	0.59
1:B:344:CYS:HB3	1:B:367:CYS:SG	2.42	0.59
6:7:104:SER:O	6:7:108:GLN:HG2	2.03	0.59
1:2:220:ASP:HB2	1:2:226:VAL:HG13	1.84	0.59
3:D:342:MET:HE3	5:F:450:TYR:HE1	1.67	0.59
4:E:91:GLU:HG3	4:E:135:PHE:O	2.02	0.59
3:4:524:ARG:HH21	3:4:740:ASP:H	1.51	0.58
2:3:350:ILE:HG12	2:3:659:TYR:HD1	1.68	0.58
4:5:407:ARG:HG2	4:5:409:ASP:H	1.68	0.58
3:D:186:SER:HB3	3:D:189:GLU:HG3	1.84	0.58
3:D:367:GLU:HB3	5:F:421:LEU:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:338:LYS:HE2	1:2:348:LEU:O	2.03	0.58
6:7:586:LEU:HD12	6:7:590:LEU:HD23	1.85	0.58
2:C:434:GLY:HA2	2:C:478:MET:HE3	1.85	0.58
5:F:145:ILE:HG13	5:F:146:TYR:HD2	1.69	0.58
5:F:326:LYS:HD3	5:F:327:TYR:H	1.68	0.58
6:7:593:ARG:HA	6:7:687:ARG:HH21	1.68	0.58
3:D:594:LYS:HG2	6:G:535:THR:HG21	1.85	0.58
3:D:621:LEU:HD13	3:D:648:VAL:HG21	1.83	0.58
4:E:136:GLN:HG3	4:E:280:ARG:HE	1.68	0.58
1:2:267:MET:HG2	1:2:268:LEU:H	1.67	0.58
6:7:652:MET:HE1	6:7:693:ILE:HG23	1.86	0.58
6:G:150:ASN:HB2	6:G:191:LEU:HD22	1.84	0.58
5:6:629:MET:SD	5:6:672:LEU:HD21	2.43	0.58
5:6:737:LYS:HD2	5:6:740:GLU:HG2	1.84	0.58
6:7:685:THR:HG22	6:7:688:THR:HG23	1.85	0.58
3:D:368:PRO:HG2	3:D:382:MET:HG3	1.86	0.58
3:D:394:LYS:HZ3	5:F:414:GLY:HA3	1.68	0.58
4:E:626:PHE:CD2	4:E:653:LEU:HB2	2.39	0.58
3:4:686:LEU:HD12	3:4:687:PRO:HD2	1.84	0.58
4:5:444:SER:HB2	4:5:447:ALA:HB3	1.86	0.57
2:3:570:ARG:HB3	4:5:613:ARG:HH12	1.68	0.57
3:4:231:ASN:O	3:4:235:GLU:HG3	2.04	0.57
6:7:157:ARG:HG3	6:7:185:VAL:HG12	1.86	0.57
1:B:353:GLN:HE21	1:B:358:GLU:HA	1.68	0.57
3:D:417:LEU:HD21	3:D:435:VAL:HG21	1.85	0.57
4:E:454:GLN:HG3	4:E:465:GLU:OE1	2.03	0.57
1:B:213:SER:O	1:B:217:GLU:HG3	2.04	0.57
5:6:334:PRO:HD3	5:6:344:TRP:CH2	2.38	0.57
1:B:245:ASN:HB3	1:B:248:HIS:CD2	2.40	0.57
5:F:599:SER:HB3	5:F:602:ALA:HB3	1.87	0.57
5:F:732:VAL:HG12	5:F:736:MET:HE3	1.86	0.57
3:4:179:ILE:HG22	3:4:186:SER:HB2	1.87	0.57
6:7:161:ILE:HD12	4:E:100:ARG:HD3	1.86	0.57
5:F:529:LEU:HD11	5:F:754:TYR:CE2	2.40	0.57
6:G:621:MET:HE3	6:G:622:HIS:CE1	2.40	0.57
1:B:690:GLU:HA	1:B:693:GLU:HG2	1.86	0.57
3:4:502:THR:HG23	3:4:505:ASP:H	1.70	0.57
5:6:497:ASN:HB2	5:6:503:VAL:HG21	1.85	0.57
6:7:456:VAL:HG12	6:7:596:ILE:HG22	1.87	0.57
1:B:458:ARG:HG2	1:B:460:GLU:H	1.70	0.57
5:F:157:HIS:HA	5:F:160:MET:HG2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:335:LYS:HE2	1:2:383:ARG:HB3	1.87	0.57
2:3:434:GLY:HA2	2:3:478:MET:HE3	1.87	0.57
3:4:480:THR:HG22	5:6:370:THR:HG21	1.87	0.57
5:F:711:LEU:HD11	5:F:806:LEU:HD21	1.85	0.57
4:5:88:PRO:O	4:5:92:THR:HG23	2.05	0.57
4:5:75:ILE:HA	4:5:78:LYS:HG2	1.87	0.56
6:7:642:ILE:O	6:7:646:LYS:HG3	2.05	0.56
1:B:332:PRO:HG2	4:E:300:ILE:HD12	1.86	0.56
1:B:786:VAL:HA	1:B:789:VAL:HG12	1.87	0.56
2:C:667:VAL:HG12	2:C:669:PRO:HD3	1.87	0.56
1:2:789:VAL:O	1:2:793:LEU:HD12	2.05	0.56
3:4:268:VAL:O	3:4:272:MET:HG3	2.04	0.56
3:4:724:LEU:HD12	6:7:689:LEU:HD22	1.86	0.56
5:F:534:ALA:HB3	5:F:544:LYS:HD3	1.87	0.56
2:3:687:ARG:HD3	6:7:609:ASP:OD2	2.05	0.56
3:4:478:THR:HG21	3:4:756:GLU:HG3	1.86	0.56
5:6:186:ARG:HH12	5:6:260:GLU:HB2	1.71	0.56
6:7:520:ILE:HG13	6:7:562:SER:HB2	1.87	0.56
6:G:593:ARG:HA	6:G:687:ARG:HE	1.70	0.56
3:4:217:ASN:HB3	3:4:220:THR:HG22	1.87	0.56
4:5:442:LYS:HG3	4:5:484:LYS:HE3	1.87	0.56
6:7:442:LYS:HB3	6:7:450:ILE:HB	1.88	0.56
1:B:336:TYR:HB2	1:B:381:VAL:HB	1.87	0.56
1:B:409:ILE:HG13	1:B:450:ILE:HD12	1.87	0.56
2:C:354:SER:HB3	2:C:717:LEU:HD12	1.86	0.56
8:Y:188:LEU:HD12	8:Y:247:VAL:HG22	1.87	0.56
1:2:631:ILE:HD12	4:5:446:ALA:HB3	1.88	0.56
7:8:529:GLN:HA	7:8:532:GLN:HG3	1.87	0.56
1:B:511:ILE:HG21	1:B:552:ILE:HD13	1.87	0.56
3:D:198:LEU:HD11	3:D:276:ILE:HD13	1.88	0.56
6:G:584:ILE:HG13	6:G:586:LEU:HD23	1.86	0.56
6:G:586:LEU:HD12	6:G:590:LEU:HD23	1.88	0.56
1:2:793:LEU:HD21	1:2:842:VAL:HG22	1.86	0.56
6:7:318:LEU:HB2	6:7:321:GLN:HG3	1.88	0.56
2:C:444:ALA:HB3	2:C:497:ILE:HD11	1.87	0.56
5:F:424:ARG:HH12	6:G:294:THR:HG23	1.71	0.56
6:G:78:VAL:HG13	6:G:202:LEU:HD12	1.86	0.56
1:2:327:ARG:HB3	1:2:386:GLN:HE21	1.70	0.56
1:2:576:LEU:HD23	1:2:616:ASP:HB3	1.88	0.56
3:4:452:VAL:HG13	6:7:277:THR:HG23	1.86	0.56
3:D:701:ARG:HE	3:D:796:ARG:CZ	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:397:LYS:NZ	4:5:516:ARG:HD3	2.21	0.56
3:D:391:PHE:HB2	5:F:281:SER:HB2	1.88	0.56
1:2:832:TYR:CZ	1:2:836:ARG:HD2	2.41	0.56
3:D:394:LYS:NZ	5:F:414:GLY:HA3	2.21	0.56
2:3:360:PHE:CE2	2:3:379:LYS:HD3	2.41	0.55
2:3:386:MET:HE1	2:3:663:ALA:HB3	1.88	0.55
5:6:778:LYS:O	5:6:782:LYS:HG3	2.05	0.55
4:E:444:SER:HB2	4:E:447:ALA:HB3	1.87	0.55
1:B:202:ASN:HA	1:B:205:ARG:HG2	1.87	0.55
2:C:166:LEU:HD12	2:C:171:LEU:HD23	1.88	0.55
2:3:535:LEU:HD22	2:3:539:LEU:HD23	1.87	0.55
3:D:443:PRO:HG3	3:D:457:TYR:CZ	2.41	0.55
1:B:197:TRP:CD1	1:B:203:VAL:HG11	2.41	0.55
4:E:13:VAL:HG22	4:E:14:LEU:HG	1.87	0.55
5:F:165:ALA:HB1	7:X:503:LEU:HD12	1.88	0.55
3:4:794:THR:HG22	3:4:796:ARG:H	1.72	0.55
6:7:246:THR:HG22	6:7:247:ARG:HG3	1.88	0.55
6:G:104:SER:O	6:G:108:GLN:HG2	2.05	0.55
3:4:333:LEU:HD11	3:4:400:GLN:HB2	1.88	0.55
4:E:253:GLN:HE21	4:E:277:THR:HG23	1.71	0.55
3:4:609:VAL:HA	3:4:612:LYS:HD3	1.89	0.55
6:7:575:ASN:HD21	6:7:577:ARG:NH1	2.04	0.55
6:7:656:VAL:HG12	6:7:710:ILE:HD13	1.89	0.55
8:Y:193:LEU:O	8:Y:197:ARG:HG2	2.06	0.55
2:C:334:THR:HG22	2:C:336:VAL:H	1.71	0.55
3:D:665:LEU:HD21	5:F:374:PRO:HD3	1.89	0.55
1:2:300:PHE:HB3	1:2:319:ARG:HD3	1.89	0.55
3:4:203:TYR:HE2	3:4:207:LYS:HE3	1.71	0.55
4:5:487:ASP:HA	4:5:490:ARG:HB2	1.88	0.55
5:6:141:GLU:HA	5:6:144:LYS:HG2	1.89	0.55
1:B:820:PHE:HA	1:B:823:MET:HG3	1.88	0.55
2:C:114:ILE:HD13	2:C:121:PHE:HB3	1.88	0.55
3:4:775:VAL:HG11	5:6:725:THR:HG22	1.88	0.55
4:5:489:ASP:O	4:5:493:ILE:HG12	2.07	0.55
6:7:414:LEU:HD11	6:7:641:TYR:HD2	1.72	0.55
3:D:732:LYS:HD3	3:D:733:PRO:HD2	1.88	0.55
1:2:206:THR:HA	1:2:209:ARG:HG2	1.89	0.54
1:2:289:ILE:HG22	1:2:290:HIS:CE1	2.42	0.54
1:2:245:ASN:HB2	1:2:248:HIS:CD2	2.42	0.54
6:G:401:VAL:O	6:G:405:ILE:HG13	2.07	0.54
6:G:452:GLY:H	6:G:694:ARG:HH11	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:574:ASN:HB3	4:5:580:ALA:HB3	1.89	0.54
1:B:769:TYR:HE1	1:B:773:LYS:HE3	1.73	0.54
4:E:678:ASP:HA	4:E:681:ILE:HD12	1.89	0.54
5:F:141:GLU:HG3	8:Y:175:VAL:HG22	1.89	0.54
6:G:580:PRO:HB2	6:G:681:PHE:HD1	1.72	0.54
3:4:718:ARG:HE	3:4:722:LYS:HE3	1.73	0.54
4:5:397:LYS:NZ	4:5:405:ARG:HE	2.05	0.54
6:7:497:VAL:HA	6:7:508:LEU:HA	1.88	0.54
1:B:834:LEU:O	1:B:838:ILE:HG13	2.08	0.54
1:2:327:ARG:HH11	1:2:386:GLN:HE22	1.55	0.54
3:D:180:ILE:HD12	3:D:185:VAL:HG13	1.88	0.54
2:3:444:ALA:HB3	2:3:497:ILE:HD11	1.90	0.54
6:7:574:TYR:CE2	6:7:599:LEU:HD21	2.42	0.54
3:D:217:ASN:HB3	3:D:220:THR:HG22	1.90	0.54
5:F:505:LEU:HD21	8:Y:156:ILE:HD11	1.89	0.54
6:G:141:VAL:O	6:G:145:GLN:HG3	2.08	0.54
6:7:411:TYR:CZ	6:7:430:LYS:HD3	2.42	0.54
3:D:688:VAL:O	3:D:692:ILE:HG12	2.08	0.54
6:G:414:LEU:HD11	6:G:641:TYR:CD2	2.43	0.54
1:2:533:ILE:HG21	4:5:576:HIS:CD2	2.43	0.54
6:7:685:THR:OG1	6:7:686:PRO:HD2	2.08	0.54
2:C:621:VAL:HG23	2:C:622:PHE:HD1	1.72	0.54
2:3:43:ARG:HD2	2:3:136:MET:HE3	1.90	0.54
3:D:704:LEU:HD23	3:D:706:TYR:CE2	2.42	0.54
6:G:544:GLN:OE1	6:G:560:ARG:HA	2.07	0.54
1:2:364:CYS:HB3	1:2:373:PHE:HE2	1.73	0.53
2:3:538:SER:O	2:3:542:ARG:HG2	2.07	0.53
3:4:203:TYR:CE2	3:4:207:LYS:HE3	2.43	0.53
1:B:200:GLN:HE22	1:B:202:ASN:ND2	2.06	0.53
1:2:539:VAL:HG12	1:2:679:ILE:HB	1.89	0.53
2:3:566:LEU:O	2:3:570:ARG:HG3	2.08	0.53
5:6:481:GLU:HA	5:6:484:MET:HE2	1.90	0.53
6:7:638:MET:O	6:7:642:ILE:HG12	2.08	0.53
5:F:309:PHE:HB3	5:F:344:TRP:HE3	1.73	0.53
8:Y:197:ARG:HH12	8:Y:203:ASN:HB3	1.74	0.53
3:4:435:VAL:HG12	3:4:466:VAL:HG22	1.90	0.53
3:D:758:ILE:HG13	3:D:813:LEU:HD23	1.90	0.53
4:5:253:GLN:HE21	4:5:277:THR:HG23	1.73	0.53
5:6:759:ARG:HA	5:6:812:ARG:HH11	1.73	0.53
4:E:74:ASP:HA	4:E:77:LYS:HZ3	1.73	0.53
6:7:139:LEU:O	6:7:143:LEU:HG	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:798:LEU:O	3:D:802:ILE:HD12	2.09	0.53
4:E:574:ASN:HB3	4:E:580:ALA:HB3	1.89	0.53
1:2:486:LYS:HA	1:2:489:ARG:HD2	1.91	0.53
2:3:299:LYS:HG3	2:3:322:LEU:HD13	1.90	0.53
2:C:413:THR:HG21	2:C:549:VAL:HB	1.91	0.53
4:E:90:PHE:CE2	4:E:94:ILE:HD11	2.43	0.53
1:2:790:TYR:CD2	1:2:810:LEU:HB2	2.44	0.53
5:6:673:ASN:H	5:6:673:ASN:HD22	1.56	0.53
6:7:437:VAL:HG21	6:7:702:LEU:HD21	1.90	0.53
1:B:707:HIS:CG	1:B:708:PRO:HD2	2.43	0.53
3:D:442:ILE:HG23	3:D:460:TYR:HE1	1.74	0.53
5:F:755:ILE:O	5:F:759:ARG:HG3	2.09	0.53
1:2:310:ARG:HD2	5:6:355:ASP:OD1	2.08	0.53
4:5:276:MET:HE1	4:5:294:ILE:HG13	1.91	0.53
6:7:542:GLU:HG2	6:7:593:ARG:HD2	1.91	0.53
1:B:267:MET:HG2	1:B:268:LEU:H	1.74	0.53
1:B:494:ILE:O	1:B:498:ILE:HG12	2.09	0.53
4:E:74:ASP:HA	4:E:77:LYS:NZ	2.24	0.53
3:4:271:ILE:HD13	7:8:525:MET:HE2	1.91	0.53
3:D:622:VAL:HG12	5:F:371:GLY:HA2	1.89	0.53
5:F:663:ILE:O	5:F:669:HIS:HA	2.09	0.53
3:4:443:PRO:HG3	3:4:457:TYR:CZ	2.44	0.53
3:D:548:THR:HB	3:D:760:PRO:HD2	1.90	0.53
1:2:852:SER:HA	1:2:855:ARG:HH11	1.74	0.52
5:6:151:ILE:HG23	5:6:265:ILE:HA	1.91	0.52
1:B:707:HIS:ND1	1:B:709:GLU:HG3	2.25	0.52
2:C:701:THR:HG23	2:C:733:LEU:HD21	1.90	0.52
5:F:629:MET:HE3	5:F:672:LEU:HB3	1.91	0.52
1:2:789:VAL:O	1:2:792:ASP:HB2	2.09	0.52
1:B:446:VAL:HB	5:F:301:ARG:HD3	1.91	0.52
6:G:180:ALA:O	6:G:184:VAL:HG23	2.10	0.52
6:G:481:VAL:HG12	6:G:516:ALA:HB2	1.91	0.52
6:G:537:ILE:HA	6:G:540:VAL:HG12	1.92	0.52
1:2:397:VAL:HG21	1:2:403:PRO:HG3	1.91	0.52
6:7:180:ALA:O	6:7:183:GLU:HG2	2.08	0.52
1:B:502:ALA:HB3	1:B:512:LYS:HE2	1.91	0.52
4:E:542:PHE:HB2	4:E:546:ILE:HD12	1.92	0.52
5:6:118:PHE:HD2	5:6:161:ARG:HG2	1.74	0.52
1:B:486:LYS:HA	1:B:489:ARG:HE	1.75	0.52
1:2:493:ILE:O	1:2:497:ILE:HG13	2.09	0.52
4:5:352:GLU:O	4:5:356:GLU:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:537:VAL:HG11	5:6:584:PHE:CZ	2.44	0.52
1:B:494:ILE:HG23	1:B:823:MET:SD	2.49	0.52
4:E:32:LYS:NZ	4:E:100:ARG:HH22	2.08	0.52
5:F:517:LYS:O	5:F:521:LYS:HG3	2.10	0.52
5:F:537:VAL:HG11	5:F:584:PHE:CZ	2.45	0.52
5:F:658:GLN:HB2	5:F:660:THR:HG22	1.92	0.52
2:C:687:ARG:HG3	2:C:687:ARG:HH11	1.74	0.52
8:Y:226:GLU:HA	8:Y:229:ARG:HE	1.74	0.52
2:3:187:THR:HG21	2:3:259:GLN:OE1	2.10	0.52
4:5:198:ASN:C	4:5:198:ASN:HD22	2.12	0.52
4:5:396:SER:H	4:5:661:GLU:CD	2.18	0.52
6:7:249:SER:HB3	6:7:312:GLU:H	1.75	0.52
8:Y:192:ILE:HG23	8:Y:251:LEU:HD21	1.91	0.52
4:5:430:GLU:OE2	4:5:438:TYR:HB2	2.10	0.52
6:7:543:GLN:HB3	6:7:545:THR:HG22	1.92	0.52
1:B:218:TYR:CE2	1:B:248:HIS:HB3	2.45	0.52
2:C:712:HIS:HD2	2:C:728:VAL:HG11	1.75	0.52
5:F:446:ARG:NH1	5:F:446:ARG:HA	2.25	0.52
5:F:759:ARG:HA	5:F:812:ARG:HH11	1.75	0.52
1:2:766:TYR:CE1	1:2:825:LEU:HD11	2.45	0.52
4:5:64:ASN:HB3	4:5:67:HIS:ND1	2.24	0.52
4:5:690:ASP:O	4:5:694:GLN:HG3	2.10	0.52
1:2:338:LYS:CD	1:2:379:LYS:HZ1	2.14	0.51
3:4:801:MET:HE3	3:4:826:VAL:HG12	1.91	0.51
2:C:498:ALA:HA	2:C:503:HIS:HA	1.90	0.51
4:E:437:VAL:HG23	4:E:472:ALA:HB2	1.92	0.51
6:G:725:GLU:HA	6:G:728:TYR:CD1	2.44	0.51
1:2:410:LEU:HD22	1:2:414:LEU:HB3	1.92	0.51
3:4:255:GLU:O	3:4:258:TYR:HB3	2.10	0.51
5:6:613:VAL:HG22	5:6:614:ARG:H	1.74	0.51
2:C:350:ILE:HG21	2:C:662:TYR:CD1	2.46	0.51
4:E:282:LEU:HD13	4:E:330:ILE:HG22	1.92	0.51
4:E:433:SER:HB3	4:E:436:ALA:HB2	1.91	0.51
2:3:359:ILE:HA	2:3:362:ILE:HG22	1.93	0.51
5:6:318:VAL:HG13	5:6:334:PRO:HB3	1.91	0.51
6:7:290:SER:HA	6:7:295:LYS:HZ2	1.74	0.51
1:2:494:ILE:HG23	1:2:823:MET:HE2	1.92	0.51
2:3:26:ARG:O	2:3:30:GLU:HG3	2.10	0.51
2:3:266:PRO:HA	4:5:343:TRP:CH2	2.46	0.51
3:4:417:LEU:HD21	3:4:435:VAL:HG21	1.92	0.51
1:B:536:ASP:HB3	1:B:645:SER:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:88:TYR:O	6:G:92:LYS:HG2	2.11	0.51
2:3:537:ASP:HB2	6:7:572:GLY:HA3	1.91	0.51
3:4:345:ALA:HB2	3:4:365:ILE:HD13	1.92	0.51
4:5:136:GLN:HG3	4:5:280:ARG:HH21	1.76	0.51
5:6:139:GLN:HG2	5:6:151:ILE:HD12	1.92	0.51
6:7:150:ASN:HB2	6:7:191:LEU:HD22	1.93	0.51
1:B:795:ARG:HG3	1:B:796:GLU:N	2.25	0.51
2:C:226:PRO:HD3	4:E:242:ILE:HD13	1.91	0.51
3:D:527:ALA:O	3:D:530:ILE:HG22	2.10	0.51
4:E:258:LEU:HB2	4:E:276:MET:SD	2.50	0.51
1:2:596:LEU:HD11	1:2:620:ILE:HD13	1.93	0.51
2:3:281:ASP:C	2:3:283:VAL:H	2.19	0.51
3:4:349:CYS:HA	3:4:381:SER:O	2.11	0.51
6:7:141:VAL:O	6:7:145:GLN:HG3	2.10	0.51
6:7:589:ALA:HB1	6:7:593:ARG:HH21	1.76	0.51
1:B:520:PHE:CE2	1:B:767:ILE:HG12	2.42	0.51
4:E:664:ALA:HA	4:E:676:HIS:CE1	2.46	0.51
1:2:409:ILE:HG13	1:2:450:ILE:HD12	1.92	0.51
3:4:808:HIS:CD2	3:4:812:LYS:HE2	2.46	0.51
4:5:350:THR:HG23	4:5:353:GLU:H	1.75	0.51
5:6:532:SER:HA	5:6:745:PRO:HD2	1.93	0.51
6:7:514:VAL:HG12	6:7:559:ALA:HB2	1.92	0.51
1:B:273:LEU:O	1:B:277:GLU:HG2	2.10	0.51
1:B:612:MET:HG2	1:B:616:ASP:HB2	1.93	0.51
4:E:183:CYS:SG	4:E:240:PRO:HB2	2.51	0.51
6:G:426:LEU:O	6:G:430:LYS:HG2	2.11	0.51
4:5:33:ASN:O	4:5:37:GLU:HG2	2.11	0.51
2:C:573:PRO:HG2	2:C:576:TYR:HB2	1.93	0.51
3:D:393:ASP:HB2	3:D:421:ASP:HA	1.92	0.51
5:F:770:ARG:O	5:F:774:VAL:HG23	2.10	0.51
3:D:243:LEU:O	3:D:305:PRO:HA	2.11	0.51
3:4:229:GLN:O	3:4:233:MET:HG3	2.10	0.51
3:D:315:ARG:HH21	3:D:413:HIS:HB2	1.75	0.51
3:D:554:LYS:HG2	5:F:739:ASP:OD2	2.11	0.51
4:E:633:LEU:O	4:E:637:GLU:HG2	2.11	0.51
4:5:585:ASN:HA	4:5:588:GLU:HG2	1.93	0.50
5:6:784:ASP:OD1	5:6:794:ARG:HD2	2.11	0.50
1:B:790:TYR:CD2	1:B:810:LEU:HB2	2.46	0.50
3:D:350:ASN:HD21	5:F:331:THR:HG23	1.76	0.50
4:E:489:ASP:O	4:E:493:ILE:HG12	2.11	0.50
5:F:776:LYS:HD2	5:F:828:TYR:CD2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:566:LEU:HD21	4:5:653:LEU:HD11	1.93	0.50
4:5:618:ALA:HB1	4:5:677:VAL:HG21	1.93	0.50
5:6:733:ASP:HB3	5:6:741:ALA:HB1	1.93	0.50
1:B:363:PHE:HE1	1:B:368:LYS:HG3	1.77	0.50
1:B:481:GLU:O	1:B:485:ARG:HG2	2.11	0.50
1:B:530:LYS:HE2	4:E:376:PRO:HD2	1.92	0.50
3:D:232:GLU:HA	3:D:235:GLU:HG2	1.92	0.50
6:G:157:ARG:HG3	6:G:185:VAL:HG12	1.93	0.50
6:G:665:ILE:O	6:G:669:GLN:HG2	2.12	0.50
4:5:433:SER:HB3	4:5:436:ALA:HB2	1.92	0.50
6:7:78:VAL:HG13	6:7:202:LEU:HD12	1.93	0.50
5:F:591:PHE:HZ	5:F:751:LEU:HD22	1.76	0.50
8:Y:187:THR:HA	8:Y:190:LYS:HE3	1.94	0.50
1:2:268:LEU:HD21	1:2:297:ILE:HD11	1.93	0.50
1:2:369:SER:HB3	1:2:373:PHE:HZ	1.76	0.50
4:5:393:MET:HG3	4:5:666:LEU:HB3	1.92	0.50
4:5:397:LYS:HZ3	4:5:516:ARG:HD3	1.75	0.50
1:B:539:VAL:HG22	1:B:647:ILE:HG12	1.92	0.50
3:D:267:GLU:O	3:D:271:ILE:HG12	2.12	0.50
4:E:436:ALA:HA	4:E:476:VAL:O	2.11	0.50
5:F:134:LYS:HE3	5:F:137:ARG:HG3	1.92	0.50
5:F:333:CYS:SG	5:F:334:PRO:HD2	2.51	0.50
2:3:462:MET:HE2	2:3:489:VAL:HG11	1.94	0.50
3:4:726:ASN:HA	3:4:729:LEU:HG	1.93	0.50
6:7:493:LEU:HD23	6:7:512:ALA:HB3	1.93	0.50
3:D:346:PHE:CE1	3:D:355:THR:HB	2.47	0.50
3:D:609:VAL:HG21	6:G:505:GLU:HA	1.93	0.50
4:E:494:HIS:NE2	4:E:546:ILE:HG12	2.27	0.50
4:E:571:HIS:O	4:E:575:ILE:HG12	2.12	0.50
5:F:806:LEU:O	5:F:810:ILE:HG12	2.11	0.50
1:2:707:HIS:CG	1:2:708:PRO:HD2	2.47	0.50
1:2:851:VAL:O	1:2:855:ARG:HG3	2.12	0.50
3:4:579:GLN:HB2	6:7:448:MET:HE1	1.94	0.50
4:E:300:ILE:HG12	4:E:324:ARG:HB2	1.93	0.50
2:3:621:VAL:HG23	2:3:622:PHE:HD1	1.77	0.50
3:4:243:LEU:O	3:4:305:PRO:HA	2.12	0.50
5:6:516:LEU:HD11	5:6:753:ARG:HG2	1.93	0.50
1:B:501:MET:HB3	1:B:555:TYR:CE2	2.47	0.50
3:D:249:LEU:HD21	3:D:258:TYR:CD2	2.46	0.50
3:D:272:MET:O	3:D:276:ILE:HG12	2.12	0.50
3:D:407:PRO:HD2	3:D:410:GLN:NE2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:177:ILE:O	8:Y:181:ARG:HD3	2.10	0.50
1:2:785:LYS:O	1:2:788:ARG:HG2	2.11	0.50
5:6:500:ASP:HB3	5:6:503:VAL:HG22	1.93	0.50
5:F:750:GLN:HA	5:F:753:ARG:HG2	1.92	0.50
6:G:264:GLN:NE2	6:G:265:CYS:HB3	2.27	0.50
1:2:511:ILE:HG21	1:2:552:ILE:HD13	1.93	0.49
2:3:282:LEU:HA	2:3:285:LYS:HD2	1.94	0.49
5:6:141:GLU:O	5:6:144:LYS:HG2	2.12	0.49
3:D:548:THR:HG22	3:D:806:GLU:OE1	2.11	0.49
2:3:413:THR:HG21	2:3:549:VAL:HB	1.95	0.49
3:4:248:LEU:HD11	3:4:272:MET:HE1	1.94	0.49
2:C:100:LEU:HD13	2:C:115:LEU:HD21	1.94	0.49
3:D:352:CYS:SG	3:D:373:ARG:HD3	2.52	0.49
5:F:308:SER:OG	5:F:347:ASN:HB3	2.12	0.49
2:3:276:VAL:HG22	2:3:321:ILE:HB	1.93	0.49
3:4:604:TYR:CE1	3:4:617:GLU:HB3	2.47	0.49
4:5:571:HIS:O	4:5:575:ILE:HG12	2.12	0.49
4:E:473:ASP:OD1	4:E:516:ARG:HG2	2.12	0.49
5:F:651:ALA:O	5:F:654:GLU:HG3	2.12	0.49
1:2:523:VAL:HG12	1:2:818:GLU:OE2	2.12	0.49
3:4:287:ASN:HB3	3:4:289:LEU:HD12	1.95	0.49
3:4:684:PRO:HB3	3:4:845:ILE:HB	1.95	0.49
3:4:688:VAL:O	3:4:692:ILE:HG12	2.11	0.49
6:7:607:ASP:O	6:7:611:LYS:HG2	2.13	0.49
3:4:527:ALA:O	3:4:530:ILE:HG22	2.11	0.49
4:5:350:THR:O	4:5:354:GLU:HG2	2.13	0.49
5:6:158:LEU:HD11	5:6:166:LEU:HG	1.95	0.49
2:C:462:MET:HG2	2:C:470:VAL:HG21	1.94	0.49
4:E:46:TYR:CE2	4:E:63:VAL:HG12	2.48	0.49
4:E:46:TYR:HE2	4:E:63:VAL:HA	1.77	0.49
6:G:179:ASP:HA	6:G:182:ARG:HG2	1.95	0.49
6:G:497:VAL:HA	6:G:508:LEU:HA	1.95	0.49
1:B:782:ASP:HB3	1:B:834:LEU:HD11	1.94	0.49
3:D:244:ASP:HB2	3:D:306:TYR:CZ	2.47	0.49
4:E:93:ALA:O	4:E:97:VAL:HG23	2.12	0.49
5:F:177:PHE:O	5:F:181:LEU:HG	2.12	0.49
1:2:832:TYR:O	1:2:836:ARG:HG3	2.13	0.49
2:3:573:PRO:HG2	2:3:576:TYR:HD2	1.78	0.49
3:4:548:THR:HG22	3:4:806:GLU:OE1	2.12	0.49
3:4:742:LEU:HD13	3:4:746:PHE:CD2	2.47	0.49
6:G:252:LYS:HD2	6:G:503:THR:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:853:VAL:HG22	1:2:857:LEU:HD23	1.95	0.49
1:2:858:ARG:NH1	1:2:859:ARG:HG2	2.27	0.49
3:4:267:GLU:O	3:4:271:ILE:HG12	2.12	0.49
5:6:770:ARG:O	5:6:774:VAL:HG23	2.13	0.49
6:7:414:LEU:HD11	6:7:641:TYR:CD2	2.47	0.49
1:B:338:LYS:HD2	1:B:350:PRO:HG3	1.95	0.49
3:D:457:TYR:HB2	6:G:253:PRO:HG2	1.94	0.49
6:G:437:VAL:HG21	6:G:702:LEU:HD21	1.93	0.49
2:3:341:MET:HE3	2:3:592:VAL:HG23	1.94	0.49
2:3:503:HIS:CE1	6:7:481:VAL:HG21	2.48	0.49
4:5:208:PRO:HG2	4:5:241:TYR:CE2	2.47	0.49
5:6:333:CYS:SG	5:6:334:PRO:HD2	2.53	0.49
6:7:459:MET:HE3	6:7:583:ASN:HD21	1.78	0.49
1:B:837:ALA:O	1:B:841:VAL:HG23	2.13	0.49
3:D:816:VAL:HG13	3:D:818:GLU:OE1	2.13	0.49
2:3:35:PHE:CE2	2:3:102:ASP:HB3	2.48	0.49
1:B:479:GLU:HA	1:B:482:ARG:NH1	2.27	0.49
5:F:545:LYS:O	5:F:549:LEU:HG	2.13	0.49
6:G:66:MET:HE2	6:G:78:VAL:HG23	1.95	0.49
6:G:154:LEU:HD21	6:G:191:LEU:HD11	1.95	0.49
1:2:348:LEU:HD21	1:2:373:PHE:HD2	1.77	0.48
1:2:834:LEU:O	1:2:838:ILE:HG13	2.13	0.48
2:3:345:PHE:O	2:3:349:ASN:ND2	2.43	0.48
2:3:676:ILE:HD11	6:7:621:MET:HE2	1.93	0.48
5:6:373:MET:HE3	5:6:374:PRO:HD2	1.95	0.48
5:6:423:THR:OG1	6:7:295:LYS:HB2	2.13	0.48
5:6:585:LEU:HD23	5:6:637:CYS:HB3	1.95	0.48
5:6:696:ARG:NH1	5:6:703:ALA:HA	2.27	0.48
3:D:274:GLN:HG2	7:X:525:MET:HE2	1.95	0.48
3:D:579:GLN:HE21	6:G:543:GLN:NE2	2.11	0.48
6:G:514:VAL:HG12	6:G:559:ALA:HB2	1.94	0.48
1:2:814:LEU:O	1:2:818:GLU:HG3	2.13	0.48
3:4:530:ILE:HD12	3:4:576:GLN:HB2	1.94	0.48
5:6:806:LEU:O	5:6:810:ILE:HG12	2.13	0.48
6:7:177:MET:HG3	6:7:179:ASP:OD2	2.12	0.48
1:B:363:PHE:CE1	1:B:368:LYS:HG3	2.48	0.48
3:D:513:ALA:HB2	3:D:813:LEU:HD12	1.95	0.48
3:D:725:THR:HG23	6:G:657:ASN:HB3	1.94	0.48
2:3:621:VAL:HG23	2:3:622:PHE:CD1	2.48	0.48
4:5:184:ARG:NH2	4:5:240:PRO:HA	2.28	0.48
5:F:614:ARG:HA	5:F:614:ARG:HH11	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:22:THR:O	6:G:26:VAL:HG22	2.13	0.48
1:2:327:ARG:HG2	1:2:388:VAL:HG23	1.96	0.48
3:4:251:TYR:CE2	3:4:253:GLN:HB2	2.47	0.48
3:4:280:MET:O	3:4:284:ILE:HG23	2.13	0.48
4:5:552:MET:HE2	4:5:554:PHE:HE1	1.77	0.48
6:7:440:VAL:HG21	6:7:649:ARG:HD3	1.96	0.48
2:C:187:THR:HG21	2:C:259:GLN:OE1	2.12	0.48
4:E:50:LEU:O	4:E:54:ILE:HG12	2.13	0.48
2:3:400:ARG:HH11	2:3:400:ARG:HG2	1.79	0.48
3:4:649:MET:HE1	3:4:702:PHE:CZ	2.48	0.48
5:6:737:LYS:HG3	5:6:741:ALA:HB2	1.95	0.48
1:B:430:TYR:HA	1:B:451:ILE:HG22	1.94	0.48
1:B:676:ARG:HH22	1:B:808:ARG:HE	1.60	0.48
1:B:767:ILE:O	1:B:771:ARG:HG3	2.14	0.48
6:G:722:VAL:HA	6:G:725:GLU:CD	2.38	0.48
1:2:488:SER:HB3	1:2:825:LEU:HD13	1.95	0.48
2:3:683:TYR:CD2	2:3:702:LEU:HB2	2.49	0.48
6:7:539:GLU:OE1	6:7:546:ILE:HA	2.13	0.48
1:B:383:ARG:HB2	1:B:412:ALA:HB2	1.94	0.48
1:B:476:TRP:HZ2	1:B:773:LYS:HE2	1.77	0.48
1:B:769:TYR:CE1	1:B:773:LYS:HE3	2.48	0.48
2:C:261:MET:HE3	2:C:264:MET:HE1	1.96	0.48
6:G:711:ASP:HA	6:G:714:GLU:HG2	1.94	0.48
1:2:255:ILE:HG13	1:2:259:PHE:CE2	2.48	0.48
2:3:483:ARG:HG3	2:3:483:ARG:HH11	1.79	0.48
4:5:62:THR:HA	4:5:138:ILE:O	2.13	0.48
6:7:584:ILE:HG13	6:7:586:LEU:HD23	1.95	0.48
6:7:589:ALA:HB1	6:7:593:ARG:NH2	2.29	0.48
3:D:255:GLU:O	3:D:258:TYR:HB3	2.14	0.48
4:5:358:LEU:O	4:5:362:ARG:HG2	2.14	0.48
5:F:614:ARG:NH1	5:F:621:TYR:HA	2.29	0.48
5:F:644:MET:HG2	5:F:648:ASP:HB2	1.95	0.48
2:3:156:SER:HB3	2:3:325:THR:OG1	2.14	0.48
2:3:278:LEU:HD13	2:3:282:LEU:O	2.14	0.48
5:6:379:VAL:HG22	5:6:454:PHE:HB3	1.95	0.48
5:6:626:GLY:H	5:6:629:MET:HB2	1.78	0.48
6:7:193:PRO:HD2	6:7:196:LEU:HD12	1.95	0.48
2:C:209:PHE:CG	6:G:10:LEU:HD12	2.48	0.48
4:E:201:THR:HG22	4:E:255:PHE:HE1	1.79	0.48
5:F:780:LEU:HG	5:F:828:TYR:HE1	1.78	0.48
2:3:209:PHE:CG	6:7:10:LEU:HD12	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:278:LEU:HD23	2:3:323:GLY:HA3	1.95	0.48
3:4:835:ASP:HA	3:4:838:THR:HG22	1.96	0.48
2:C:621:VAL:HG23	2:C:622:PHE:CD1	2.48	0.48
3:D:682:TYR:CD1	3:D:709:LEU:HD21	2.49	0.48
6:7:664:TYR:CD2	6:7:689:LEU:HB2	2.49	0.47
2:C:308:GLN:HB2	4:E:209:ARG:HH22	1.79	0.47
3:D:354:HIS:HB2	3:D:373:ARG:HD2	1.96	0.47
5:F:608:LEU:HD13	5:F:652:ILE:HD11	1.95	0.47
6:G:446:ASP:OD2	6:G:448:MET:HG2	2.13	0.47
2:3:360:PHE:HE2	2:3:379:LYS:HD3	1.78	0.47
4:5:360:LEU:O	4:5:366:LEU:HD21	2.14	0.47
6:7:290:SER:HA	6:7:295:LYS:NZ	2.28	0.47
1:B:763:LEU:O	1:B:767:ILE:HG13	2.14	0.47
2:C:307:ASN:HB3	4:E:207:LEU:HD12	1.95	0.47
2:C:662:TYR:CD2	2:C:666:ARG:HG3	2.49	0.47
4:E:208:PRO:HG2	4:E:241:TYR:CE2	2.49	0.47
6:G:464:VAL:HG12	6:G:600:MET:HE2	1.97	0.47
1:2:696:ALA:O	1:2:700:VAL:HG22	2.13	0.47
2:3:563:GLU:HG3	2:3:567:ARG:NH1	2.26	0.47
6:7:196:LEU:HD21	6:7:257:VAL:HG11	1.96	0.47
2:C:281:ASP:C	2:C:283:VAL:H	2.22	0.47
3:4:395:GLN:HB3	3:4:419:VAL:CG2	2.45	0.47
5:6:529:LEU:HD11	5:6:754:TYR:CE1	2.49	0.47
3:D:340:PRO:HB2	3:D:391:PHE:CD1	2.49	0.47
6:G:177:MET:HG3	6:G:179:ASP:OD1	2.15	0.47
2:3:261:MET:HG2	2:3:263:GLU:OE1	2.13	0.47
4:5:628:THR:O	4:5:632:GLN:HG2	2.15	0.47
2:C:296:GLY:HA3	2:C:322:LEU:O	2.15	0.47
2:C:461:ALA:HB2	4:E:505:ALA:HB1	1.97	0.47
6:G:489:SER:O	6:G:493:LEU:HD12	2.14	0.47
1:2:266:GLU:HA	1:2:269:LYS:HE2	1.97	0.47
3:4:314:MET:SD	3:4:315:ARG:HG3	2.55	0.47
3:4:827:ARG:HH11	3:4:827:ARG:HG2	1.79	0.47
4:5:605:TYR:HE2	4:5:668:LEU:HD11	1.77	0.47
5:6:176:ARG:HH21	5:6:177:PHE:HE2	1.63	0.47
5:6:277:ARG:HD3	5:6:375:ARG:HD2	1.97	0.47
5:6:751:LEU:O	5:6:755:ILE:HG12	2.15	0.47
6:7:497:VAL:O	6:7:498:MET:HE2	2.15	0.47
6:7:529:MET:HE3	6:7:533:ASP:HB3	1.95	0.47
1:B:334:LEU:HD12	1:B:337:VAL:HG22	1.96	0.47
4:E:464:LEU:HD21	4:E:470:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:594:ILE:HG23	4:E:598:LYS:HZ2	1.80	0.47
6:G:688:THR:O	6:G:692:ILE:HG12	2.15	0.47
1:2:690:GLU:HB2	1:2:694:ARG:HH12	1.80	0.47
1:2:855:ARG:O	1:2:858:ARG:HD3	2.15	0.47
4:5:181:ILE:HD12	4:5:241:TYR:CG	2.49	0.47
5:6:538:PHE:CE2	5:6:726:GLU:HG3	2.50	0.47
6:7:252:LYS:HD2	6:7:503:THR:HG21	1.97	0.47
6:7:358:ALA:HB3	6:7:373:GLU:HB2	1.97	0.47
1:B:539:VAL:HG12	1:B:679:ILE:HB	1.96	0.47
3:D:524:ARG:HH21	3:D:740:ASP:H	1.63	0.47
4:E:582:ALA:O	4:E:586:GLN:HG2	2.15	0.47
5:F:142:PHE:HA	5:F:145:ILE:HG12	1.96	0.47
5:F:321:VAL:HG21	5:F:330:PRO:HD3	1.96	0.47
5:F:695:LEU:HD21	5:F:793:TYR:HB3	1.95	0.47
6:G:348:ILE:HG22	6:G:384:HIS:CD2	2.49	0.47
6:G:396:ASP:HA	6:G:399:GLU:HG3	1.97	0.47
6:G:435:LEU:HD21	6:G:520:ILE:HD12	1.97	0.47
8:Y:196:LEU:HD21	8:Y:251:LEU:HD22	1.96	0.47
8:Y:196:LEU:HD13	8:Y:203:ASN:HA	1.97	0.47
1:2:307:ARG:HH12	1:2:396:THR:HG22	1.80	0.47
4:5:13:VAL:HG11	6:G:268:GLU:HG3	1.97	0.47
1:B:703:HIS:CE1	5:F:565:LEU:HD13	2.50	0.47
3:D:515:ARG:NH1	3:D:521:LEU:HD22	2.30	0.47
3:D:835:ASP:HA	3:D:838:THR:HG22	1.97	0.47
5:F:116:GLU:OE2	5:F:184:GLY:HA2	2.14	0.47
5:F:550:GLN:HB2	5:F:571:ILE:HD12	1.95	0.47
8:Y:155:ILE:O	8:Y:158:GLN:HG3	2.15	0.47
1:2:554:LYS:O	1:2:558:LYS:HG3	2.15	0.47
3:4:350:ASN:HD21	5:6:331:THR:HG23	1.80	0.47
4:5:64:ASN:HA	4:5:140:ASN:O	2.15	0.47
4:5:65:MET:SD	4:5:139:LEU:HD13	2.55	0.47
4:5:553:ILE:HB	4:5:688:THR:HG22	1.96	0.47
6:7:537:ILE:HA	6:7:540:VAL:HG12	1.96	0.47
8:Y:173:ARG:HH21	8:Y:233:GLY:HA2	1.79	0.47
1:2:676:ARG:NH1	1:2:808:ARG:HH22	2.11	0.47
4:5:53:ASN:HB3	4:5:58:ASN:O	2.15	0.47
5:6:137:ARG:HH12	5:6:191:LYS:HZ1	1.61	0.47
1:B:704:VAL:HG11	5:F:770:ARG:HH11	1.80	0.47
3:D:826:VAL:O	3:D:830:ARG:HG2	2.15	0.47
5:F:150:THR:HG22	5:F:264:GLN:HB3	1.97	0.47
6:G:142:ILE:O	6:G:146:ARG:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:525:MET:HG3	7:X:529:GLN:HE22	1.80	0.47
4:5:470:VAL:HG23	4:5:471:LEU:HD12	1.97	0.46
1:B:657:TYR:CD2	1:B:684:ARG:HD3	2.50	0.46
6:G:400:ARG:HD2	6:G:637:LYS:HE3	1.96	0.46
8:Y:253:LEU:HA	8:Y:256:LYS:HE2	1.96	0.46
1:2:200:GLN:HE22	1:2:202:ASN:ND2	2.13	0.46
5:6:412:LEU:HG	5:6:413:PRO:HD2	1.96	0.46
2:C:470:VAL:HG12	2:C:472:ILE:HG13	1.97	0.46
3:D:185:VAL:HG23	3:D:190:CYS:SG	2.56	0.46
4:E:24:ASN:O	4:E:28:ILE:HG13	2.16	0.46
5:F:517:LYS:HG2	8:Y:153:ILE:HD11	1.97	0.46
5:F:591:PHE:CZ	5:F:751:LEU:HD22	2.50	0.46
1:2:319:ARG:HG2	1:2:427:THR:OG1	2.15	0.46
3:4:704:LEU:HD23	3:4:706:TYR:HE2	1.79	0.46
4:5:258:LEU:HB2	4:5:276:MET:SD	2.55	0.46
4:5:411:ASN:ND2	4:5:497:MET:HG2	2.31	0.46
5:6:798:ARG:HA	5:6:801:GLU:OE1	2.15	0.46
1:B:662:PRO:HG2	1:B:665:GLN:OE1	2.15	0.46
2:C:171:LEU:HD11	2:C:182:VAL:HG21	1.96	0.46
2:C:295:VAL:HB	2:C:325:THR:HB	1.96	0.46
2:3:296:GLY:HA3	2:3:322:LEU:O	2.15	0.46
4:5:149:ARG:HH21	4:5:266:PRO:HD2	1.80	0.46
6:7:265:CYS:HB3	6:7:289:CYS:HB3	1.97	0.46
1:B:198:ILE:HD11	1:B:259:PHE:CD1	2.50	0.46
3:D:696:PRO:N	3:D:697:PRO:HD2	2.30	0.46
1:2:759:PRO:HB2	1:2:761:GLU:OE1	2.16	0.46
1:2:803:PHE:HB2	1:2:849:GLN:OE1	2.15	0.46
5:6:297:THR:HG23	5:6:359:VAL:HG12	1.97	0.46
6:7:664:TYR:CG	6:7:689:LEU:HD12	2.50	0.46
1:B:374:ARG:NE	1:B:374:ARG:HA	2.30	0.46
1:B:589:TRP:HE1	4:E:458:MET:HE2	1.81	0.46
2:C:344:ASP:O	2:C:348:ARG:HG3	2.16	0.46
3:D:371:CYS:SG	3:D:373:ARG:HG2	2.56	0.46
5:F:170:ILE:HD13	5:F:177:PHE:HD1	1.80	0.46
1:2:332:PRO:HD2	4:5:326:PRO:HG3	1.97	0.46
1:2:419:LYS:O	1:2:422:GLU:HG2	2.15	0.46
2:3:341:MET:HG2	2:3:592:VAL:HG21	1.98	0.46
4:5:204:THR:HG22	4:5:205:VAL:HG23	1.98	0.46
6:7:394:THR:O	6:7:398:GLU:HB2	2.15	0.46
7:8:502:PHE:O	7:8:506:GLU:HG2	2.16	0.46
3:D:244:ASP:HB3	3:D:247:ASN:OD1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:549:ASN:ND2	3:D:559:ARG:HE	2.14	0.46
4:E:254:GLN:HB2	4:E:283:THR:HG22	1.97	0.46
4:E:384:ILE:HD11	4:E:556:VAL:HG11	1.97	0.46
6:G:679:PHE:HB3	6:G:728:TYR:CE2	2.51	0.46
2:3:349:ASN:H	2:3:349:ASN:HD22	1.64	0.46
4:E:605:TYR:O	4:E:609:LYS:HG2	2.15	0.46
4:E:681:ILE:HG23	4:E:685:GLN:HE21	1.81	0.46
5:F:529:LEU:HD11	5:F:754:TYR:HE2	1.79	0.46
8:Y:249:THR:HA	8:Y:252:LYS:HZ3	1.80	0.46
2:3:225:ILE:HD11	4:5:184:ARG:HA	1.96	0.46
2:3:233:THR:HB	4:E:5:ARG:HB2	1.98	0.46
2:3:334:THR:HG22	2:3:336:VAL:H	1.79	0.46
3:4:244:ASP:OD2	3:4:307:ASN:HB3	2.15	0.46
7:8:501:GLU:HG3	7:8:502:PHE:CD1	2.51	0.46
2:C:586:LEU:HD23	2:C:588:LEU:HD22	1.98	0.46
3:D:718:ARG:HE	3:D:722:LYS:HE3	1.81	0.46
5:F:479:GLU:HG2	5:F:482:LEU:H	1.81	0.46
6:G:455:ASN:ND2	6:G:541:MET:HB2	2.31	0.46
6:G:465:ALA:HB2	9:G:1001:ADP:C8	2.51	0.46
2:3:681:LYS:HG3	2:3:682:ASN:N	2.31	0.46
4:5:384:ILE:HD11	4:5:556:VAL:HG11	1.98	0.46
5:6:781:ARG:HH12	5:6:794:ARG:HH21	1.63	0.46
1:B:632:SER:HA	1:B:636:ILE:O	2.16	0.46
5:F:162:GLU:HG3	5:F:165:ALA:HB3	1.98	0.46
3:4:767:LYS:HE3	5:6:733:ASP:OD1	2.16	0.46
4:5:575:ILE:HD13	4:5:581:ASN:HB3	1.98	0.46
2:C:662:TYR:CE2	2:C:666:ARG:HG3	2.51	0.46
3:D:715:LYS:HE3	3:D:715:LYS:HA	1.97	0.46
4:E:53:ASN:HB3	4:E:58:ASN:O	2.14	0.46
1:2:854:ARG:HA	1:2:857:LEU:HB2	1.97	0.45
4:5:636:ASN:O	4:5:639:GLU:HG3	2.15	0.45
1:B:268:LEU:HD21	1:B:297:ILE:HD11	1.98	0.45
4:E:344:ASN:O	4:E:344:ASN:ND2	2.37	0.45
1:2:853:VAL:O	1:2:857:LEU:HD23	2.16	0.45
3:4:249:LEU:HD13	3:4:258:TYR:CD1	2.51	0.45
3:4:401:GLU:HG3	3:4:403:PRO:HD3	1.97	0.45
4:5:9:TYR:CE1	6:G:193:PRO:HG3	2.51	0.45
4:5:546:ILE:HD12	4:5:546:ILE:H	1.81	0.45
5:6:168:MET:O	5:6:172:GLU:HG2	2.17	0.45
6:7:248:VAL:HG13	6:7:313:CYS:SG	2.56	0.45
2:C:202:TYR:HD1	2:C:209:PHE:CE2	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:830:ARG:HG3	3:D:830:ARG:HH11	1.81	0.45
4:E:285:LYS:HB2	4:E:285:LYS:HE2	1.83	0.45
6:G:438:GLY:HA2	6:G:454:ILE:HG12	1.98	0.45
8:Y:164:LYS:O	8:Y:168:LYS:HG2	2.16	0.45
2:3:18:ASP:OD2	2:3:20:VAL:HG22	2.16	0.45
3:4:370:ARG:HG3	3:4:377:ASN:HA	1.98	0.45
4:5:346:VAL:HG22	4:5:348:MET:HB3	1.97	0.45
5:6:277:ARG:CZ	5:6:375:ARG:HH11	2.29	0.45
6:7:90:ASN:ND2	6:7:215:TYR:HE1	2.06	0.45
3:D:342:MET:HE3	5:F:450:TYR:CE1	2.49	0.45
6:G:618:TYR:HD2	6:G:626:PRO:HB3	1.81	0.45
1:2:606:ILE:HG21	1:2:609:PHE:HD1	1.80	0.45
2:3:226:PRO:HD3	4:5:242:ILE:HD13	1.98	0.45
2:3:712:HIS:HD2	2:3:728:VAL:HG11	1.80	0.45
3:4:343:LYS:HE2	3:4:392:ALA:HB3	1.99	0.45
3:4:622:VAL:HG12	5:6:371:GLY:HA2	1.97	0.45
1:B:696:ALA:HB3	5:F:774:VAL:HG13	1.99	0.45
2:C:554:ASN:HB3	2:C:557:ARG:HB2	1.99	0.45
3:4:433:ILE:HG22	3:4:468:LYS:HG2	1.98	0.45
5:6:166:LEU:O	5:6:170:ILE:HG12	2.16	0.45
5:6:532:SER:HB2	5:6:745:PRO:HB2	1.99	0.45
6:7:422:ILE:HG21	6:7:469:LEU:HD21	1.98	0.45
1:B:675:SER:HB2	1:B:808:ARG:NH1	2.31	0.45
4:E:182:MET:HB2	4:E:189:THR:HG22	1.99	0.45
5:F:519:MET:O	5:F:525:ILE:HD12	2.17	0.45
2:3:553:ILE:HG21	4:5:634:LEU:HB2	1.98	0.45
3:4:809:ALA:HB2	3:4:817:VAL:HG23	1.99	0.45
6:7:164:GLU:HG3	6:7:166:LEU:HD21	1.98	0.45
6:7:618:TYR:HD2	6:7:626:PRO:HB3	1.81	0.45
6:7:646:LYS:HA	6:7:701:LYS:NZ	2.32	0.45
2:C:413:THR:HG22	2:C:413:THR:O	2.17	0.45
3:D:371:CYS:HB3	3:D:376:CYS:SG	2.57	0.45
4:E:681:ILE:O	4:E:685:GLN:HG2	2.16	0.45
1:2:549:LYS:HB2	1:2:549:LYS:HE3	1.78	0.45
2:3:667:VAL:HG12	2:3:669:PRO:HD3	1.99	0.45
3:4:354:HIS:HB2	3:4:373:ARG:HH21	1.81	0.45
4:5:299:SER:HB2	4:5:329:LYS:HE3	1.99	0.45
5:6:296:ARG:NH2	5:6:622:THR:HG21	2.26	0.45
5:6:780:LEU:HD13	5:6:828:TYR:CE1	2.52	0.45
5:6:790:ARG:HH11	5:6:838:VAL:HB	1.80	0.45
1:B:335:LYS:HD2	1:B:383:ARG:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:761:GLU:O	1:B:765:LYS:HG3	2.16	0.45
2:C:712:HIS:CD2	2:C:728:VAL:HG11	2.52	0.45
4:E:559:ASP:HB3	4:E:564:ARG:HG2	1.98	0.45
5:F:305:TYR:CD2	5:F:306:LYS:HG2	2.52	0.45
5:F:567:GLY:C	5:F:805:ARG:HD3	2.42	0.45
1:2:324:VAL:HB	1:2:420:PRO:HA	1.98	0.45
1:2:408:VAL:HG22	1:2:451:ILE:HD11	1.99	0.45
4:5:413:LEU:HD23	4:5:553:ILE:HG12	1.99	0.45
5:6:502:GLU:HA	5:6:505:LEU:HG	1.98	0.45
6:7:164:GLU:CD	4:E:36:LEU:HD13	2.42	0.45
1:B:241:SER:HB3	1:B:413:ASP:OD2	2.16	0.45
1:B:304:TYR:HE2	1:B:313:ASN:ND2	2.15	0.45
2:C:97:ILE:HG21	2:C:158:LYS:HD3	1.99	0.45
3:D:199:MET:O	3:D:224:LEU:HD13	2.17	0.45
3:D:604:TYR:CE1	3:D:617:GLU:HB3	2.52	0.45
6:G:657:ASN:O	6:G:661:VAL:HG23	2.16	0.45
1:2:306:LEU:HB2	1:2:392:GLU:HG2	1.98	0.45
1:2:613:ASN:HB2	1:2:616:ASP:OD1	2.17	0.45
2:3:259:GLN:NE2	2:3:271:PRO:HG2	2.14	0.45
5:6:409:GLN:HB3	5:6:449:THR:HB	1.98	0.45
5:6:549:LEU:HD21	5:6:810:ILE:HD13	1.99	0.45
3:D:306:TYR:HB3	3:D:465:HIS:CD2	2.52	0.45
4:E:302:ASN:HB3	4:E:324:ARG:NH2	2.28	0.45
6:G:264:GLN:HE22	6:G:289:CYS:CB	2.30	0.45
1:2:310:ARG:HD3	1:2:310:ARG:HA	1.75	0.45
1:2:336:TYR:HA	1:2:351:PHE:O	2.17	0.45
1:2:763:LEU:HD12	1:2:766:TYR:HD2	1.82	0.45
3:4:198:LEU:HD11	3:4:276:ILE:HD13	1.99	0.45
3:4:767:LYS:HE2	5:6:732:VAL:HB	1.99	0.45
1:B:255:ILE:HG13	1:B:259:PHE:CE2	2.52	0.45
2:C:509:ARG:HE	2:C:509:ARG:HB2	1.61	0.45
6:G:215:TYR:O	6:G:216:ARG:HB2	2.17	0.45
1:2:612:MET:HG3	1:2:616:ASP:HB2	1.99	0.44
3:D:557:ARG:NH1	3:D:668:ARG:HD3	2.33	0.44
6:G:290:SER:HA	6:G:295:LYS:NZ	2.31	0.44
6:G:496:ALA:O	6:G:509:GLU:HG3	2.17	0.44
1:2:267:MET:C	1:2:269:LYS:H	2.25	0.44
1:2:638:THR:HG21	4:5:165:ILE:HD11	1.99	0.44
6:7:465:ALA:HB2	9:7:1001:ADP:C8	2.52	0.44
1:B:600:ASP:OD2	4:E:263:GLU:HG2	2.17	0.44
4:E:564:ARG:HD2	4:E:568:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:488:SER:CB	1:2:825:LEU:HD13	2.47	0.44
1:2:540:LEU:HD23	1:2:680:LEU:HD22	1.98	0.44
1:2:690:GLU:HB2	1:2:694:ARG:NH1	2.32	0.44
3:4:364:VAL:HG11	6:7:299:PHE:CE1	2.52	0.44
3:4:451:ARG:HD3	6:7:280:PRO:HD2	1.98	0.44
4:5:32:LYS:HE3	4:5:100:ARG:HH12	1.81	0.44
6:7:710:ILE:O	6:7:714:GLU:HG2	2.18	0.44
1:B:242:LEU:HB2	1:B:293:ILE:HD11	1.99	0.44
4:E:181:ILE:HD12	4:E:241:TYR:CG	2.52	0.44
3:4:340:PRO:HG3	5:6:452:ILE:HG13	1.99	0.44
3:4:713:ASP:OD1	3:4:716:ASN:HB3	2.18	0.44
3:4:778:ARG:HD2	3:4:793:ALA:HB3	1.98	0.44
5:6:596:VAL:HG21	5:6:630:LEU:HB2	1.99	0.44
1:B:493:ILE:O	1:B:497:ILE:HG13	2.18	0.44
3:D:334:ARG:NH2	3:D:398:LYS:HZ3	2.15	0.44
3:D:596:SER:HB2	3:D:601:LEU:HD21	1.98	0.44
3:D:612:LYS:HD3	3:D:612:LYS:HA	1.84	0.44
3:D:650:GLU:HB2	3:D:701:ARG:NH2	2.32	0.44
5:F:392:GLY:HA3	5:F:630:LEU:HD22	1.99	0.44
5:F:515:GLU:O	5:F:518:GLU:HG3	2.16	0.44
5:F:613:VAL:HG22	5:F:614:ARG:H	1.82	0.44
8:Y:167:THR:O	8:Y:171:VAL:HG23	2.16	0.44
4:5:421:ALA:HB2	9:5:1001:ADP:C8	2.52	0.44
6:7:265:CYS:SG	6:7:267:TYR:HB2	2.58	0.44
6:7:717:LEU:HA	6:7:720:VAL:HG22	1.99	0.44
1:B:343:LYS:HB2	1:B:367:CYS:SG	2.58	0.44
1:B:761:GLU:HG2	1:B:762:LEU:N	2.33	0.44
5:F:484:MET:HE3	5:F:484:MET:HA	1.98	0.44
6:G:139:LEU:O	6:G:143:LEU:HG	2.16	0.44
1:2:181:LEU:HD22	1:2:202:ASN:OD1	2.17	0.44
1:2:269:LYS:HE3	1:2:269:LYS:HB2	1.70	0.44
1:2:458:ARG:NH1	1:2:459:ARG:HB2	2.32	0.44
2:3:572:LEU:HD11	2:3:578:GLU:HA	1.99	0.44
6:7:435:LEU:HD13	6:7:456:VAL:HG22	2.00	0.44
3:D:183:THR:OG1	3:D:185:VAL:HG12	2.18	0.44
3:D:375:ASP:HB2	5:F:100:VAL:HG12	1.99	0.44
3:D:559:ARG:HD2	3:D:559:ARG:HA	1.72	0.44
5:F:737:LYS:HB2	5:F:741:ALA:HB2	1.99	0.44
2:3:43:ARG:HE	2:3:47:VAL:HG13	1.83	0.44
2:3:363:LEU:HD11	2:3:659:TYR:CE2	2.53	0.44
2:3:577:LEU:HG	2:3:580:GLU:OE2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:732:LYS:HD3	3:4:733:PRO:HD2	1.99	0.44
4:5:685:GLN:O	4:5:689:MET:HB2	2.17	0.44
5:6:533:ILE:O	5:6:544:LYS:HD3	2.18	0.44
6:7:596:ILE:HD11	6:7:723:SER:OG	2.17	0.44
2:C:683:TYR:CD2	2:C:702:LEU:HB2	2.53	0.44
4:E:137:LEU:HD12	4:E:137:LEU:HA	1.65	0.44
5:F:309:PHE:HE2	5:F:346:LEU:HD13	1.82	0.44
5:F:632:ASP:HA	5:F:676:THR:HG22	2.00	0.44
6:G:289:CYS:HA	6:G:292:ASN:ND2	2.32	0.44
8:Y:156:ILE:HA	8:Y:159:GLN:HG2	1.99	0.44
1:2:256:LEU:HD23	1:2:256:LEU:HA	1.88	0.44
1:2:458:ARG:HD3	1:2:460:GLU:N	2.33	0.44
1:2:502:ALA:HB3	1:2:512:LYS:HE2	2.00	0.44
1:2:758:ILE:CD1	1:2:759:PRO:HD2	2.44	0.44
2:3:176:LEU:HD12	4:5:250:PHE:HB2	1.99	0.44
3:4:767:LYS:HB2	5:6:736:MET:CE	2.48	0.44
4:5:36:LEU:HD13	6:G:164:GLU:OE1	2.18	0.44
5:6:301:ARG:HD3	5:6:356:TRP:HZ3	1.83	0.44
6:7:440:VAL:HG12	6:7:697:GLN:OE1	2.17	0.44
1:B:850:LYS:O	1:B:854:ARG:HG3	2.18	0.44
3:D:760:PRO:HD3	3:D:810:LYS:HG3	2.00	0.44
5:F:749:GLU:HG2	5:F:750:GLN:N	2.33	0.44
1:2:795:ARG:HB3	4:5:562:GLU:OE2	2.18	0.44
3:4:621:LEU:HD23	3:4:621:LEU:HA	1.79	0.44
6:7:216:ARG:HD3	6:7:216:ARG:HA	1.82	0.44
1:B:794:ARG:O	1:B:798:ILE:HG12	2.18	0.44
2:C:26:ARG:O	2:C:30:GLU:HG3	2.17	0.44
2:C:557:ARG:O	2:C:561:ILE:HG13	2.17	0.44
3:D:708:VAL:O	3:D:709:LEU:HD23	2.17	0.44
4:E:575:ILE:HD13	4:E:581:ASN:HB3	1.99	0.44
4:E:634:LEU:HD23	4:E:638:LEU:HD23	1.98	0.44
5:F:424:ARG:HH12	6:G:294:THR:HA	1.82	0.44
1:2:276:MET:HE2	1:2:276:MET:HB3	1.86	0.43
2:3:220:THR:HG21	2:3:224:ARG:HD2	2.00	0.43
3:4:370:ARG:HG2	3:4:371:CYS:N	2.33	0.43
4:5:628:THR:HA	4:5:631:LYS:HE3	1.99	0.43
1:B:407:GLU:HB2	1:B:450:ILE:HG22	1.99	0.43
3:D:393:ASP:HB3	3:D:424:VAL:HG11	2.00	0.43
5:F:423:THR:OG1	6:G:295:LYS:HB2	2.17	0.43
6:G:227:VAL:HG22	6:G:317:GLU:CG	2.45	0.43
1:2:598:LEU:HD21	4:5:267:VAL:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:756:SER:OG	1:2:757:PRO:HD3	2.18	0.43
2:3:161:PHE:HB3	2:3:164:HIS:HB2	1.99	0.43
2:3:470:VAL:HG12	2:3:472:ILE:HG13	1.99	0.43
2:3:491:GLU:HG2	2:3:700:ARG:HH22	1.83	0.43
3:4:773:ALA:O	3:4:777:MET:HG3	2.18	0.43
1:B:263:CYS:SG	1:B:266:GLU:HB2	2.57	0.43
2:C:332:ARG:HH22	2:C:420:ARG:HD2	1.82	0.43
3:D:181:TRP:HA	7:X:533:PHE:HE1	1.82	0.43
1:2:851:VAL:HA	1:2:854:ARG:HB3	2.01	0.43
2:3:545:LEU:HD21	2:3:708:LEU:HD11	2.01	0.43
3:4:594:LYS:HB3	6:7:535:THR:HG21	2.00	0.43
3:4:611:THR:O	3:4:613:GLN:HG2	2.17	0.43
5:6:572:CYS:HB2	5:6:709:PHE:CE1	2.53	0.43
6:7:398:GLU:O	6:7:402:MET:HG2	2.18	0.43
4:E:594:ILE:HG23	4:E:598:LYS:NZ	2.33	0.43
6:G:207:LEU:HD21	6:G:219:ALA:HB1	2.00	0.43
1:2:267:MET:HG2	1:2:268:LEU:N	2.32	0.43
1:2:325:THR:HB	1:2:389:THR:HB	2.00	0.43
2:3:700:ARG:O	2:3:704:THR:HG23	2.18	0.43
4:5:100:ARG:HD3	6:G:161:ILE:HD12	2.01	0.43
5:6:294:VAL:HG21	5:6:389:ALA:HB1	1.99	0.43
1:B:419:LYS:O	1:B:422:GLU:HG2	2.19	0.43
2:3:687:ARG:HG3	2:3:687:ARG:HH11	1.83	0.43
3:4:559:ARG:HE	3:4:668:ARG:HB3	1.82	0.43
3:4:704:LEU:HD23	3:4:706:TYR:CE2	2.53	0.43
4:5:40:LEU:HD22	4:5:67:HIS:HE2	1.84	0.43
6:7:472:ALA:O	6:7:476:ILE:HD12	2.19	0.43
1:B:327:ARG:HG3	1:B:420:PRO:HG3	2.01	0.43
1:B:585:ILE:HG13	1:B:586:THR:HG23	2.01	0.43
3:D:618:SER:HA	5:F:373:MET:HE3	1.99	0.43
3:D:712:VAL:HG11	6:G:672:LYS:HB2	2.01	0.43
4:E:167:ILE:HD11	4:E:257:LYS:HG2	2.01	0.43
6:G:289:CYS:HA	6:G:292:ASN:HD22	1.83	0.43
8:Y:197:ARG:NH1	8:Y:203:ASN:HB3	2.34	0.43
8:Y:248:GLU:C	8:Y:252:LYS:HZ3	2.27	0.43
1:2:300:PHE:HB3	1:2:319:ARG:CD	2.48	0.43
1:2:566:ALA:O	1:2:606:ILE:HA	2.18	0.43
2:3:483:ARG:HG3	2:3:483:ARG:NH1	2.34	0.43
2:3:538:SER:HB3	2:3:542:ARG:NH2	2.33	0.43
3:4:326:ILE:HD13	3:4:439:PHE:HB2	2.00	0.43
5:6:301:ARG:HD3	5:6:356:TRP:CZ3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:63:TYR:O	6:7:67:LEU:HD23	2.19	0.43
6:7:367:LYS:HE3	6:7:369:GLY:O	2.18	0.43
6:7:493:LEU:HB3	6:7:513:LEU:HD23	1.99	0.43
1:B:425:GLU:OE2	1:B:457:LYS:HG3	2.19	0.43
2:C:569:HIS:CE1	4:E:406:LEU:HD23	2.53	0.43
4:E:363:ASN:O	4:E:366:LEU:HG	2.19	0.43
8:Y:181:ARG:HH12	8:Y:230:ILE:HG21	1.83	0.43
8:Y:245:GLU:O	8:Y:249:THR:HG23	2.19	0.43
2:3:382:LEU:O	2:3:386:MET:HG2	2.19	0.43
2:3:712:HIS:CD2	2:3:728:VAL:HG11	2.54	0.43
3:4:519:TYR:CZ	3:4:538:LYS:HD3	2.54	0.43
6:7:402:MET:HA	6:7:405:ILE:HG22	2.01	0.43
1:B:341:CYS:HB3	1:B:344:CYS:SG	2.57	0.43
1:B:566:ALA:O	1:B:606:ILE:HA	2.18	0.43
1:B:779:HIS:HB3	1:B:781:MET:SD	2.58	0.43
2:C:423:LEU:HD13	2:C:431:ALA:HB2	1.99	0.43
3:D:311:CYS:O	3:D:312:LYS:HG2	2.19	0.43
5:F:335:ASN:HB2	5:F:338:CYS:SG	2.58	0.43
5:F:552:LEU:HD23	5:F:755:ILE:HG23	2.00	0.43
8:Y:192:ILE:HD12	8:Y:251:LEU:HD21	2.01	0.43
1:2:307:ARG:HD2	5:6:493:VAL:HG21	2.01	0.43
1:2:805:ILE:HD11	1:2:845:PHE:CE2	2.54	0.43
3:4:394:LYS:NZ	5:6:414:GLY:HA3	2.34	0.43
3:4:482:GLU:HA	3:4:485:LEU:HD12	2.01	0.43
1:B:207:ILE:O	1:B:211:LEU:HG	2.18	0.43
3:D:258:TYR:CZ	3:D:262:LEU:HD11	2.54	0.43
5:F:304:LEU:HD21	5:F:307:ALA:HB2	1.99	0.43
6:G:440:VAL:HG12	6:G:697:GLN:OE1	2.19	0.43
2:3:201:HIS:HE1	2:3:231:TYR:CE2	2.37	0.43
3:4:380:ASN:ND2	1:B:365:THR:HG21	2.34	0.43
3:4:599:VAL:HG12	3:4:604:TYR:HB3	2.00	0.43
4:5:272:ARG:HG2	4:5:272:ARG:HH11	1.84	0.43
4:5:415:LEU:O	4:5:555:ILE:HA	2.18	0.43
5:6:368:ILE:HG22	5:6:369:PRO:O	2.19	0.43
4:E:650:ILE:HD12	4:E:650:ILE:H	1.83	0.43
5:F:118:PHE:HA	5:F:161:ARG:NH1	2.34	0.43
5:F:191:LYS:HD2	5:F:191:LYS:C	2.44	0.43
1:2:235:GLY:HA3	1:2:283:TYR:CE2	2.54	0.43
1:2:494:ILE:O	1:2:498:ILE:HG13	2.19	0.43
1:2:557:GLU:OE1	1:2:565:PHE:HB2	2.19	0.43
2:3:393:LEU:HD12	2:3:397:SER:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:687:PRO:HG2	3:4:690:GLU:HG2	2.01	0.43
4:5:685:GLN:HA	4:5:689:MET:HG3	2.01	0.43
5:6:412:LEU:HB3	5:6:416:LYS:NZ	2.34	0.43
5:6:669:HIS:CE1	5:6:671:THR:HG23	2.54	0.43
2:C:18:ASP:OD2	2:C:20:VAL:HG22	2.19	0.43
2:C:442:LEU:HD13	2:C:486:ILE:HD11	2.00	0.43
4:E:62:THR:HA	4:E:138:ILE:O	2.19	0.43
4:E:360:LEU:O	4:E:366:LEU:HD21	2.18	0.43
5:F:629:MET:HE2	5:F:629:MET:HA	2.01	0.43
8:Y:181:ARG:HH12	8:Y:230:ILE:CG2	2.32	0.43
1:2:778:LEU:HD12	1:2:779:HIS:H	1.84	0.42
2:3:355:LYS:HA	2:3:355:LYS:HD3	1.89	0.42
2:3:413:THR:O	2:3:413:THR:HG22	2.18	0.42
2:3:456:ARG:HG2	2:3:456:ARG:HH11	1.84	0.42
2:3:570:ARG:HB3	4:5:613:ARG:NH1	2.32	0.42
3:4:178:ARG:HG3	3:4:178:ARG:HH11	1.84	0.42
3:4:344:VAL:HG12	3:4:390:SER:OG	2.18	0.42
3:4:483:GLN:HA	3:4:486:MET:HE2	2.00	0.42
3:4:800:SER:O	3:4:804:LEU:HD23	2.18	0.42
4:5:575:ILE:HA	4:5:581:ASN:ND2	2.34	0.42
5:6:184:GLY:O	5:6:188:VAL:HG23	2.19	0.42
5:6:658:GLN:HB2	5:6:660:THR:HG22	2.01	0.42
6:7:268:GLU:HG3	4:E:13:VAL:HG11	2.00	0.42
2:C:475:PHE:HB2	2:C:514:ALA:HB1	2.01	0.42
3:D:343:LYS:HA	3:D:343:LYS:HD2	1.80	0.42
4:E:562:GLU:OE2	4:E:562:GLU:HA	2.19	0.42
1:2:325:THR:HG23	5:6:669:HIS:ND1	2.34	0.42
3:4:388:ARG:HA	3:4:388:ARG:HD2	1.88	0.42
3:D:340:PRO:HB3	5:F:281:SER:HB3	2.00	0.42
3:D:452:VAL:CG1	6:G:277:THR:HG23	2.49	0.42
3:D:456:LEU:HD12	3:D:456:LEU:HA	1.85	0.42
3:D:526:ILE:HD11	3:D:541:LEU:HD13	2.01	0.42
3:D:682:TYR:CE1	3:D:707:LEU:HD21	2.54	0.42
4:E:69:ILE:HB	4:E:76:TYR:CD1	2.54	0.42
4:E:684:PHE:O	4:E:689:MET:HG2	2.20	0.42
5:F:765:LEU:HD22	5:F:819:ILE:HD12	2.01	0.42
6:G:397:VAL:O	6:G:401:VAL:HG13	2.19	0.42
6:G:471:LYS:HD2	6:G:475:LYS:NZ	2.33	0.42
1:2:701:ASP:HA	1:2:704:VAL:HG22	2.01	0.42
4:5:630:ARG:HD2	4:5:630:ARG:HA	1.86	0.42
4:5:660:THR:HG22	4:5:677:VAL:HA	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:187:ARG:NH1	5:6:187:ARG:HB3	2.34	0.42
5:6:521:LYS:HA	5:6:521:LYS:HD3	1.81	0.42
6:7:674:GLU:HB3	6:7:677:SER:HB3	2.00	0.42
4:E:299:SER:HB2	4:E:329:LYS:HE3	2.01	0.42
4:E:301:TYR:HD1	4:E:327:TYR:CD1	2.37	0.42
4:E:344:ASN:C	4:E:344:ASN:ND2	2.69	0.42
5:F:111:VAL:HG12	7:X:499:LEU:HD11	2.02	0.42
5:F:305:TYR:CE2	5:F:306:LYS:HE3	2.55	0.42
5:F:500:ASP:HB3	5:F:503:VAL:HG12	2.01	0.42
6:G:144:ASN:O	6:G:147:ARG:HG2	2.19	0.42
6:G:700:ALA:HA	6:G:703:ARG:HH11	1.84	0.42
2:3:687:ARG:HD3	6:7:609:ASP:CG	2.44	0.42
3:4:202:LYS:HE3	3:4:222:GLU:HA	2.01	0.42
3:4:347:PHE:O	3:4:355:THR:HA	2.19	0.42
5:6:150:THR:HG22	5:6:264:GLN:HB3	2.01	0.42
6:7:405:ILE:HA	6:7:410:VAL:HG11	2.02	0.42
6:7:646:LYS:HA	6:7:701:LYS:HZ2	1.83	0.42
6:7:718:ARG:HG3	6:7:721:ARG:HH12	1.85	0.42
5:F:276:ILE:HD12	5:F:363:GLU:HA	2.00	0.42
6:G:157:ARG:HH11	6:G:157:ARG:HG2	1.85	0.42
6:G:265:CYS:SG	6:G:267:TYR:HB2	2.60	0.42
6:G:534:ARG:NH1	6:G:586:LEU:HD13	2.33	0.42
3:4:393:ASP:OD2	5:6:280:ARG:HD2	2.20	0.42
3:4:685:ASN:HA	3:4:844:LYS:HD3	2.01	0.42
3:4:794:THR:O	3:4:797:GLN:HB2	2.20	0.42
4:5:436:ALA:HA	4:5:476:VAL:O	2.19	0.42
4:5:649:THR:H	4:5:652:GLN:HG2	1.83	0.42
6:7:446:ASP:OD2	6:7:448:MET:HG2	2.19	0.42
1:B:194:TYR:O	1:B:198:ILE:HG12	2.19	0.42
3:D:642:ARG:HD3	3:D:698:LEU:HD22	2.01	0.42
3:D:721:ALA:HB3	6:G:661:VAL:HG13	2.00	0.42
5:F:585:LEU:O	5:F:589:VAL:HG12	2.20	0.42
8:Y:154:ASP:HA	8:Y:157:ILE:HG12	2.00	0.42
1:2:616:ASP:O	1:2:620:ILE:HG12	2.19	0.42
1:2:697:THR:HA	1:2:700:VAL:HG22	2.01	0.42
1:2:857:LEU:O	1:2:861:PHE:HD1	2.02	0.42
4:5:553:ILE:H	4:5:688:THR:HG23	1.85	0.42
6:7:264:GLN:HE22	6:7:289:CYS:HB2	1.85	0.42
6:7:599:LEU:HD23	6:7:726:SER:O	2.20	0.42
6:7:693:ILE:O	6:7:697:GLN:HG3	2.20	0.42
1:B:476:TRP:CZ2	1:B:773:LYS:HE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:75:ILE:HD12	4:E:78:LYS:HD3	2.00	0.42
1:2:209:ARG:HA	1:2:212:LYS:HE3	2.02	0.42
4:5:32:LYS:NZ	4:5:100:ARG:HH22	2.18	0.42
6:7:158:THR:HG23	6:7:181:LEU:HD22	2.02	0.42
6:7:295:LYS:HA	6:7:295:LYS:HD2	1.67	0.42
3:D:391:PHE:HE1	5:F:450:TYR:HD1	1.66	0.42
3:D:633:GLU:OE1	3:D:636:LYS:HG3	2.19	0.42
4:E:420:THR:HG22	4:E:420:THR:O	2.19	0.42
6:G:713:VAL:O	6:G:717:LEU:HD23	2.20	0.42
3:4:508:LYS:HA	3:4:511:GLU:HG2	2.02	0.42
5:6:110:LYS:HA	5:6:113:GLU:CD	2.44	0.42
5:6:737:LYS:HE2	5:6:741:ALA:HA	2.02	0.42
3:D:684:PRO:HB3	3:D:845:ILE:HB	2.02	0.42
4:E:31:PHE:CB	4:E:90:PHE:HD1	2.23	0.42
4:E:45:ILE:HG13	4:E:46:TYR:CD1	2.55	0.42
4:E:516:ARG:O	4:E:516:ARG:HG3	2.20	0.42
5:F:777:TYR:CD1	5:F:800:LEU:HB2	2.54	0.42
5:F:796:THR:H	5:F:799:GLN:HG2	1.83	0.42
6:G:472:ALA:O	6:G:476:ILE:HD12	2.20	0.42
6:G:529:MET:HE3	6:G:533:ASP:HB3	2.01	0.42
2:3:385:LEU:HD23	2:3:385:LEU:HA	1.87	0.42
5:6:591:PHE:CZ	5:6:751:LEU:HD22	2.55	0.42
5:6:706:MET:HG3	5:6:712:PHE:CE1	2.55	0.42
5:6:707:SER:HB3	5:6:798:ARG:NH1	2.35	0.42
6:7:149:ARG:HG3	6:7:149:ARG:HH11	1.84	0.42
1:B:337:VAL:HB	1:B:359:ILE:HD11	2.02	0.42
3:D:596:SER:HA	6:G:549:SER:O	2.20	0.42
4:E:32:LYS:HZ1	4:E:100:ARG:HH22	1.68	0.42
4:E:185:ASN:HD22	4:E:236:CYS:HA	1.85	0.42
5:F:137:ARG:HH21	5:F:191:LYS:NZ	2.18	0.42
5:F:507:SER:C	5:F:508:LEU:HD12	2.44	0.42
6:G:437:VAL:O	6:G:646:LYS:HE2	2.19	0.42
6:G:437:VAL:HG22	6:G:642:ILE:HG23	2.01	0.42
6:G:701:LYS:O	6:G:704:LEU:HD12	2.20	0.42
2:3:367:LEU:HD11	2:3:382:LEU:HB2	2.02	0.42
3:4:272:MET:O	3:4:276:ILE:HG12	2.19	0.42
3:4:314:MET:HG3	3:4:401:GLU:OE2	2.19	0.42
5:6:673:ASN:HB2	5:6:675:ARG:HH12	1.85	0.42
5:6:706:MET:HG3	5:6:712:PHE:CZ	2.54	0.42
5:6:790:ARG:HD3	5:6:790:ARG:HA	1.80	0.42
1:B:342:LEU:H	1:B:342:LEU:HD23	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:PHE:HA	1:B:369:SER:O	2.20	0.42
1:B:419:LYS:HB3	1:B:419:LYS:HE2	1.80	0.42
2:C:118:PRO:HB3	2:C:122:ILE:HD12	2.02	0.42
3:D:474:LEU:HD21	3:D:751:ILE:HB	2.02	0.42
4:E:31:PHE:CD1	4:E:90:PHE:CD1	3.08	0.42
8:Y:181:ARG:NH2	8:Y:227:LEU:HD12	2.35	0.42
1:2:368:LYS:HZ2	5:F:342:ALA:HB2	1.85	0.41
1:2:528:ASN:ND2	4:5:585:ASN:HD22	2.18	0.41
3:4:738:GLN:HG3	3:4:741:VAL:HG23	2.01	0.41
4:5:568:ILE:O	4:5:572:VAL:HG12	2.20	0.41
5:6:191:LYS:NZ	5:6:192:TYR:HB2	2.35	0.41
6:7:534:ARG:NH2	6:7:586:LEU:HA	2.34	0.41
1:B:414:LEU:HD23	1:B:456:ILE:HG13	2.01	0.41
1:B:704:VAL:HG21	5:F:770:ARG:NH1	2.35	0.41
2:C:43:ARG:HE	2:C:47:VAL:HG13	1.85	0.41
2:C:368:ALA:HB3	2:C:378:LYS:HE2	2.02	0.41
2:C:578:GLU:HG3	4:E:613:ARG:HE	1.85	0.41
5:F:644:MET:HE3	5:F:649:GLN:HG3	2.01	0.41
6:G:31:ASP:C	6:G:62:LYS:HD3	2.45	0.41
1:2:327:ARG:HH11	1:2:386:GLN:NE2	2.18	0.41
1:2:497:ILE:O	1:2:501:MET:HG3	2.20	0.41
9:3:1001:ADP:O2A	4:5:498:GLU:HG2	2.20	0.41
3:4:443:PRO:HB2	3:4:453:LEU:HD22	2.01	0.41
3:4:772:ARG:HA	3:4:775:VAL:HG22	2.00	0.41
5:6:137:ARG:HH12	5:6:191:LYS:NZ	2.18	0.41
1:B:408:VAL:HG22	1:B:451:ILE:CG1	2.50	0.41
1:B:838:ILE:O	1:B:842:VAL:HG22	2.20	0.41
1:B:850:LYS:C	1:B:854:ARG:HG3	2.45	0.41
2:C:35:PHE:CE2	2:C:102:ASP:HB3	2.55	0.41
2:C:400:ARG:HG3	2:C:493:GLN:NE2	2.35	0.41
3:D:742:LEU:HD13	3:D:746:PHE:CD1	2.55	0.41
3:D:762:ILE:HB	5:F:736:MET:HB3	2.02	0.41
4:E:618:ALA:HB1	4:E:677:VAL:HG21	2.01	0.41
4:E:622:LEU:HD23	4:E:622:LEU:HA	1.89	0.41
5:F:614:ARG:HD3	5:F:621:TYR:CE1	2.55	0.41
6:G:473:ILE:HD13	6:G:473:ILE:HA	1.91	0.41
6:G:486:LYS:HG2	6:G:528:LYS:O	2.19	0.41
1:2:244:VAL:HG11	1:2:271:PHE:CZ	2.55	0.41
1:2:368:LYS:HE2	1:2:368:LYS:HA	2.01	0.41
1:2:494:ILE:HD11	1:2:824:ARG:HG3	2.01	0.41
1:2:518:SER:HA	1:2:537:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:374:HIS:O	2:3:378:LYS:HG3	2.20	0.41
4:5:454:GLN:HG3	4:5:465:GLU:CD	2.44	0.41
5:6:768:GLU:HG2	5:6:769:ALA:N	2.36	0.41
2:C:278:LEU:HD13	2:C:282:LEU:O	2.20	0.41
2:C:667:VAL:HG21	2:C:717:LEU:HD23	2.01	0.41
3:D:329:LYS:HG2	3:D:434:GLU:HG3	2.01	0.41
6:G:615:HIS:O	6:G:619:VAL:HG23	2.20	0.41
1:2:218:TYR:CE2	1:2:248:HIS:HB3	2.54	0.41
1:2:336:TYR:CE2	1:2:352:PHE:HD2	2.38	0.41
1:2:499:SER:HB3	1:2:509:ARG:HH12	1.85	0.41
2:3:360:PHE:HD1	2:3:715:VAL:HG11	1.86	0.41
3:4:762:ILE:HD11	3:4:802:ILE:HG23	2.03	0.41
1:B:334:LEU:HD23	1:B:334:LEU:H	1.85	0.41
2:C:43:ARG:HD2	2:C:136:MET:HE2	2.02	0.41
3:D:616:LEU:HD13	3:D:661:ILE:HD12	2.02	0.41
6:G:183:GLU:O	6:G:186:GLU:HG3	2.19	0.41
2:3:277:ILE:HD12	2:3:320:LEU:HD11	2.03	0.41
4:5:276:MET:CE	4:5:294:ILE:HG21	2.51	0.41
6:7:409:ASP:OD2	6:7:412:ASN:HB2	2.21	0.41
3:D:207:LYS:HD3	3:D:207:LYS:HA	1.76	0.41
3:D:609:VAL:HG11	6:G:505:GLU:HA	2.03	0.41
4:E:54:ILE:HD11	4:E:98:ALA:HB1	2.02	0.41
5:F:326:LYS:HE2	5:F:326:LYS:HA	2.02	0.41
5:F:749:GLU:HA	5:F:752:ARG:NH1	2.36	0.41
6:G:578:LEU:HD23	6:G:579:SER:N	2.34	0.41
6:G:653:SER:HB3	6:G:707:MET:HE1	2.02	0.41
1:2:219:THR:HG22	1:2:220:ASP:O	2.20	0.41
2:3:561:ILE:O	2:3:565:VAL:HG23	2.21	0.41
3:4:440:ARG:HD2	3:4:462:ASP:OD2	2.20	0.41
3:4:482:GLU:O	3:4:485:LEU:HB2	2.21	0.41
4:5:359:GLN:NE2	4:5:360:LEU:HD12	2.35	0.41
6:7:481:VAL:HG12	6:7:516:ALA:HB2	2.01	0.41
2:C:270:LEU:HD11	4:E:457:PRO:HD2	2.02	0.41
3:D:315:ARG:NH1	3:D:410:GLN:HB2	2.36	0.41
3:D:340:PRO:HG3	5:F:452:ILE:HG13	2.03	0.41
4:E:370:LEU:HD23	4:E:370:LEU:HA	1.86	0.41
5:F:186:ARG:HA	5:F:189:VAL:HG12	2.03	0.41
5:F:763:PRO:HA	5:F:817:ASP:O	2.20	0.41
3:4:767:LYS:HB2	5:6:736:MET:HE3	2.02	0.41
4:5:69:ILE:HB	4:5:76:TYR:CD1	2.56	0.41
6:7:17:LEU:O	6:7:21:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:854:ARG:NH1	1:B:858:ARG:HH21	2.18	0.41
2:C:417:GLN:HG2	9:C:1001:ADP:O1A	2.21	0.41
3:D:756:GLU:HG2	3:D:757:HIS:CE1	2.55	0.41
3:D:761:ILE:O	3:D:817:VAL:HG12	2.20	0.41
4:E:66:GLU:HA	4:E:69:ILE:HG22	2.03	0.41
4:E:139:LEU:HD23	4:E:331:LEU:HB3	2.02	0.41
6:G:286:SER:HB2	6:G:288:GLU:OE2	2.21	0.41
8:Y:153:ILE:HA	8:Y:156:ILE:HG12	2.03	0.41
1:2:552:ILE:O	1:2:556:VAL:HG23	2.21	0.41
4:5:490:ARG:NH2	4:5:542:PHE:HB3	2.36	0.41
5:6:585:LEU:O	5:6:589:VAL:HG12	2.21	0.41
1:B:286:TYR:HA	1:B:289:ILE:HG22	2.03	0.41
1:B:328:THR:HG23	1:B:387:ARG:O	2.20	0.41
1:B:386:GLN:HB3	1:B:415:VAL:HG12	2.03	0.41
1:B:662:PRO:HD3	1:B:850:LYS:HB3	2.02	0.41
1:B:783:MET:HB2	4:E:573:ILE:HG21	2.03	0.41
1:B:796:GLU:HG3	1:B:861:PHE:HE2	1.84	0.41
3:D:314:MET:HE3	3:D:415:ILE:HD12	2.02	0.41
3:D:701:ARG:HA	3:D:796:ARG:HD2	2.02	0.41
3:D:745:GLU:HG2	3:D:746:PHE:N	2.35	0.41
6:G:264:GLN:HE22	6:G:265:CYS:HB3	1.86	0.41
1:2:482:ARG:O	1:2:486:LYS:HG2	2.21	0.41
2:3:509:ARG:HE	2:3:509:ARG:HB2	1.64	0.41
2:3:694:LYS:HG3	2:3:737:LEU:O	2.20	0.41
3:4:628:VAL:HG22	3:4:670:SER:HB2	2.03	0.41
3:4:721:ALA:HB3	6:7:661:VAL:HG13	2.03	0.41
3:4:839:ASP:HB3	3:4:842:THR:O	2.21	0.41
4:5:32:LYS:CE	4:5:100:ARG:HH12	2.34	0.41
4:5:349:PHE:HB2	4:5:354:GLU:OE2	2.20	0.41
4:5:363:ASN:O	4:5:366:LEU:HG	2.21	0.41
4:5:420:THR:O	4:5:420:THR:HG22	2.20	0.41
5:6:641:PHE:HE2	5:6:705:ILE:HG21	1.85	0.41
5:6:672:LEU:HD23	5:6:673:ASN:N	2.36	0.41
6:7:166:LEU:HD12	4:E:100:ARG:HG2	2.03	0.41
6:7:596:ILE:HD13	6:7:720:VAL:HG12	2.03	0.41
6:7:621:MET:HG3	6:7:622:HIS:ND1	2.35	0.41
1:B:408:VAL:HG22	1:B:451:ILE:HD11	2.03	0.41
2:C:367:LEU:HD11	2:C:382:LEU:HB2	2.02	0.41
3:D:178:ARG:HA	7:X:533:PHE:O	2.21	0.41
3:D:581:VAL:HA	3:D:584:ILE:HG22	2.03	0.41
3:D:594:LYS:O	3:D:594:LYS:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:724:LEU:HD22	6:G:689:LEU:HD22	2.02	0.41
3:D:762:ILE:HA	3:D:817:VAL:CG1	2.51	0.41
3:D:767:LYS:HG3	5:F:732:VAL:CG1	2.51	0.41
6:G:90:ASN:HD21	6:G:215:TYR:HE1	1.69	0.41
6:G:295:LYS:HE3	6:G:295:LYS:HA	2.03	0.41
6:G:493:LEU:O	6:G:511:GLY:HA3	2.21	0.41
6:G:527:ASP:HB3	6:G:584:ILE:HD11	2.02	0.41
6:G:593:ARG:HB2	6:G:687:ARG:NH2	2.35	0.41
1:2:792:ASP:O	1:2:793:LEU:C	2.64	0.41
2:3:306:MET:HE2	2:3:306:MET:HB2	1.84	0.41
3:4:508:LYS:HD2	3:4:512:VAL:HG23	2.02	0.41
3:4:559:ARG:HB3	3:4:561:ASP:OD2	2.20	0.41
4:5:456:ASP:HB3	4:5:461:GLU:H	1.86	0.41
5:6:110:LYS:HE3	7:8:499:LEU:HD12	2.02	0.41
5:6:777:TYR:CD2	5:6:800:LEU:HD12	2.56	0.41
6:7:497:VAL:O	6:7:497:VAL:HG13	2.21	0.41
6:7:593:ARG:NH1	6:7:687:ARG:HH12	2.18	0.41
1:B:458:ARG:HD2	1:B:460:GLU:HG2	2.02	0.41
1:B:474:PHE:HB3	1:B:768:HIS:CD2	2.55	0.41
1:B:570:GLY:HA2	5:F:650:VAL:HG11	2.03	0.41
1:B:759:PRO:HG2	1:B:762:LEU:HB3	2.03	0.41
3:D:506:LEU:HD23	3:D:510:ARG:HD3	2.03	0.41
3:D:519:TYR:CZ	3:D:538:LYS:HD3	2.56	0.41
3:D:530:ILE:HD12	3:D:576:GLN:HB2	2.02	0.41
4:E:535:SER:HB3	4:E:696:PRO:HD2	2.02	0.41
6:G:533:ASP:O	6:G:537:ILE:HG12	2.21	0.41
3:4:508:LYS:HG3	3:4:746:PHE:CE1	2.56	0.40
3:4:554:LYS:HE2	5:6:742:ILE:HG21	2.02	0.40
4:5:276:MET:HG2	4:5:328:ILE:HB	2.01	0.40
5:6:276:ILE:HD12	5:6:363:GLU:HA	2.03	0.40
5:6:748:ALA:O	5:6:752:ARG:HG3	2.21	0.40
6:7:183:GLU:O	6:7:186:GLU:HG3	2.21	0.40
6:7:523:ILE:HG21	6:7:526:PHE:HD2	1.86	0.40
6:7:593:ARG:HD3	6:7:687:ARG:NH2	2.36	0.40
3:D:437:GLY:HA3	3:D:463:VAL:HA	2.04	0.40
5:F:424:ARG:HH22	6:G:294:THR:HA	1.85	0.40
6:G:535:THR:O	6:G:538:HIS:HB3	2.21	0.40
8:Y:223:HIS:HB3	8:Y:226:GLU:HB2	2.03	0.40
1:2:327:ARG:HB3	1:2:386:GLN:NE2	2.35	0.40
1:2:805:ILE:HD11	1:2:845:PHE:CD2	2.56	0.40
3:4:635:ASP:OD1	3:4:636:LYS:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:422:ASP:HB3	5:6:424:ARG:HG2	2.03	0.40
5:6:570:ASN:O	5:6:710:ASP:HB2	2.21	0.40
5:6:780:LEU:HB2	5:6:828:TYR:HE1	1.87	0.40
6:7:718:ARG:HA	6:7:721:ARG:NH1	2.36	0.40
3:D:344:VAL:HG12	3:D:390:SER:OG	2.22	0.40
3:D:365:ILE:HB	5:F:419:SER:HA	2.03	0.40
3:D:843:GLY:C	3:D:844:LYS:HD3	2.47	0.40
5:F:109:GLU:O	5:F:113:GLU:OE1	2.40	0.40
5:F:572:CYS:HB2	5:F:709:PHE:CE1	2.57	0.40
1:2:200:GLN:OE1	1:2:203:VAL:HG23	2.21	0.40
1:2:783:MET:O	1:2:784:ASP:C	2.63	0.40
2:3:308:GLN:H	4:5:209:ARG:HH22	1.68	0.40
3:4:798:LEU:HA	3:4:801:MET:HG3	2.04	0.40
6:7:676:ASP:HA	6:7:678:LYS:HE3	2.03	0.40
1:B:304:TYR:HE2	1:B:313:ASN:HD21	1.69	0.40
1:B:387:ARG:HD2	1:B:407:GLU:OE1	2.22	0.40
1:B:780:GLN:O	1:B:783:MET:HG3	2.22	0.40
2:C:154:LYS:HA	2:C:154:LYS:HD2	1.91	0.40
2:C:281:ASP:C	2:C:283:VAL:N	2.79	0.40
2:C:393:LEU:HD12	2:C:397:SER:HB2	2.03	0.40
3:D:770:LEU:HD23	3:D:770:LEU:HA	1.92	0.40
5:F:117:GLN:HA	5:F:120:GLU:HG3	2.03	0.40
5:F:311:CYS:HB2	5:F:313:MET:SD	2.60	0.40
5:F:398:THR:HB	5:F:458:HIS:CE1	2.56	0.40
5:F:703:ALA:N	5:F:704:PRO:HD2	2.36	0.40
6:G:648:LYS:HD2	6:G:704:LEU:HA	2.04	0.40
1:2:458:ARG:NH1	1:2:460:GLU:H	2.19	0.40
2:3:338:ALA:HB3	2:3:427:SER:HA	2.03	0.40
3:4:613:GLN:OE1	3:4:613:GLN:HA	2.22	0.40
3:4:777:MET:HE1	3:4:797:GLN:HB3	2.03	0.40
4:5:136:GLN:HG3	4:5:280:ARG:NH2	2.35	0.40
4:5:570:ASN:HA	4:5:573:ILE:HG22	2.03	0.40
5:6:657:GLU:CG	5:6:708:ARG:HE	2.34	0.40
6:7:66:MET:HE3	6:7:78:VAL:HG23	2.04	0.40
1:B:245:ASN:OD1	1:B:299:ASP:HB2	2.21	0.40
1:B:343:LYS:H	1:B:343:LYS:HG2	1.66	0.40
3:D:720:LEU:HD21	6:G:686:PRO:HB3	2.04	0.40
4:E:43:GLN:OE1	4:E:43:GLN:HA	2.21	0.40
5:F:117:GLN:HG2	5:F:161:ARG:HH12	1.87	0.40
5:F:323:GLN:HG3	5:F:328:THR:H	1.86	0.40
8:Y:192:ILE:CD1	8:Y:250:LEU:HD11	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:228:LYS:HD2	8:Y:232:MET:HE1	2.03	0.40
2:3:104:ARG:CZ	2:3:108:ARG:HH12	2.34	0.40
3:4:210:ASP:HB3	3:4:212:ARG:HG2	2.04	0.40
3:4:319:PRO:HB3	6:7:253:PRO:HB3	2.04	0.40
3:4:528:PRO:HB2	3:4:735:HIS:CE1	2.57	0.40
4:5:12:PRO:HB3	6:G:267:TYR:CE2	2.56	0.40
4:5:197:PHE:HB3	4:5:200:ILE:HD11	2.04	0.40
5:6:139:GLN:HG2	5:6:151:ILE:CD1	2.52	0.40
5:6:186:ARG:HH22	5:6:260:GLU:HB3	1.86	0.40
6:7:264:GLN:HE22	6:7:289:CYS:CB	2.34	0.40
1:B:306:LEU:HD12	1:B:406:ARG:CG	2.51	0.40
1:B:543:GLY:HA3	1:B:549:LYS:HD3	2.02	0.40
1:B:605:LEU:HD23	1:B:647:ILE:HB	2.02	0.40
3:D:567:CYS:HA	3:D:675:ALA:O	2.22	0.40
3:D:646:HIS:CE1	3:D:701:ARG:HH12	2.38	0.40
3:D:695:PRO:HA	3:D:696:PRO:HD2	1.95	0.40
4:E:100:ARG:HE	4:E:100:ARG:HB2	1.67	0.40
5:F:777:TYR:CE1	5:F:800:LEU:HB2	2.57	0.40
8:Y:173:ARG:HH22	8:Y:235:GLY:CA	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	616/868 (71%)	598 (97%)	18 (3%)	0	100	100
1	B	616/868 (71%)	600 (97%)	16 (3%)	0	100	100
2	3	617/971 (64%)	601 (97%)	16 (3%)	0	100	100
2	C	617/971 (64%)	603 (98%)	14 (2%)	0	100	100
3	4	664/933 (71%)	647 (97%)	17 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	664/933 (71%)	645 (97%)	19 (3%)	0	100	100
4	5	635/775 (82%)	616 (97%)	19 (3%)	0	100	100
4	E	635/775 (82%)	617 (97%)	18 (3%)	0	100	100
5	6	637/1017 (63%)	619 (97%)	18 (3%)	0	100	100
5	F	637/1017 (63%)	624 (98%)	13 (2%)	0	100	100
6	7	684/845 (81%)	667 (98%)	17 (2%)	0	100	100
6	G	684/845 (81%)	670 (98%)	14 (2%)	0	100	100
7	8	25/668 (4%)	25 (100%)	0	0	100	100
7	X	25/668 (4%)	25 (100%)	0	0	100	100
8	Y	90/257 (35%)	87 (97%)	3 (3%)	0	100	100
All	All	7846/12411 (63%)	7644 (97%)	202 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	550/770 (71%)	549 (100%)	1 (0%)	87	85
1	B	550/770 (71%)	550 (100%)	0	100	100
2	3	546/835 (65%)	545 (100%)	1 (0%)	87	85
2	C	546/835 (65%)	546 (100%)	0	100	100
3	4	608/848 (72%)	608 (100%)	0	100	100
3	D	608/848 (72%)	607 (100%)	1 (0%)	87	85
4	5	575/688 (84%)	574 (100%)	1 (0%)	87	85
4	E	575/688 (84%)	574 (100%)	1 (0%)	87	85
5	6	566/886 (64%)	565 (100%)	1 (0%)	87	85
5	F	566/886 (64%)	566 (100%)	0	100	100
6	7	609/753 (81%)	609 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	G	609/753 (81%)	609 (100%)	0	100	100
7	8	29/628 (5%)	29 (100%)	0	100	100
7	X	29/628 (5%)	29 (100%)	0	100	100
8	Y	87/234 (37%)	87 (100%)	0	100	100
All	All	7053/11050 (64%)	7047 (100%)	6 (0%)	87	87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	551	GLN
2	3	293	ASN
4	5	590	ASN
5	6	673	ASN
3	D	488	ASN
4	E	344	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	245	ASN
1	2	248	HIS
1	2	290	HIS
1	2	353	GLN
1	2	386	GLN
1	2	703	HIS
2	3	164	HIS
2	3	349	ASN
2	3	417	GLN
2	3	493	GLN
2	3	691	ASN
3	4	240	ASN
3	4	483	GLN
3	4	487	GLN
3	4	651	GLN
3	4	797	GLN
3	4	808	HIS
4	5	195	ASN
4	5	253	GLN
4	5	254	GLN
4	5	284	ASN

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Mol	Chain	Res	Type
4	5	411	ASN
4	5	514	ASN
4	5	576	HIS
4	5	584	GLN
4	5	585	ASN
4	5	636	ASN
5	6	690	ASN
5	6	700	ASN
6	7	90	ASN
6	7	107	GLN
6	7	229	GLN
6	7	264	GLN
6	7	293	GLN
6	7	543	GLN
6	7	544	GLN
7	8	500	ASN
1	B	200	GLN
1	B	248	HIS
1	B	366	ASN
1	B	405	HIS
1	B	454	ASN
1	B	849	GLN
2	C	151	HIS
2	C	392	ASN
2	C	673	GLN
2	C	722	ASN
3	D	193	ASN
3	D	492	HIS
3	D	579	GLN
3	D	691	ASN
3	D	723	HIS
3	D	757	HIS
3	D	851	GLN
4	E	245	HIS
4	E	499	GLN
4	E	524	ASN
4	E	581	ASN
4	E	636	ASN
4	E	676	HIS
5	F	514	ASN
5	F	653	HIS
6	G	90	ASN

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Mol	Chain	Res	Type
6	G	229	GLN
6	G	264	GLN
6	G	311	GLN
6	G	379	GLN
6	G	412	ASN
6	G	538	HIS
6	G	554	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 10 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	ADP	G	1001	-	27,29,29	1.33	4 (14%)	42,45,45	1.97	9 (21%)
9	ADP	2	1001	-	27,29,29	1.34	4 (14%)	42,45,45	2.00	11 (26%)
9	ADP	7	1001	-	27,29,29	1.32	4 (14%)	42,45,45	1.99	9 (21%)
9	ADP	B	1001	-	27,29,29	1.34	4 (14%)	42,45,45	1.97	9 (21%)
9	ADP	3	1001	-	27,29,29	1.34	4 (14%)	42,45,45	1.95	11 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	ADP	E	1001	-	27,29,29	1.34	4 (14%)	42,45,45	1.95	10 (23%)
9	ADP	C	1001	-	27,29,29	1.35	4 (14%)	42,45,45	1.96	10 (23%)
9	ADP	5	1001	-	27,29,29	1.34	4 (14%)	42,45,45	1.93	10 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ADP	G	1001	-	-	4/16/32/32	0/3/3/3
9	ADP	2	1001	-	-	7/16/32/32	0/3/3/3
9	ADP	7	1001	-	-	5/16/32/32	0/3/3/3
9	ADP	B	1001	-	-	5/16/32/32	0/3/3/3
9	ADP	3	1001	-	-	5/16/32/32	0/3/3/3
9	ADP	E	1001	-	-	5/16/32/32	0/3/3/3
9	ADP	C	1001	-	-	4/16/32/32	0/3/3/3
9	ADP	5	1001	-	-	5/16/32/32	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	1001	ADP	C5-C4	4.43	1.47	1.39
9	B	1001	ADP	C5-C4	4.39	1.47	1.39
9	G	1001	ADP	C5-C4	4.38	1.47	1.39
9	7	1001	ADP	C5-C4	4.36	1.47	1.39
9	C	1001	ADP	C5-C4	4.36	1.47	1.39
9	3	1001	ADP	C5-C4	4.36	1.47	1.39
9	5	1001	ADP	C5-C4	4.35	1.47	1.39
9	E	1001	ADP	C5-C4	4.31	1.47	1.39
9	E	1001	ADP	C5-C6	2.57	1.48	1.41
9	3	1001	ADP	C5-C6	2.56	1.48	1.41
9	2	1001	ADP	C5-C6	2.56	1.48	1.41
9	5	1001	ADP	C5-C6	2.56	1.48	1.41
9	C	1001	ADP	C5-C6	2.54	1.48	1.41
9	B	1001	ADP	C5-C6	2.53	1.48	1.41
9	7	1001	ADP	C5-C6	2.48	1.48	1.41
9	G	1001	ADP	C5-C6	2.46	1.47	1.41
9	3	1001	ADP	C8-N7	2.42	1.36	1.31
9	E	1001	ADP	C8-N7	2.39	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1001	ADP	C8-N7	2.39	1.36	1.31
9	2	1001	ADP	C8-N7	2.34	1.36	1.31
9	5	1001	ADP	C8-N7	2.32	1.36	1.31
9	G	1001	ADP	C5-N7	-2.32	1.34	1.39
9	B	1001	ADP	C8-N7	2.31	1.36	1.31
9	C	1001	ADP	C5-N7	-2.30	1.34	1.39
9	B	1001	ADP	C5-N7	-2.30	1.34	1.39
9	7	1001	ADP	C8-N7	2.29	1.35	1.31
9	G	1001	ADP	C8-N7	2.28	1.35	1.31
9	E	1001	ADP	C5-N7	-2.25	1.34	1.39
9	5	1001	ADP	C5-N7	-2.24	1.34	1.39
9	7	1001	ADP	C5-N7	-2.23	1.34	1.39
9	2	1001	ADP	C5-N7	-2.22	1.34	1.39
9	3	1001	ADP	C5-N7	-2.21	1.34	1.39

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	7	1001	ADP	C5-C4-N3	-6.37	118.44	126.75
9	B	1001	ADP	C5-C4-N3	-6.22	118.64	126.75
9	5	1001	ADP	C5-C4-N3	-6.16	118.71	126.75
9	2	1001	ADP	C5-C4-N3	-6.13	118.75	126.75
9	G	1001	ADP	C5-C4-N3	-6.12	118.77	126.75
9	C	1001	ADP	C5-C4-N3	-6.10	118.79	126.75
9	E	1001	ADP	C5-C4-N3	-6.09	118.81	126.75
9	3	1001	ADP	C5-C4-N3	-5.98	118.94	126.75
9	7	1001	ADP	N3-C4-N9	5.13	135.53	127.08
9	G	1001	ADP	N3-C4-N9	5.04	135.39	127.08
9	B	1001	ADP	N3-C4-N9	4.92	135.19	127.08
9	5	1001	ADP	N3-C4-N9	4.88	135.12	127.08
9	2	1001	ADP	N3-C4-N9	4.83	135.04	127.08
9	E	1001	ADP	N3-C4-N9	4.77	134.94	127.08
9	C	1001	ADP	N3-C4-N9	4.74	134.88	127.08
9	3	1001	ADP	N3-C4-N9	4.58	134.62	127.08
9	7	1001	ADP	C2-N3-C4	3.96	121.10	111.75
9	C	1001	ADP	C2-N3-C4	3.84	120.83	111.75
9	2	1001	ADP	C2-N3-C4	3.84	120.82	111.75
9	E	1001	ADP	C2-N3-C4	3.83	120.81	111.75
9	3	1001	ADP	C2-N3-C4	3.82	120.78	111.75
9	5	1001	ADP	C2-N3-C4	3.82	120.77	111.75
9	G	1001	ADP	C2-N3-C4	3.80	120.72	111.75
9	B	1001	ADP	C2-N3-C4	3.79	120.69	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	1001	ADP	PA-O3A-PB	-3.72	120.06	132.83
9	2	1001	ADP	PA-O3A-PB	-3.58	120.55	132.83
9	C	1001	ADP	PA-O3A-PB	-3.54	120.66	132.83
9	G	1001	ADP	PA-O3A-PB	-3.50	120.80	132.83
9	E	1001	ADP	PA-O3A-PB	-3.41	121.12	132.83
9	3	1001	ADP	C4-C5-N7	-3.33	106.56	110.62
9	3	1001	ADP	N3-C2-N1	-3.24	123.53	128.60
9	7	1001	ADP	N3-C2-N1	-3.23	123.56	128.60
9	C	1001	ADP	C4-C5-N7	-3.21	106.71	110.62
9	C	1001	ADP	N3-C2-N1	-3.20	123.59	128.60
9	2	1001	ADP	C4-C5-N7	-3.19	106.73	110.62
9	5	1001	ADP	C4-C5-N7	-3.17	106.75	110.62
9	E	1001	ADP	C4-C5-N7	-3.17	106.76	110.62
9	7	1001	ADP	PA-O3A-PB	-3.16	121.97	132.83
9	E	1001	ADP	N3-C2-N1	-3.16	123.66	128.60
9	3	1001	ADP	PA-O3A-PB	-3.16	121.99	132.83
9	2	1001	ADP	N3-C2-N1	-3.15	123.68	128.60
9	G	1001	ADP	N3-C2-N1	-3.13	123.70	128.60
9	B	1001	ADP	C4-C5-N7	-3.09	106.85	110.62
9	5	1001	ADP	N3-C2-N1	-3.09	123.77	128.60
9	5	1001	ADP	PA-O3A-PB	-3.02	122.46	132.83
9	7	1001	ADP	C4-C5-N7	-3.02	106.94	110.62
9	B	1001	ADP	N3-C2-N1	-3.00	123.92	128.60
9	G	1001	ADP	C4-C5-N7	-2.86	107.14	110.62
9	3	1001	ADP	C5-N7-C8	2.75	107.41	103.51
9	G	1001	ADP	C4-N9-C8	2.72	108.68	105.73
9	5	1001	ADP	C5-N7-C8	2.71	107.36	103.51
9	E	1001	ADP	C5-N7-C8	2.71	107.36	103.51
9	C	1001	ADP	C5-N7-C8	2.70	107.34	103.51
9	2	1001	ADP	C5-N7-C8	2.70	107.34	103.51
9	5	1001	ADP	C4-N9-C8	2.67	108.62	105.73
9	2	1001	ADP	C4-N9-C8	2.66	108.61	105.73
9	E	1001	ADP	C4-N9-C8	2.65	108.60	105.73
9	7	1001	ADP	C4-N9-C8	2.64	108.58	105.73
9	7	1001	ADP	C5-N7-C8	2.63	107.25	103.51
9	2	1001	ADP	C3'-C2'-C1'	2.62	106.41	101.43
9	B	1001	ADP	C5-N7-C8	2.61	107.22	103.51
9	3	1001	ADP	C4-N9-C8	2.58	108.53	105.73
9	B	1001	ADP	C4-N9-C8	2.58	108.53	105.73
9	C	1001	ADP	C4-N9-C8	2.54	108.48	105.73
9	G	1001	ADP	C5-N7-C8	2.49	107.05	103.51
9	G	1001	ADP	C3'-C2'-C1'	2.45	106.08	101.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	1001	ADP	C3'-C2'-C1'	2.33	105.86	101.43
9	3	1001	ADP	C6-C5-N7	2.28	136.27	132.02
9	7	1001	ADP	C3'-C2'-C1'	2.25	105.71	101.43
9	E	1001	ADP	C6-C5-N7	2.16	136.05	132.02
9	C	1001	ADP	C6-C5-N7	2.15	136.03	132.02
9	E	1001	ADP	N9-C8-N7	-2.11	111.03	113.91
9	5	1001	ADP	C6-C5-N7	2.10	135.94	132.02
9	3	1001	ADP	O4'-C1'-N9	2.10	112.20	108.06
9	2	1001	ADP	C6-C5-N7	2.10	135.93	132.02
9	3	1001	ADP	N9-C8-N7	-2.09	111.06	113.91
9	5	1001	ADP	N9-C8-N7	-2.06	111.09	113.91
9	2	1001	ADP	N9-C8-N7	-2.05	111.11	113.91
9	C	1001	ADP	N9-C8-N7	-2.04	111.13	113.91

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	2	1001	ADP	C5'-O5'-PA-O1A
9	2	1001	ADP	C5'-O5'-PA-O2A
9	3	1001	ADP	PA-O3A-PB-O2B
9	3	1001	ADP	C5'-O5'-PA-O1A
9	3	1001	ADP	C5'-O5'-PA-O2A
9	5	1001	ADP	PA-O3A-PB-O2B
9	5	1001	ADP	PA-O3A-PB-O3B
9	5	1001	ADP	C5'-O5'-PA-O1A
9	5	1001	ADP	C5'-O5'-PA-O2A
9	7	1001	ADP	C5'-O5'-PA-O2A
9	B	1001	ADP	C5'-O5'-PA-O1A
9	B	1001	ADP	C5'-O5'-PA-O2A
9	C	1001	ADP	C5'-O5'-PA-O1A
9	C	1001	ADP	C5'-O5'-PA-O2A
9	E	1001	ADP	C5'-O5'-PA-O1A
9	E	1001	ADP	C5'-O5'-PA-O2A
9	G	1001	ADP	PA-O3A-PB-O2B
9	G	1001	ADP	PA-O3A-PB-O3B
9	E	1001	ADP	PA-O3A-PB-O1B
9	7	1001	ADP	PA-O3A-PB-O2B
9	E	1001	ADP	PA-O3A-PB-O2B
9	5	1001	ADP	C5'-O5'-PA-O3A
9	7	1001	ADP	C5'-O5'-PA-O3A
9	7	1001	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
9	2	1001	ADP	PA-O3A-PB-O1B
9	C	1001	ADP	PB-O3A-PA-O2A
9	G	1001	ADP	O4'-C4'-C5'-O5'
9	2	1001	ADP	PA-O3A-PB-O2B
9	2	1001	ADP	PA-O3A-PB-O3B
9	3	1001	ADP	PA-O3A-PB-O3B
9	7	1001	ADP	PA-O3A-PB-O3B
9	B	1001	ADP	PA-O3A-PB-O3B
9	2	1001	ADP	C5'-O5'-PA-O3A
9	3	1001	ADP	C5'-O5'-PA-O3A
9	B	1001	ADP	C5'-O5'-PA-O3A
9	C	1001	ADP	C5'-O5'-PA-O3A
9	E	1001	ADP	C5'-O5'-PA-O3A
9	B	1001	ADP	O4'-C4'-C5'-O5'
9	G	1001	ADP	C5'-O5'-PA-O1A
9	2	1001	ADP	O4'-C4'-C5'-O5'

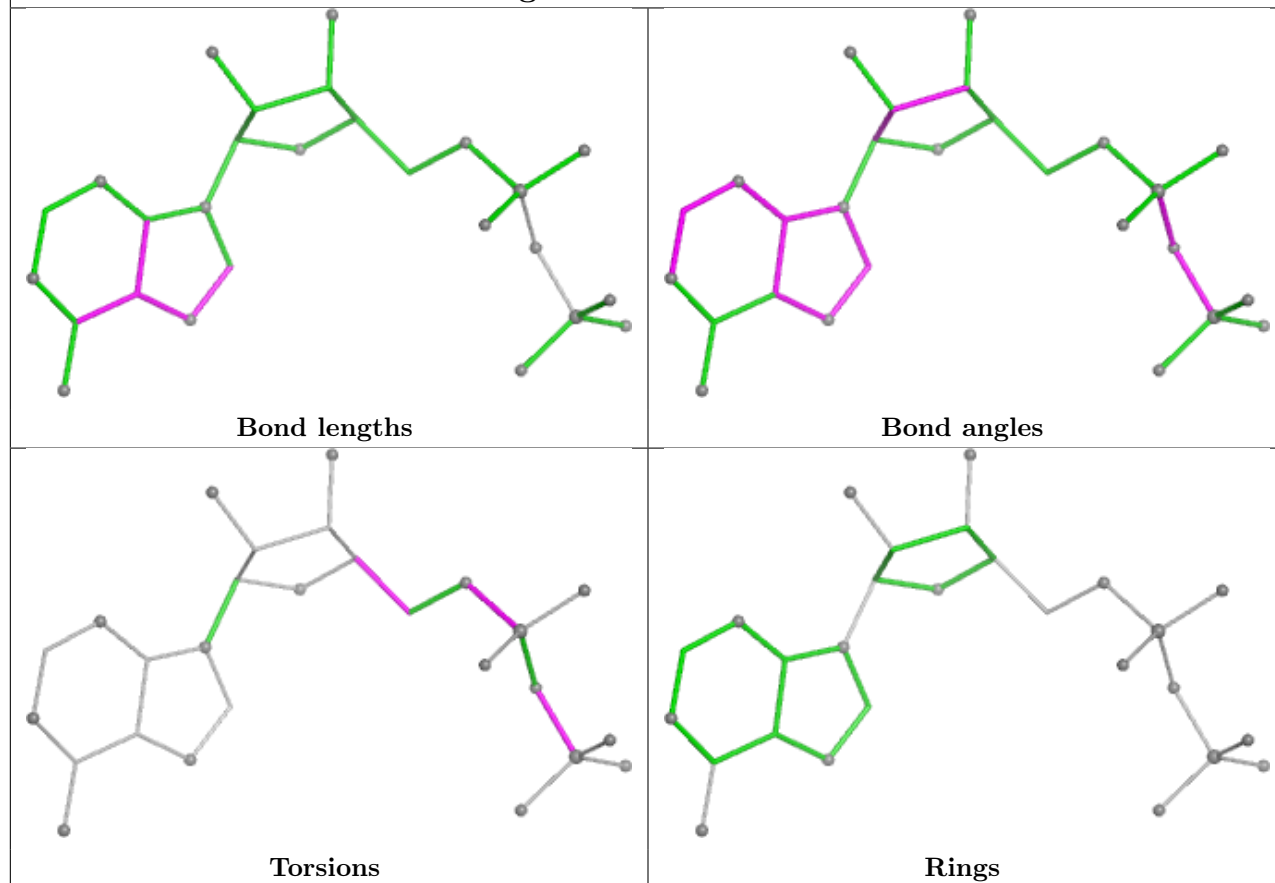
There are no ring outliers.

5 monomers are involved in 5 short contacts:

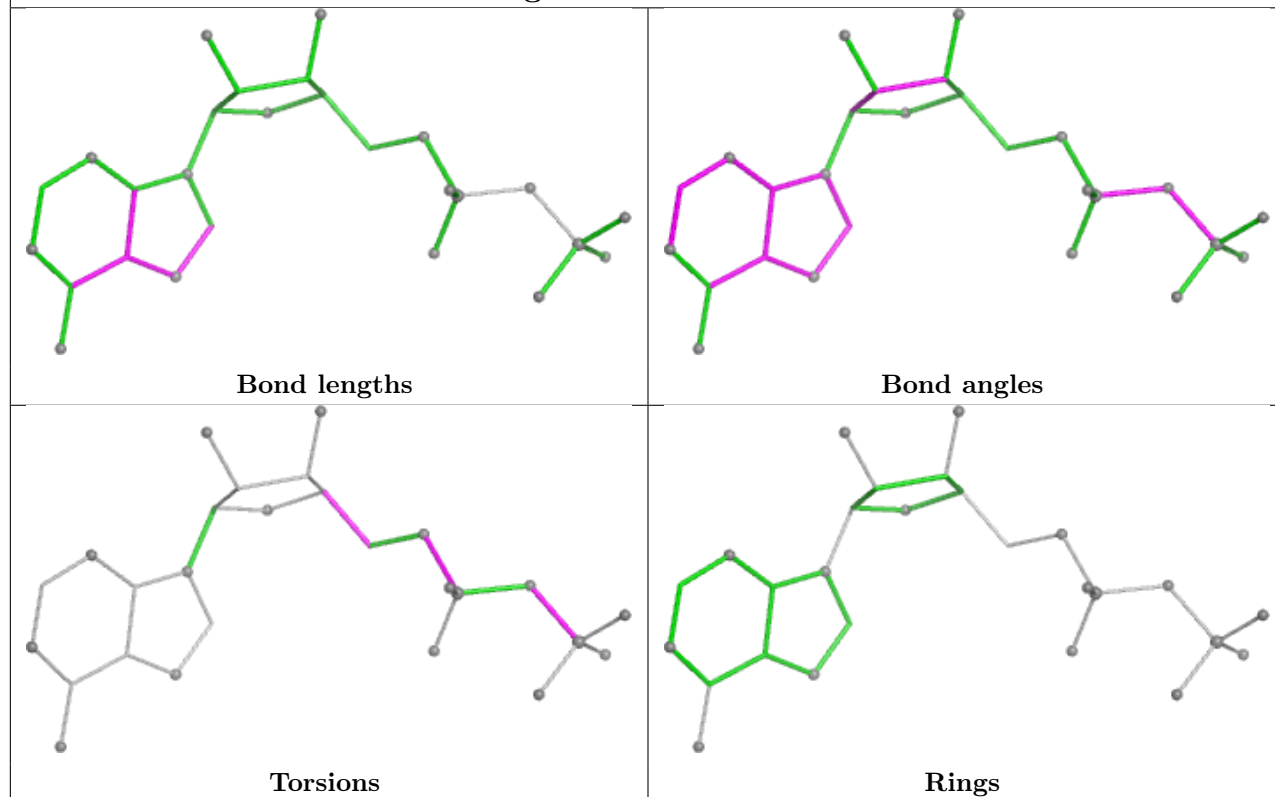
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	G	1001	ADP	1	0
9	7	1001	ADP	1	0
9	3	1001	ADP	1	0
9	C	1001	ADP	1	0
9	5	1001	ADP	1	0

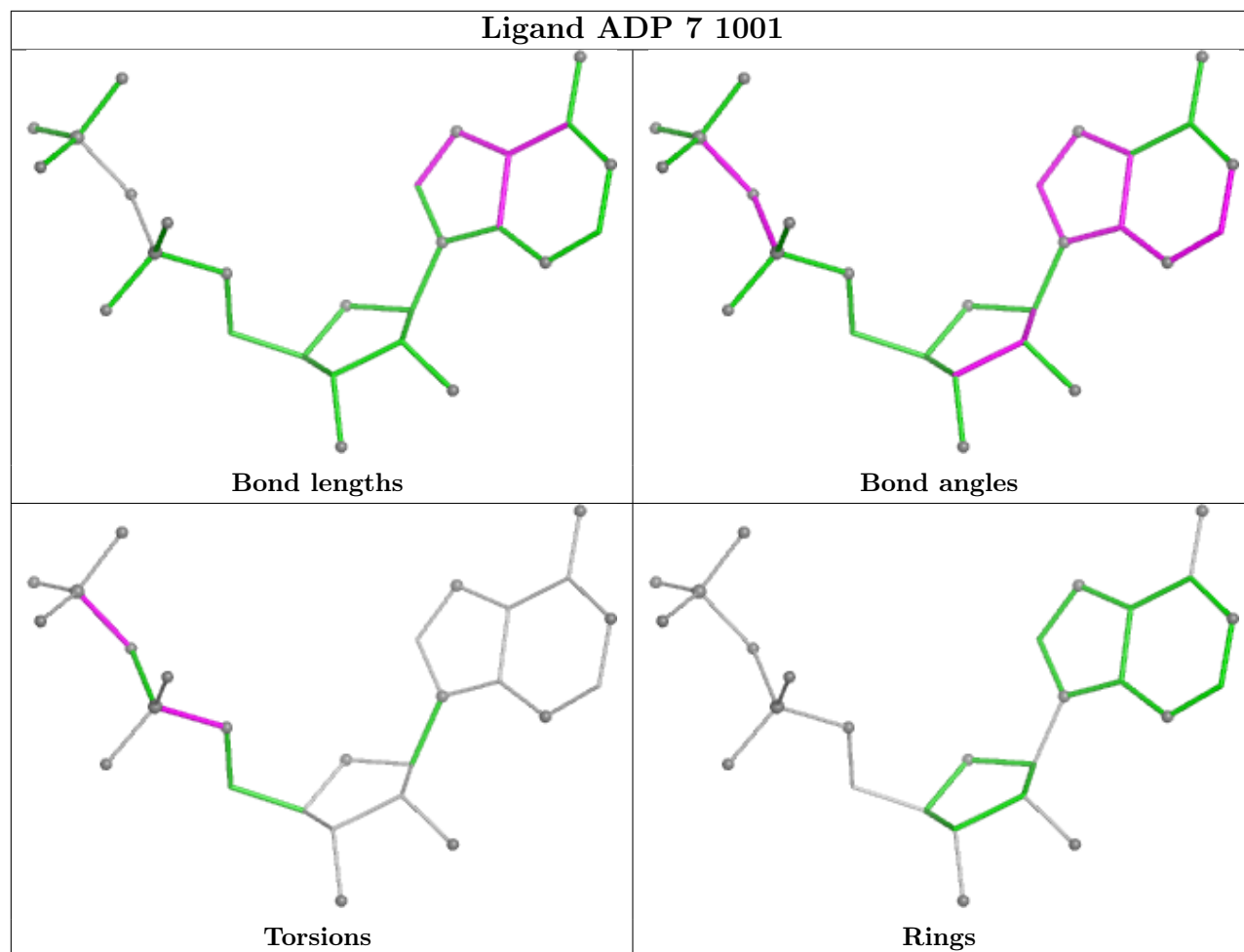
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

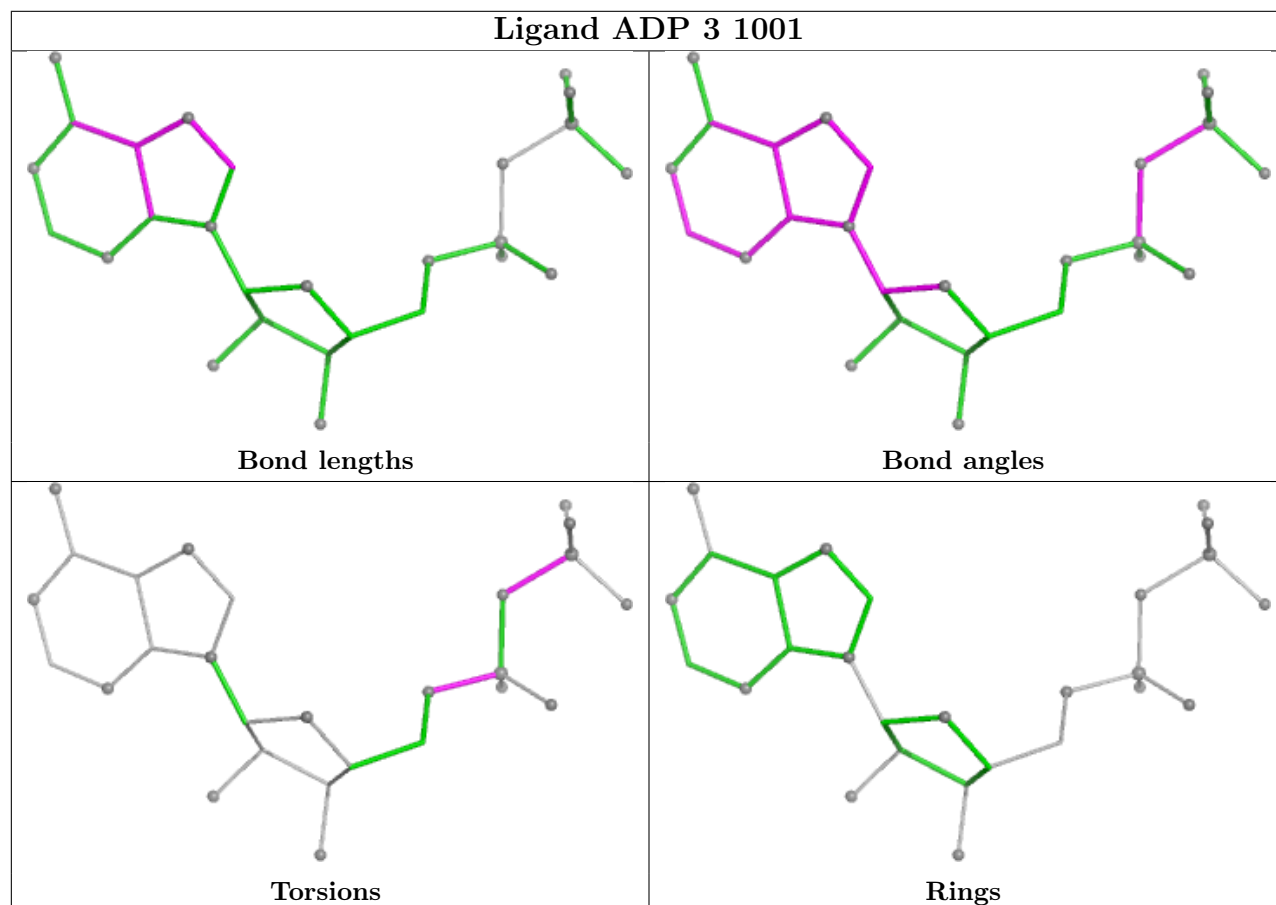
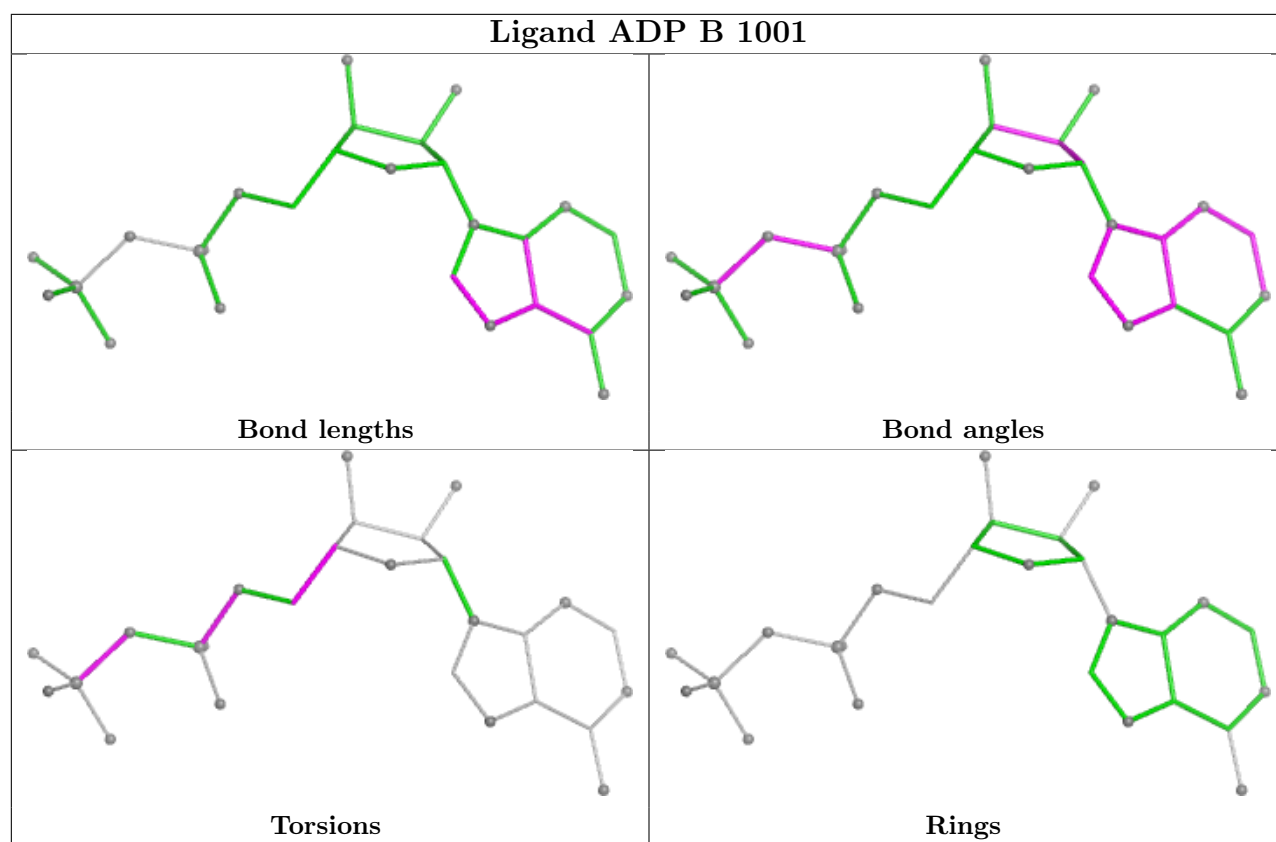
Ligand ADP G 1001

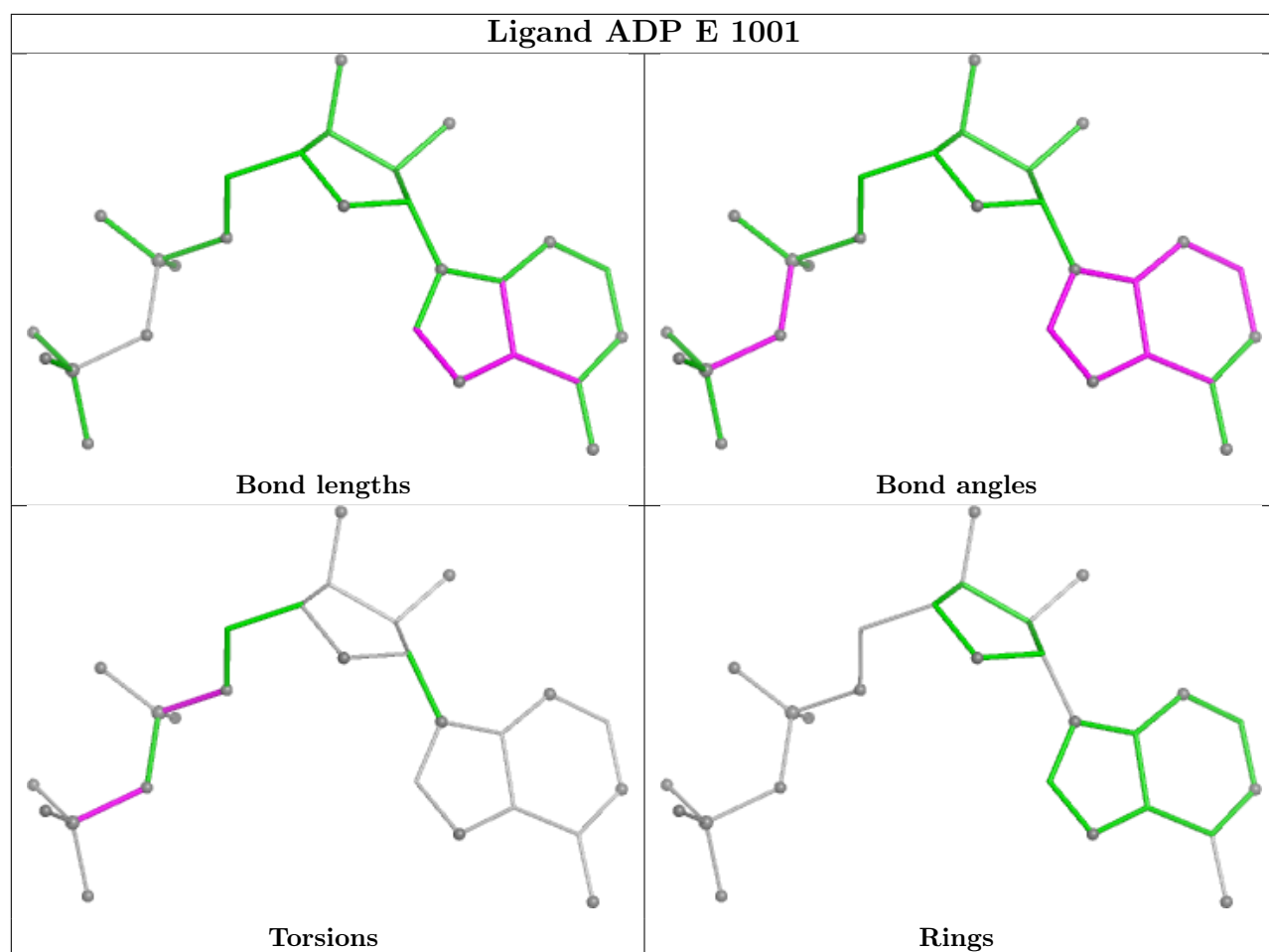


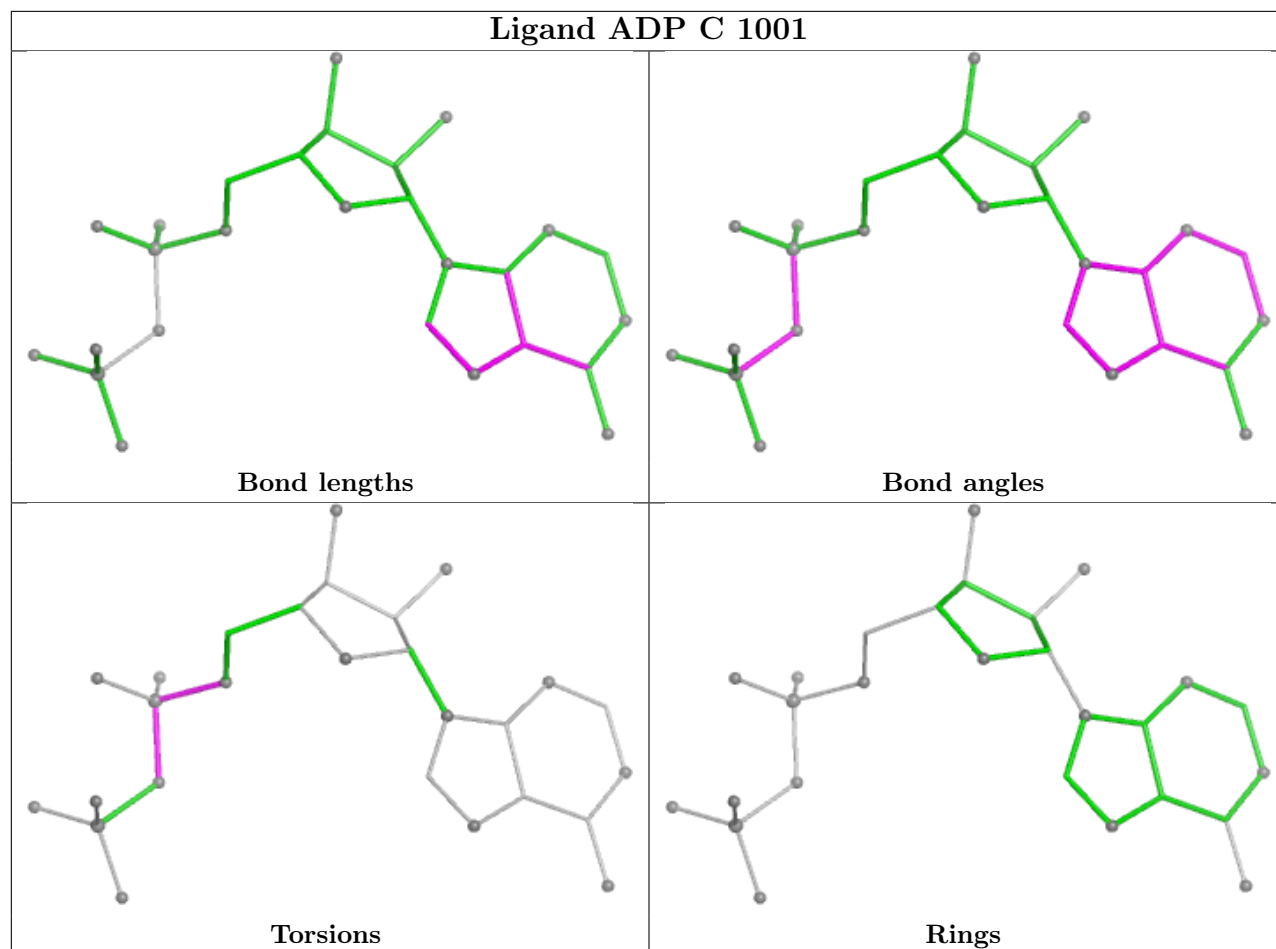
Ligand ADP 2 1001

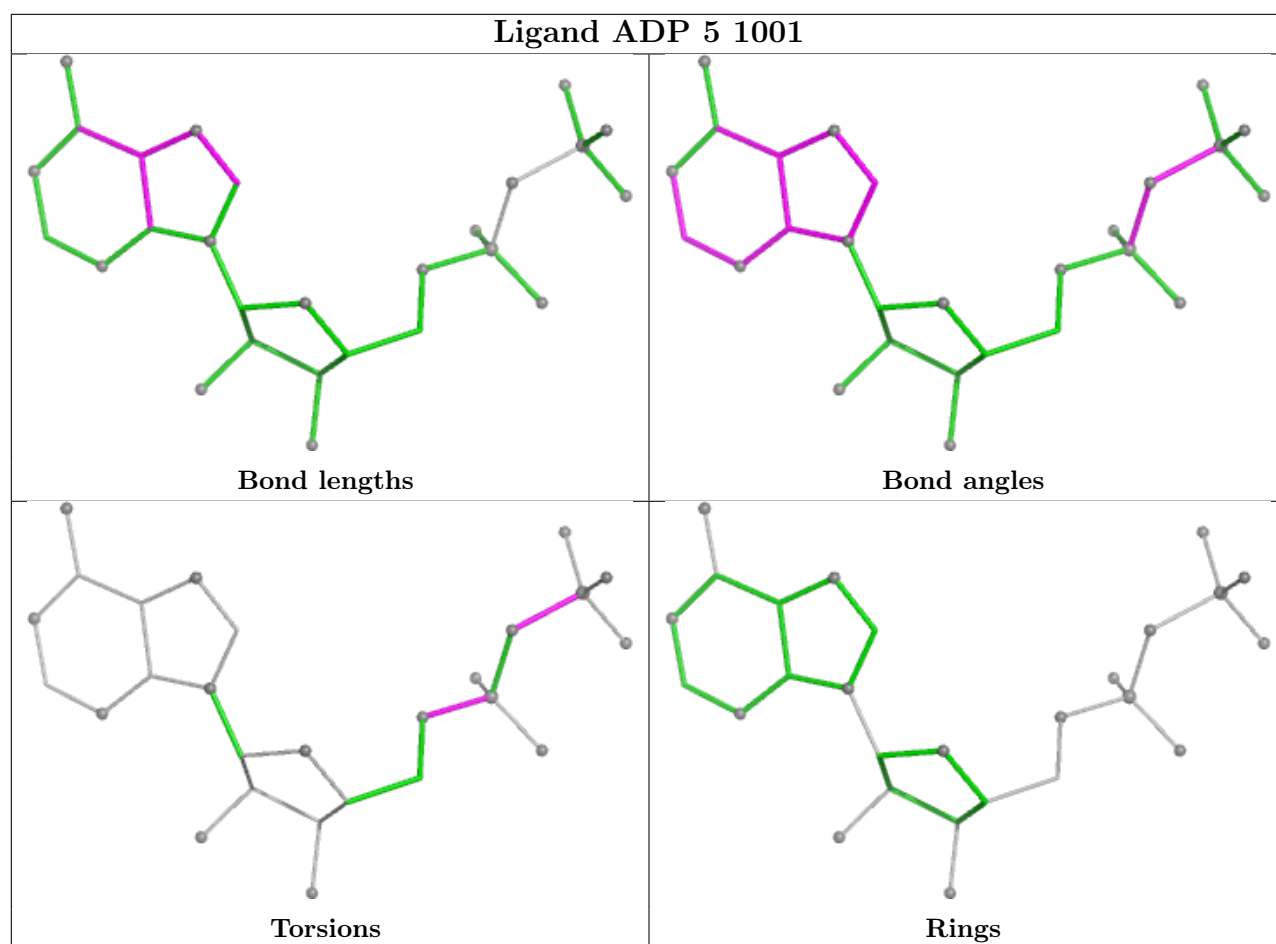












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

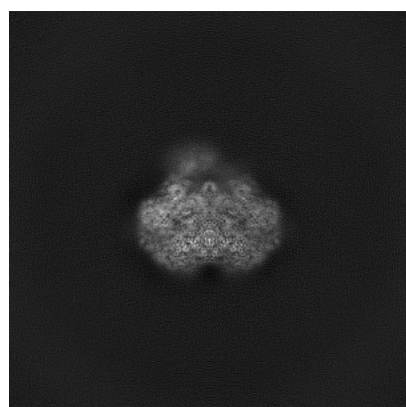
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55904. These allow visual inspection of the internal detail of the map and identification of artifacts.

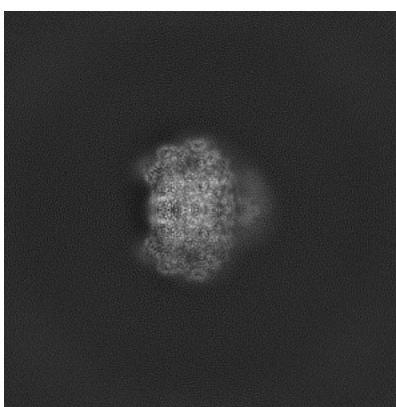
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

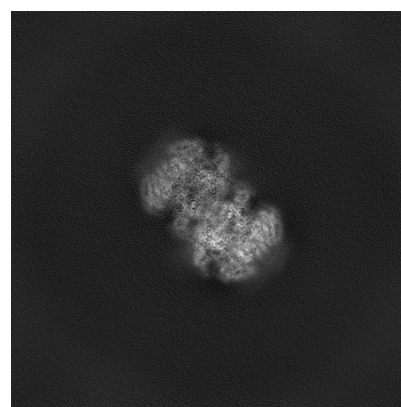
6.1.1 Primary map



X



Y

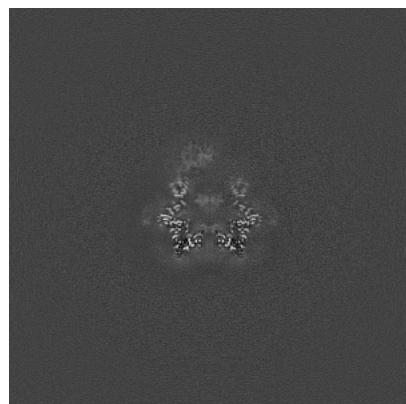


Z

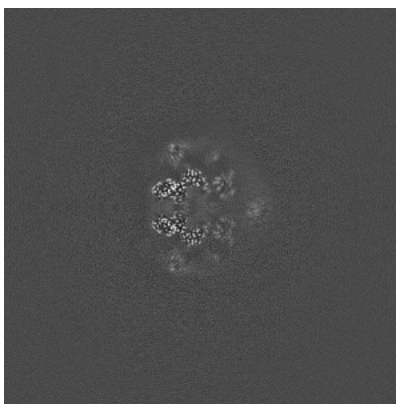
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

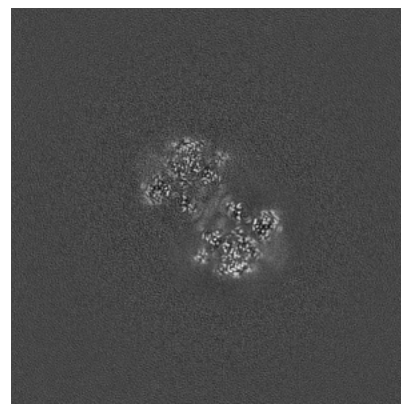
6.2.1 Primary map



X Index: 188



Y Index: 188

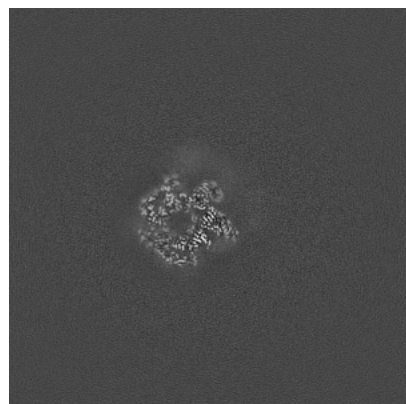


Z Index: 188

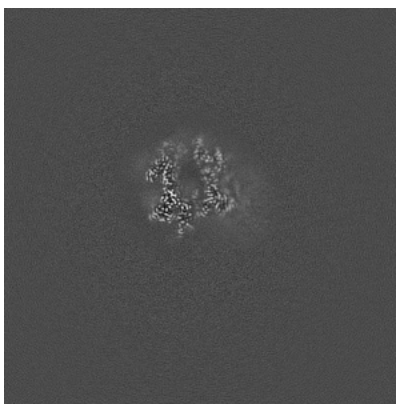
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

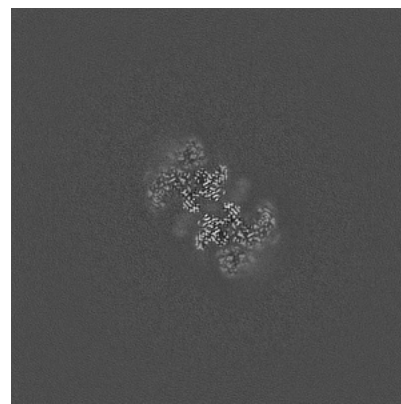
6.3.1 Primary map



X Index: 214



Y Index: 160

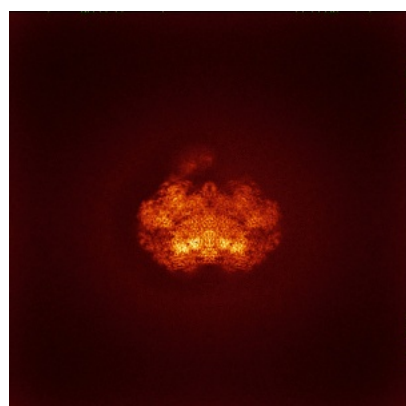


Z Index: 155

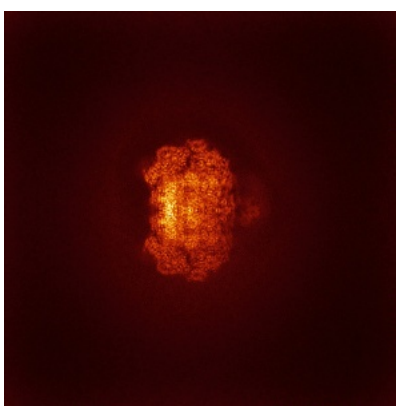
The images above show the largest variance slices of the map in three orthogonal directions.

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

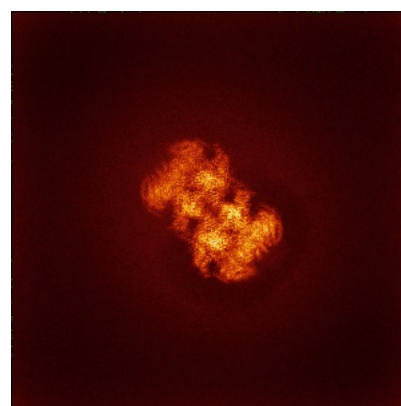
6.4.1 Primary map



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



X



Y



Z

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

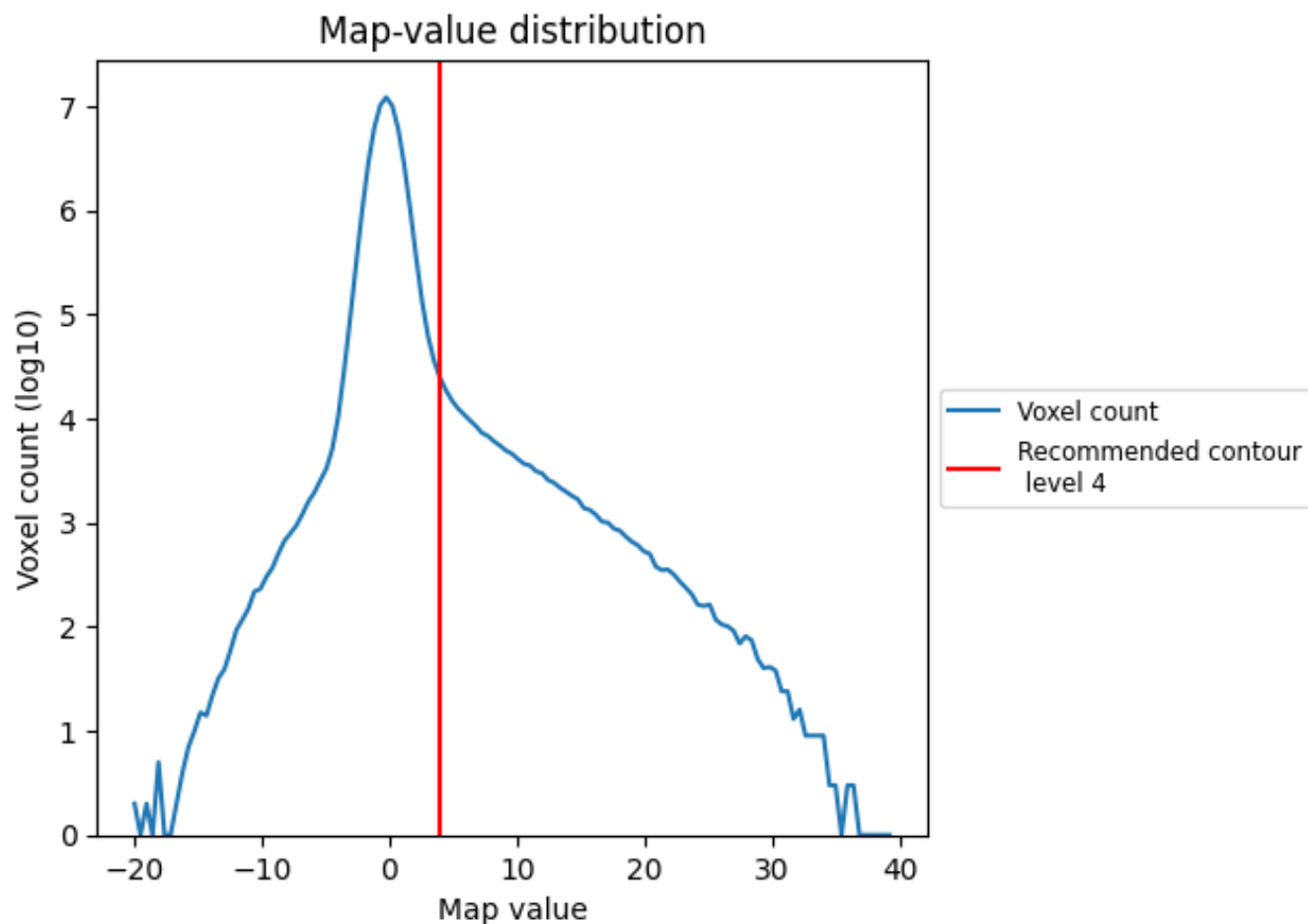
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

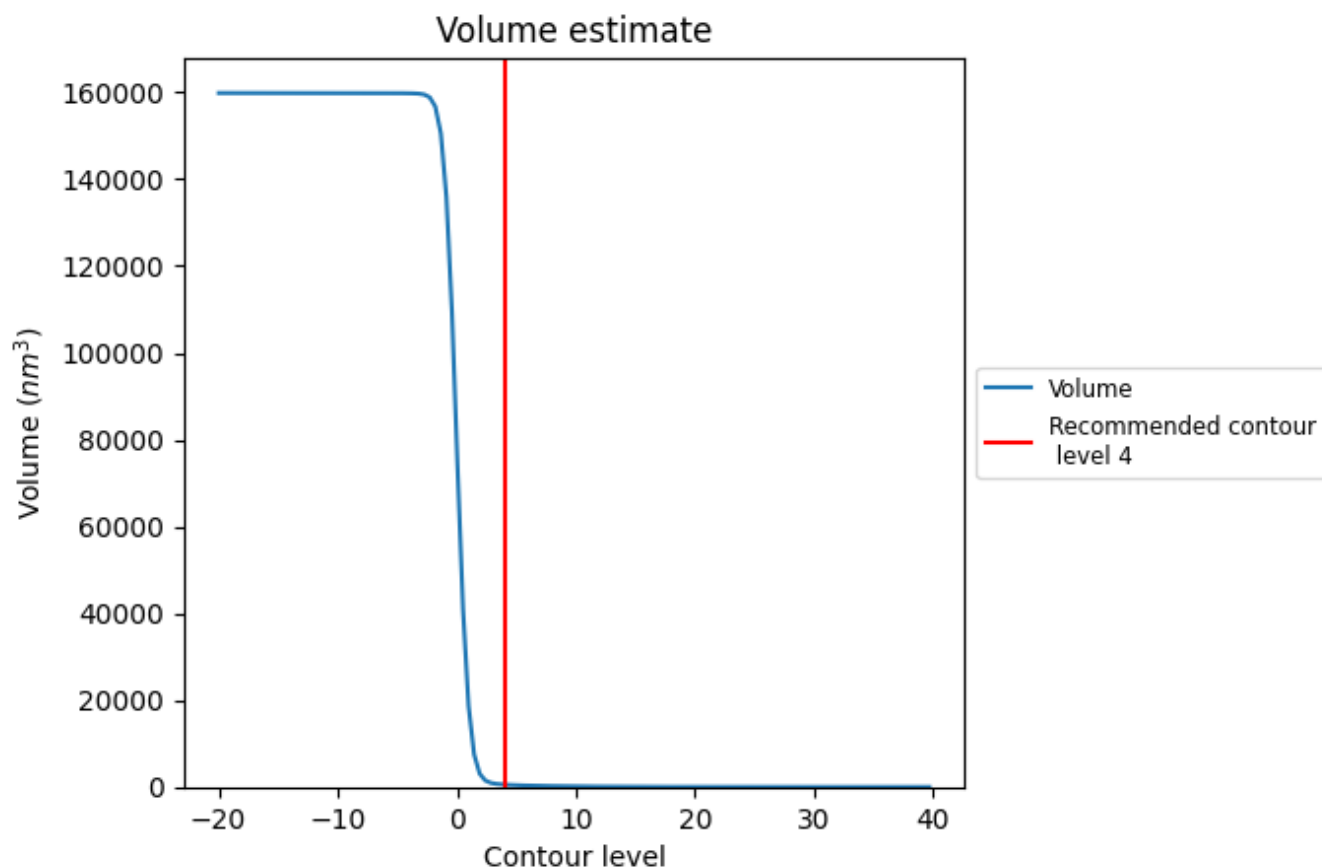
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

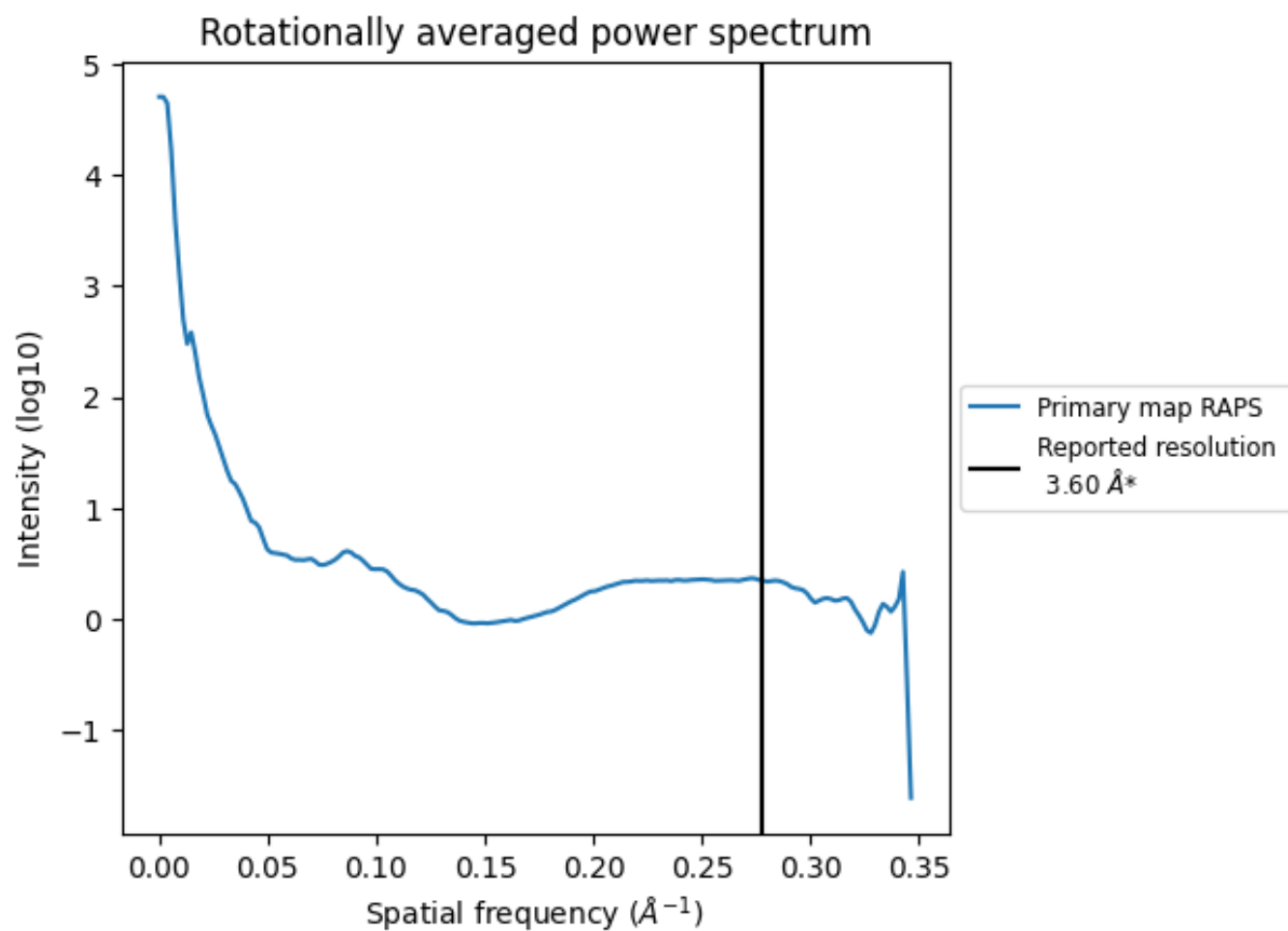
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 534 nm^3 ; this corresponds to an approximate mass of 482 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 0.278 Å⁻¹

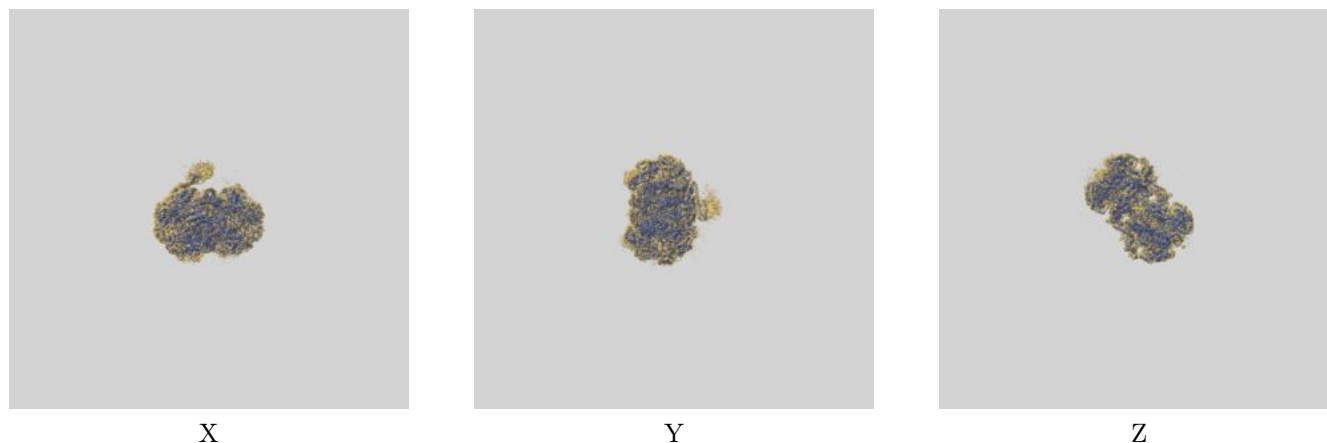
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

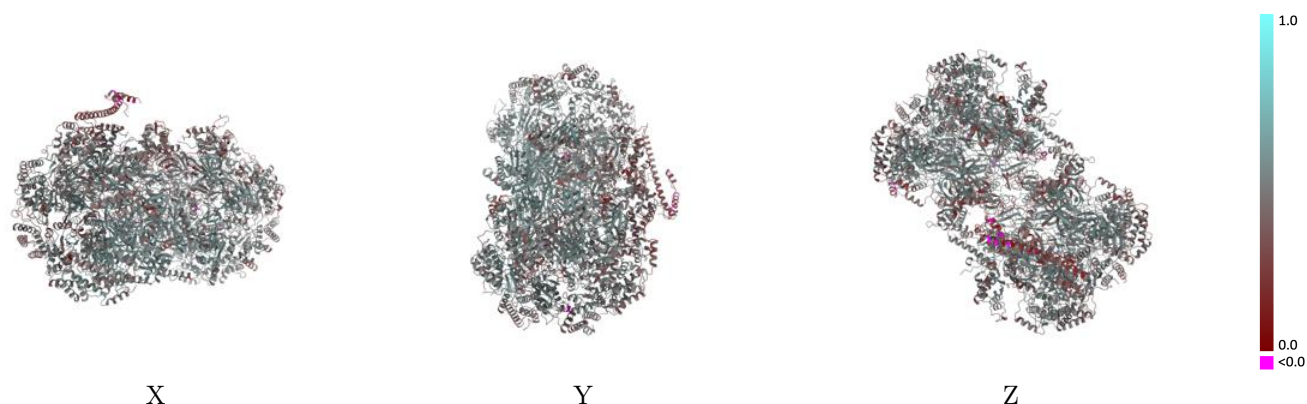
This section contains information regarding the fit between EMDB map EMD-55904 and PDB model 9TGM. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



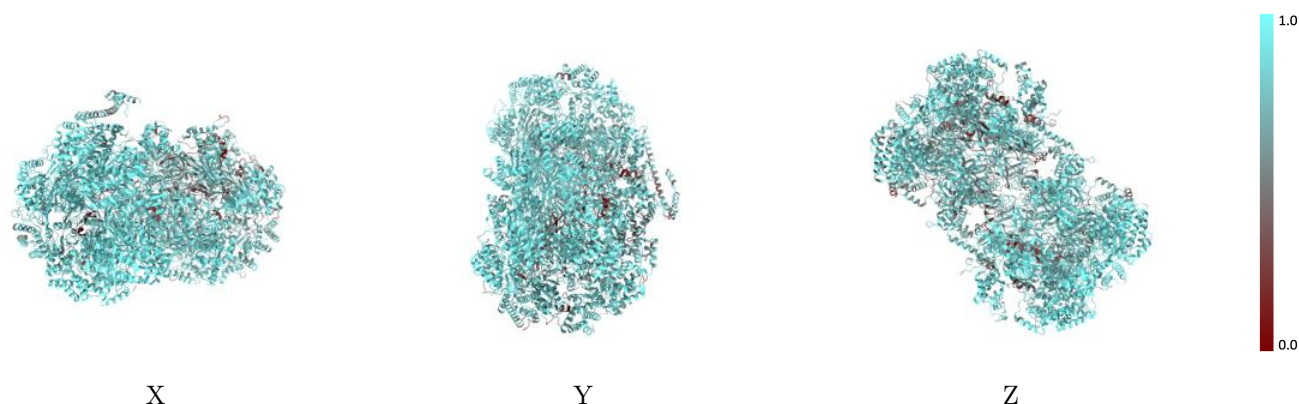
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



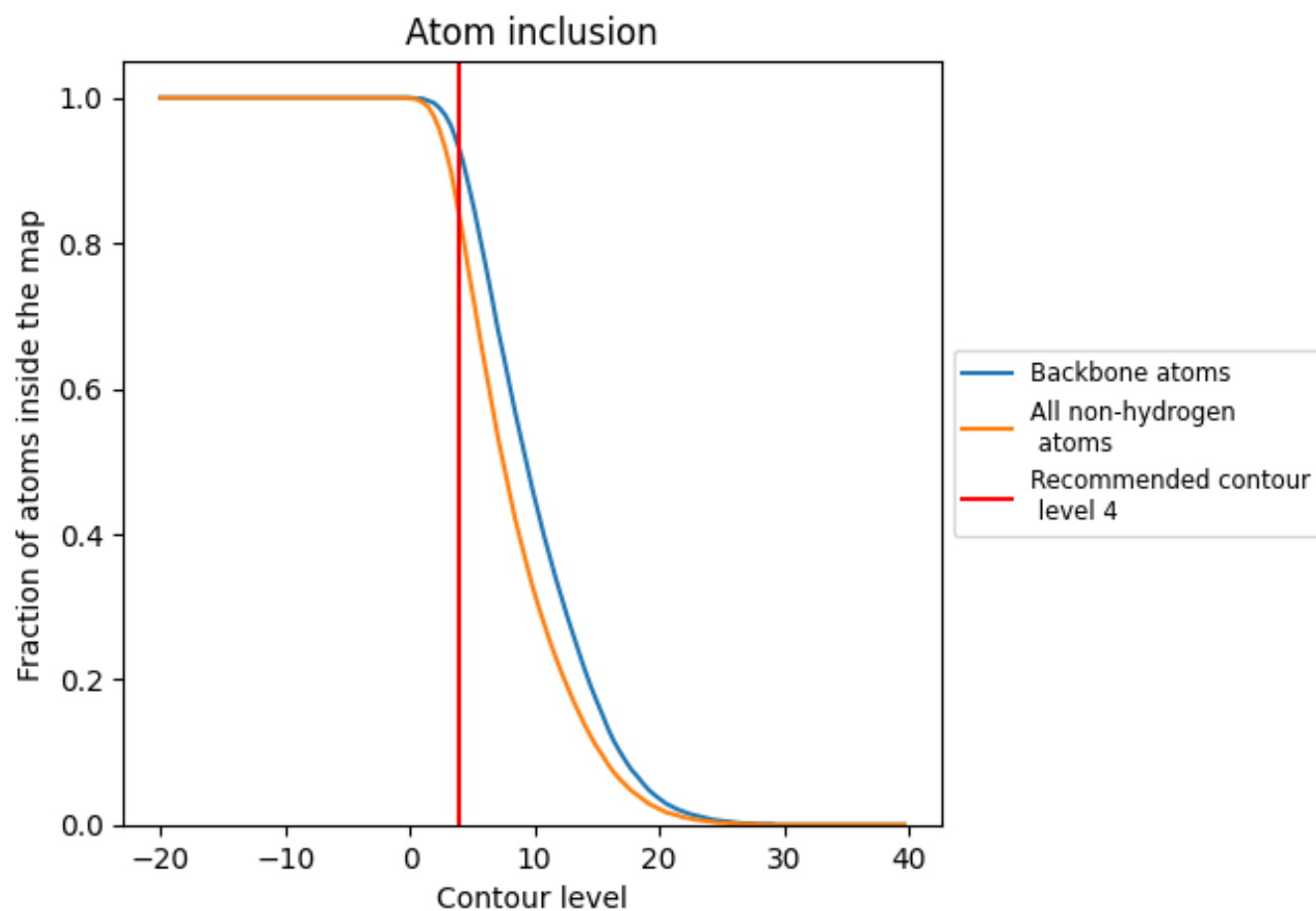
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	0.8360	0.4770
2	0.7510	0.4530
3	0.8820	0.5270
4	0.7980	0.4780
5	0.8090	0.4880
6	0.7280	0.4530
7	0.8330	0.4880
8	0.3550	0.3700
B	0.8660	0.4530
C	0.9260	0.5310
D	0.8870	0.4710
E	0.8700	0.4920
F	0.8570	0.4450
G	0.8780	0.4910
X	0.5560	0.3680
Y	0.6930	0.2350

