



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:10 PM UTC

PDB ID : 6WQH / pdb_00006wqh
EMDB ID : EMD-21870
Title : Molecular basis for the ATPase-powered substrate translocation by the Lon AAA+ protease
Authors : Zhang, K.; Li, S.; Hsiehb, K.; Sub, S.; Pintilie, G.; Chiu, W.; Chang, C.
Deposited on : 2020-04-28
Resolution : 3.60 Å(reported)
Based on initial model : 4YPL

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

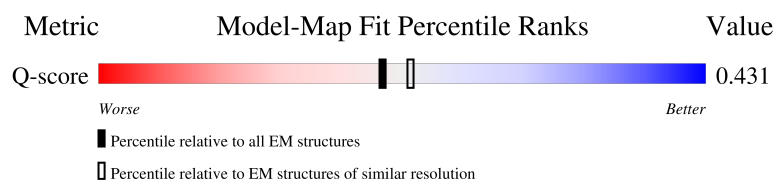
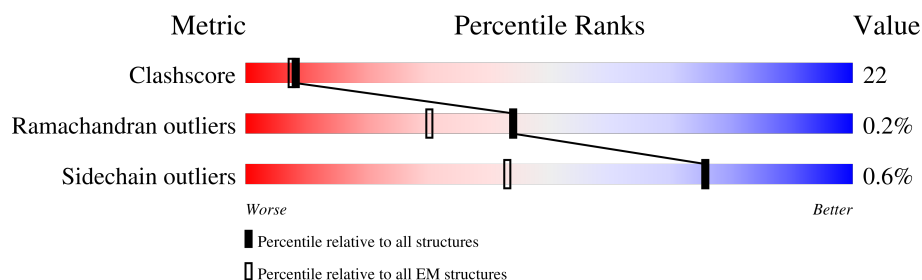
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	794	7% 42% 25% 32%
1	B	794	• 45% 22% • 32%
1	C	794	7% 42% 25% • 32%
1	D	794	14% 41% 26% • 32%

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Mol	Chain	Length	Quality of chain
1	E	794	
1	F	794	
2	S	11	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AGS	A	801	-	-	X	-
3	AGS	B	801	-	-	X	-
3	AGS	C	801	-	-	X	-
5	ADP	D	801	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25471 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 Lon protease.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	537	Total	C	N	O	S	0	0
			4179	2643	731	789	16		
1	B	537	Total	C	N	O	S	0	0
			4179	2643	731	789	16		
1	C	538	Total	C	N	O	S	0	0
			4188	2648	733	791	16		
1	F	537	Total	C	N	O	S	0	0
			4179	2643	731	789	16		
1	D	537	Total	C	N	O	S	0	0
			4179	2643	731	789	16		
1	E	537	Total	C	N	O	S	0	0
			4179	2643	731	789	16		

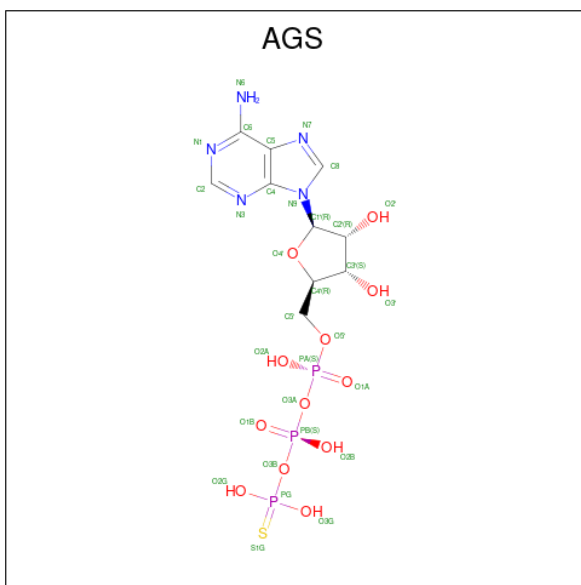
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	PHE	-	insertion	UNP A0A059VAZ3
B	92	PHE	-	insertion	UNP A0A059VAZ3
C	92	PHE	-	insertion	UNP A0A059VAZ3
F	92	PHE	-	insertion	UNP A0A059VAZ3
D	92	PHE	-	insertion	UNP A0A059VAZ3
E	92	PHE	-	insertion	UNP A0A059VAZ3

- Molecule 2 is a protein called Ig2 substrate.

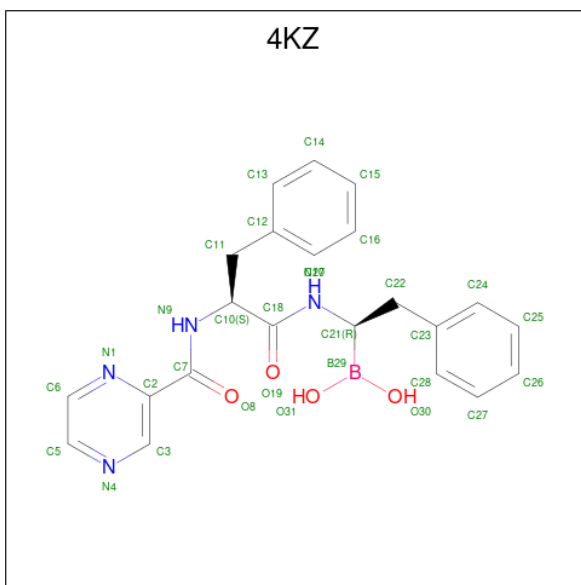
Mol	Chain	Residues	Atoms				AltConf	Trace
2	S	11	Total	C	N	O	0	0
			55	33	11	11		

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).



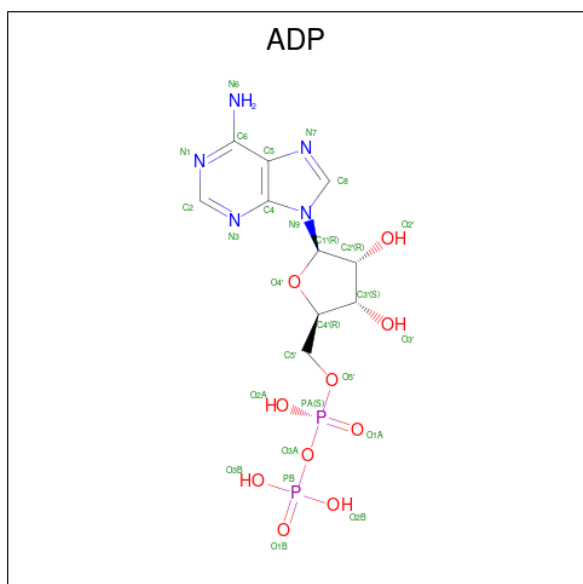
Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

- Molecule 4 is N-[(1R)-1-(dihydroxyboranyl)-2-phenylethyl]-Nalpha-(pyrazin-2-ylcarbon yl)-L-phenylalaninamide (CCD ID: 4KZ) (formula: $C_{22}H_{23}BN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	B	C	N	O	0
			31	1	22	4	4	
4	B	1	Total	B	C	N	O	0
			31	1	22	4	4	
4	C	1	Total	B	C	N	O	0
			31	1	22	4	4	
4	F	1	Total	B	C	N	O	0
			31	1	22	4	4	
4	D	1	Total	B	C	N	O	0
			31	1	22	4	4	
4	E	1	Total	B	C	N	O	0
			31	1	22	4	4	

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

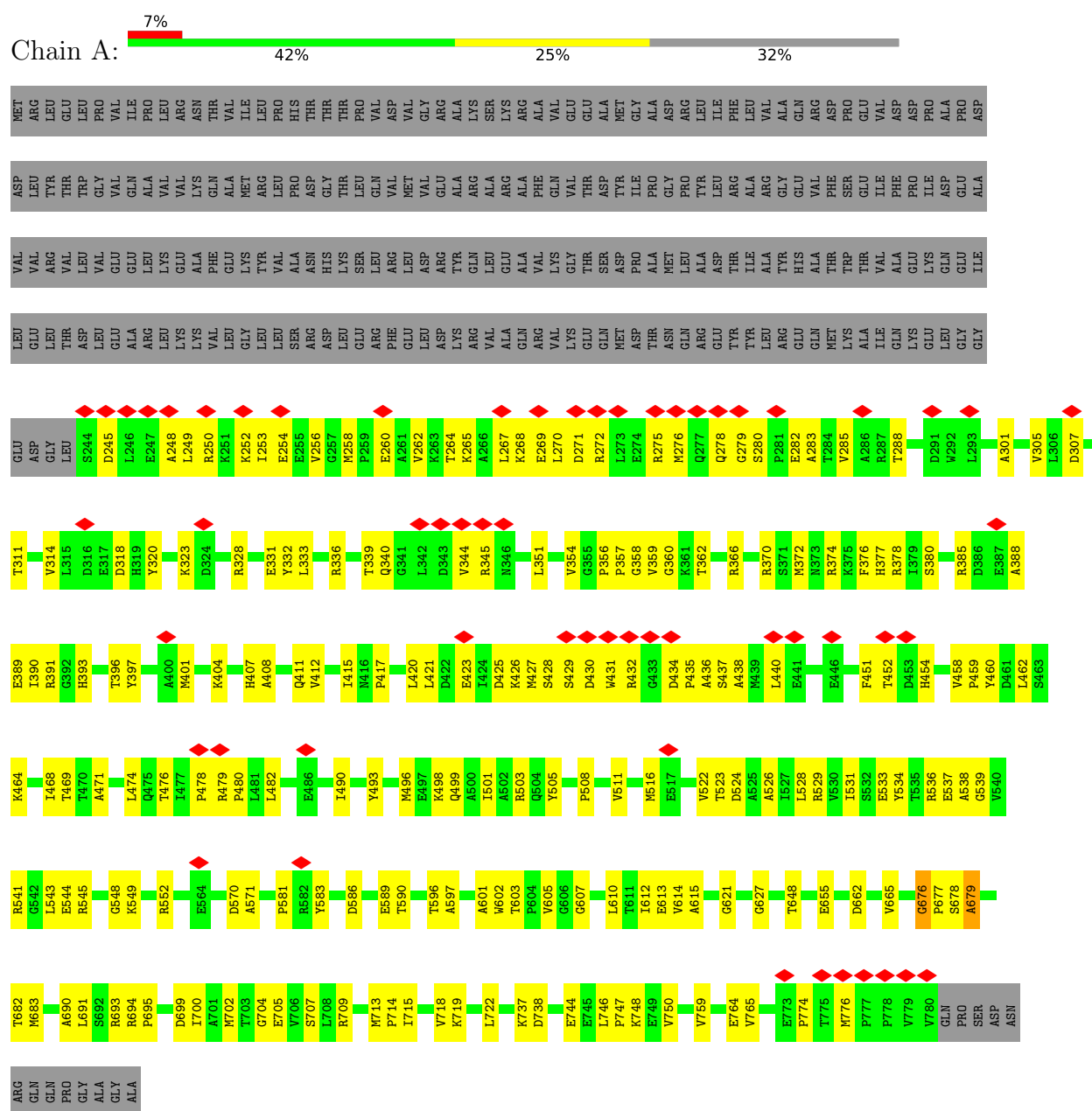


Mol	Chain	Residues	Atoms					AltConf
5	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

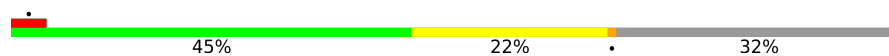
3 Residue-property plots

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

• Molecule 1: Lon protease

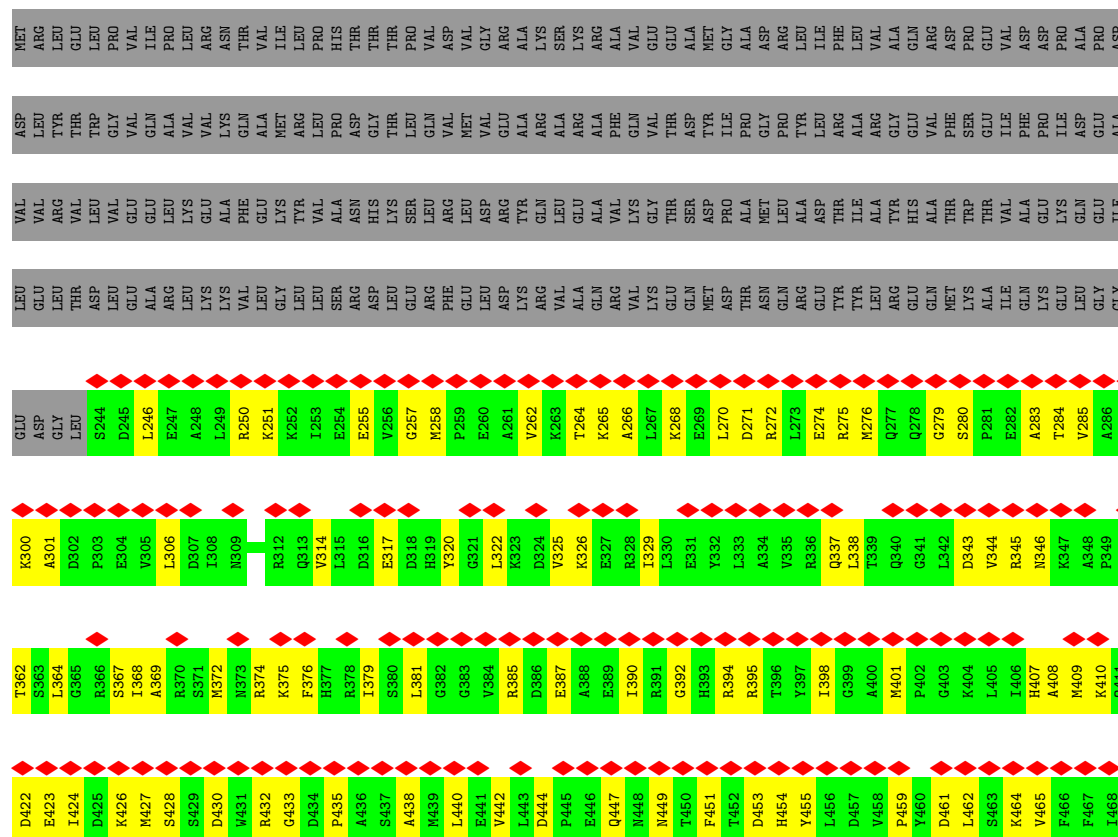


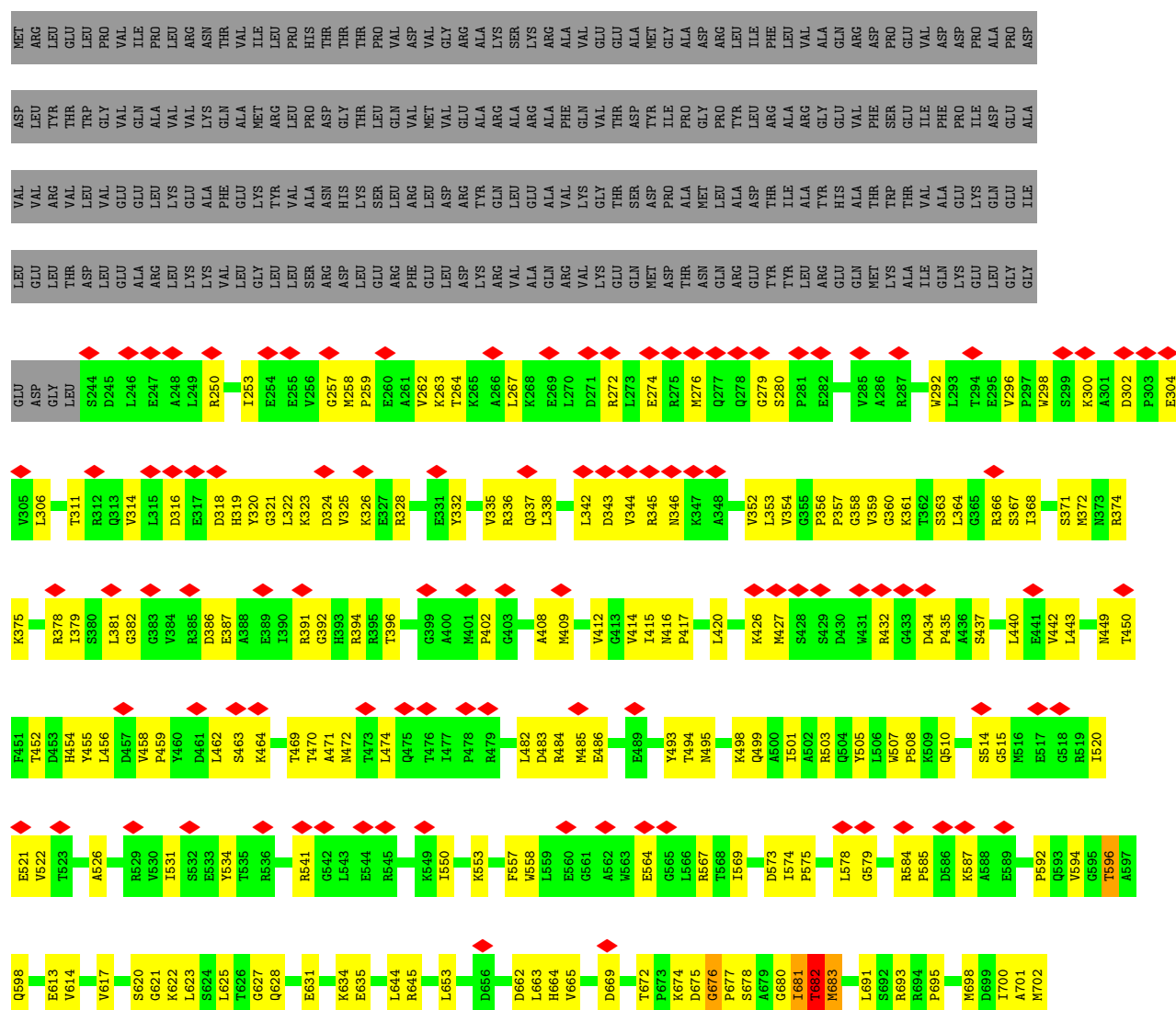
Chain B:

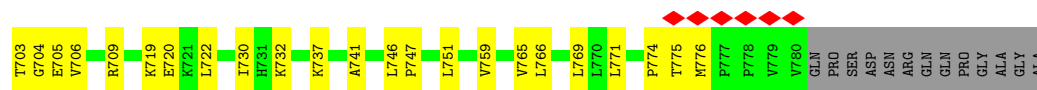
[illegible]

Chain C:

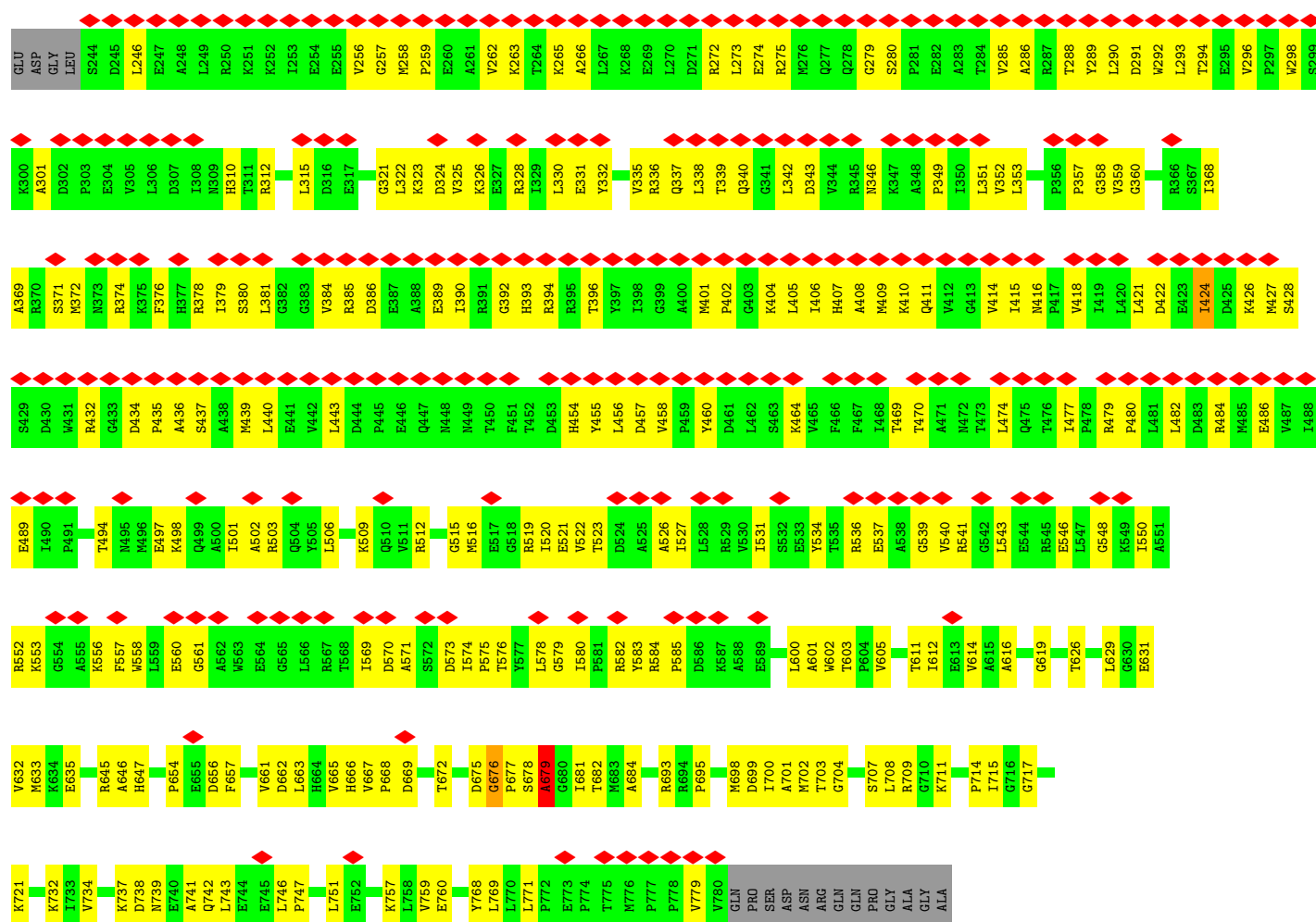
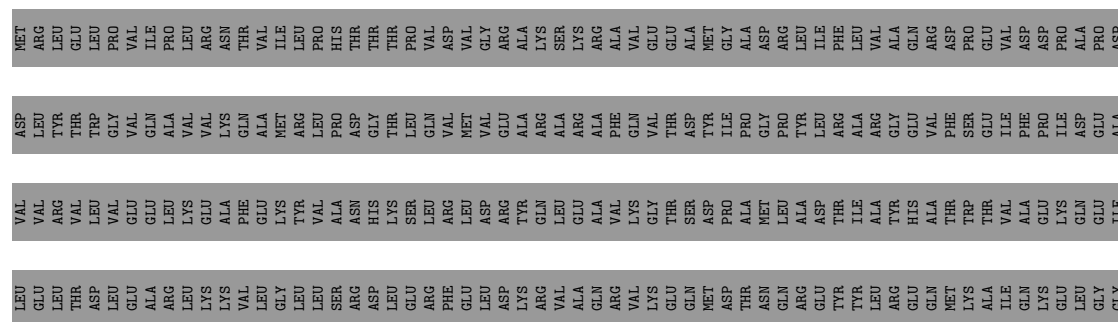
[illegible]



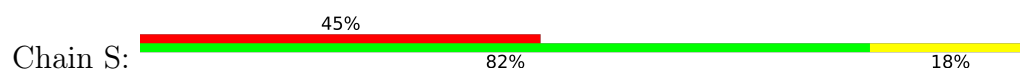


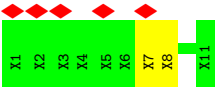


• Molecule 1: Lon protease



• Molecule 2: Ig2 substrate





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	23487	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	8.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.219	Depositor
Minimum map value	-0.637	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.076	Depositor
Recommended contour level	0.32	Depositor
Map size (Å)	218.4, 218.4, 218.4	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.65, 0.65, 0.65	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, 4KZ, AGS

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.75	2/4257 (0.0%)	0.58	5/5771 (0.1%)
1	B	0.51	1/4257 (0.0%)	0.55	7/5771 (0.1%)
1	C	0.45	1/4266 (0.0%)	0.55	6/5783 (0.1%)
1	D	0.79	1/4257 (0.0%)	0.53	5/5771 (0.1%)
1	E	0.38	1/4257 (0.0%)	0.43	1/5771 (0.0%)
1	F	0.80	1/4257 (0.0%)	0.45	5/5771 (0.1%)
All	All	0.64	7/25551 (0.0%)	0.52	29/34638 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	E	0	2
All	All	0	4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	676	GLY	C-N	49.06	1.77	1.33
1	D	676	GLY	C-N	48.40	1.71	1.33
1	A	676	GLY	C-N	40.19	1.65	1.33
1	B	676	GLY	C-N	-22.34	1.16	1.33
1	E	679	ALA	C-N	-19.71	1.04	1.33
1	A	679	ALA	C-N	-14.40	1.12	1.33
1	C	683	MET	CA-C	-5.88	1.45	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	676	GLY	O-C-N	-16.20	105.57	121.77
1	A	676	GLY	CA-C-N	13.97	137.20	121.00
1	A	676	GLY	C-N-CA	13.97	137.20	121.00
1	D	676	GLY	CA-C-N	13.40	136.21	120.94
1	D	676	GLY	C-N-CA	13.40	136.21	120.94
1	D	676	GLY	O-C-N	-10.96	110.81	121.77
1	B	435	PRO	N-CA-C	-10.51	98.93	113.53
1	C	675	ASP	N-CA-C	9.22	122.06	108.60
1	F	682	THR	CB-CA-C	-8.28	97.05	110.79
1	B	434	ASP	CA-C-N	7.44	127.31	119.05
1	B	434	ASP	C-N-CA	7.44	127.31	119.05
1	C	677	PRO	CA-C-N	7.16	132.94	121.98
1	C	677	PRO	C-N-CA	7.16	132.94	121.98
1	C	541	ARG	N-CA-C	-7.10	103.47	111.07
1	B	679	ALA	CA-C-N	-6.74	108.20	121.41
1	B	679	ALA	C-N-CA	-6.74	108.20	121.41
1	B	435	PRO	CA-C-N	-6.15	109.79	121.54
1	B	435	PRO	C-N-CA	-6.15	109.79	121.54
1	E	677	PRO	N-CA-C	6.02	121.44	114.03
1	D	681	ILE	CB-CA-C	-5.88	104.44	111.97
1	D	682	THR	N-CA-C	5.61	117.39	111.28
1	C	681	ILE	CB-CA-C	-5.22	105.09	112.14
1	C	678	SER	O-C-N	5.14	127.48	122.19
1	F	676	GLY	O-C-N	-5.13	116.64	121.77
1	F	676	GLY	CA-C-N	5.11	127.08	120.89
1	F	676	GLY	C-N-CA	5.11	127.08	120.89
1	F	681	ILE	CB-CA-C	-5.09	105.27	112.14
1	A	679	ALA	CA-C-N	5.04	131.30	121.41
1	A	679	ALA	C-N-CA	5.04	131.30	121.41

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	426	LYS	Mainchain
1	B	679	ALA	Mainchain
1	E	676	GLY	Mainchain
1	E	679	ALA	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4179	0	4259	182	0
1	B	4179	0	4261	197	0
1	C	4188	0	4267	250	0
1	D	4179	0	4261	205	0
1	E	4179	0	4260	196	0
1	F	4179	0	4261	162	0
2	S	55	0	15	8	0
3	A	31	0	12	13	0
3	B	31	0	12	10	0
3	C	31	0	12	15	0
4	A	31	0	0	7	0
4	B	31	0	0	5	0
4	C	31	0	0	8	0
4	D	31	0	0	7	0
4	E	31	0	0	2	0
4	F	31	0	0	3	0
5	D	27	0	12	14	0
5	F	27	0	12	5	0
All	All	25471	0	25644	1115	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 22.

All (1115) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:498:LYS:CA	1:C:501:ILE:HD11	1.38	1.54
1:D:676:GLY:C	1:D:677:PRO:N	1.71	1.45
1:F:676:GLY:C	1:F:677:PRO:N	1.77	1.43
1:C:378:ARG:NH1	1:C:422:ASP:HB2	1.31	1.39
1:C:667:VAL:CB	1:C:674:LYS:NZ	1.82	1.38
1:C:498:LYS:O	1:C:501:ILE:CD1	1.70	1.37
1:C:667:VAL:CG2	1:C:674:LYS:NZ	1.88	1.37
1:B:434:ASP:OD2	1:B:436:ALA:HB3	1.18	1.31
1:C:541:ARG:HH22	1:D:484:ARG:CZ	1.45	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:681:ILE:CD1	1:D:704:GLY:HA3	1.60	1.30
1:C:498:LYS:C	1:C:501:ILE:HD11	1.56	1.29
1:C:667:VAL:HG23	1:C:674:LYS:NZ	1.43	1.28
1:C:681:ILE:CD1	1:C:704:GLY:HA3	1.63	1.28
1:C:382:GLY:HA3	1:C:423:GLU:OE2	1.33	1.26
1:C:381:LEU:HB3	1:C:427:MET:CE	1.64	1.24
1:C:498:LYS:C	1:C:501:ILE:CD1	2.06	1.24
1:C:541:ARG:HH22	1:D:484:ARG:NH1	1.38	1.20
1:C:378:ARG:HH12	1:C:422:ASP:CB	1.54	1.20
1:B:434:ASP:OD2	1:B:436:ALA:CB	1.92	1.18
1:D:681:ILE:HD12	1:D:704:GLY:CA	1.76	1.14
1:C:541:ARG:NH1	3:C:801:AGS:S1G	2.20	1.14
1:C:667:VAL:HB	1:C:674:LYS:NZ	1.57	1.14
1:A:541:ARG:HD3	1:B:483:ASP:OD2	1.50	1.10
1:C:681:ILE:HD12	1:C:704:GLY:CA	1.79	1.09
1:B:385:ARG:HD2	1:B:430:ASP:HB2	1.15	1.09
1:C:498:LYS:O	1:C:501:ILE:HD12	1.49	1.08
1:C:498:LYS:HA	1:C:501:ILE:CD1	1.83	1.08
1:C:541:ARG:NH2	1:D:484:ARG:NH1	1.99	1.08
1:D:681:ILE:HD12	1:D:704:GLY:HA3	1.24	1.08
1:C:498:LYS:CA	1:C:501:ILE:CD1	2.33	1.06
1:B:435:PRO:O	1:B:437:SER:N	1.88	1.06
1:B:435:PRO:O	1:B:438:ALA:N	1.89	1.05
1:C:667:VAL:HG23	1:C:674:LYS:CE	1.85	1.05
1:A:432:ARG:HD3	2:S:7:UNK:CB	1.88	1.02
1:C:360:GLY:HA3	3:C:801:AGS:H8	1.38	1.01
1:D:681:ILE:HD11	1:D:704:GLY:HA3	1.39	1.01
1:C:681:ILE:HD12	1:C:704:GLY:HA3	1.01	1.00
1:B:610:LEU:HD12	4:B:802:4KZ:C26	1.90	1.00
1:C:378:ARG:NH1	1:C:422:ASP:CB	2.15	0.99
1:A:430:ASP:OD2	1:B:432:ARG:HA	1.63	0.98
1:D:681:ILE:CD1	1:D:704:GLY:CA	2.38	0.97
1:C:498:LYS:HA	1:C:501:ILE:HD11	0.97	0.97
1:B:385:ARG:CD	1:B:430:ASP:HB2	1.95	0.96
1:C:379:ILE:HG22	1:C:381:LEU:HG	1.45	0.96
1:A:432:ARG:HH21	2:S:7:UNK:CB	1.80	0.95
1:C:381:LEU:HB3	1:C:427:MET:HE3	1.46	0.94
1:C:498:LYS:O	1:C:501:ILE:HD13	1.67	0.94
1:C:541:ARG:NH2	1:D:484:ARG:CZ	2.27	0.93
1:C:360:GLY:CA	3:C:801:AGS:H8	1.98	0.93
1:C:378:ARG:HH12	1:C:422:ASP:CG	1.76	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:GLY:CA	1:C:423:GLU:OE2	2.16	0.93
1:B:435:PRO:O	1:B:436:ALA:C	2.06	0.92
1:A:541:ARG:CD	1:B:483:ASP:OD2	2.17	0.92
1:C:676:GLY:HA2	4:C:802:4KZ:C16	1.99	0.91
1:A:423:GLU:OE2	3:A:801:AGS:O3G	1.87	0.91
1:B:385:ARG:HD3	1:B:428:SER:OG	1.70	0.91
1:B:615:ALA:HB2	1:C:708:LEU:HD21	1.52	0.91
1:E:601:ALA:HB2	4:E:801:4KZ:C27	2.00	0.91
1:B:430:ASP:OD1	1:C:431:TRP:HA	1.70	0.90
1:A:676:GLY:CA	4:A:802:4KZ:C14	2.50	0.90
1:D:681:ILE:HD12	1:D:704:GLY:N	1.87	0.89
1:C:612:ILE:HD12	1:C:682:THR:HG21	1.51	0.89
1:C:502:ALA:HA	1:C:506:LEU:HB2	1.55	0.88
1:D:681:ILE:HG13	1:D:704:GLY:O	1.74	0.86
1:A:677:PRO:HB2	1:A:705:GLU:OE2	1.74	0.86
1:D:682:THR:HG23	1:D:702:MET:CG	2.06	0.86
1:D:682:THR:CG2	1:D:702:MET:HG2	2.06	0.86
1:A:677:PRO:O	1:A:705:GLU:OE2	1.94	0.85
1:A:430:ASP:OD2	1:B:432:ARG:CA	2.24	0.85
1:D:681:ILE:HD12	1:D:703:THR:C	2.02	0.84
1:B:345:ARG:HG3	1:B:464:LYS:HA	1.60	0.84
1:A:360:GLY:HA3	3:A:801:AGS:H8	1.60	0.84
1:B:610:LEU:CD1	4:B:802:4KZ:C26	2.56	0.84
1:A:676:GLY:HA2	4:A:802:4KZ:C14	2.09	0.83
1:B:444:ASP:HA	1:B:484:ARG:HD3	1.59	0.83
1:B:430:ASP:CG	1:C:431:TRP:HA	2.04	0.83
1:C:680:GLY:HA3	1:C:706:VAL:HG12	1.61	0.82
1:C:667:VAL:HG23	1:C:674:LYS:HE3	1.61	0.82
1:C:612:ILE:HD12	1:C:682:THR:CG2	2.09	0.82
1:C:678:SER:C	1:C:704:GLY:O	2.23	0.81
1:C:378:ARG:HH12	1:C:422:ASP:HB2	1.02	0.81
1:C:501:ILE:HG22	3:C:801:AGS:C2	2.11	0.80
1:A:615:ALA:HB2	1:B:708:LEU:HD21	1.64	0.79
1:A:429:SER:HA	1:A:434:ASP:CG	2.08	0.79
1:C:501:ILE:CG2	3:C:801:AGS:N1	2.46	0.79
1:D:320:TYR:O	5:D:801:ADP:N6	2.15	0.79
1:B:385:ARG:HD2	1:B:430:ASP:CB	2.06	0.79
1:F:597:ALA:CB	1:F:682:THR:HG22	2.13	0.79
1:F:610:LEU:HD12	4:F:802:4KZ:C26	2.13	0.79
1:D:325:VAL:HA	1:D:328:ARG:HH21	1.48	0.79
1:C:715:ILE:H	1:C:739:ASN:HD21	1.32	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:600:LEU:HD11	1:E:701:ALA:HB1	1.66	0.78
1:A:498:LYS:HA	1:A:501:ILE:HG22	1.66	0.77
1:C:318:ASP:OD2	1:C:370:ARG:NH2	2.16	0.77
1:F:597:ALA:HB3	1:F:682:THR:HG22	1.65	0.77
1:A:432:ARG:CD	2:S:7:UNK:CB	2.61	0.77
1:E:582:ARG:HG3	1:E:583:TYR:HD1	1.50	0.77
1:C:667:VAL:HG23	1:C:674:LYS:HZ2	1.49	0.77
1:C:676:GLY:CA	4:C:802:4KZ:C16	2.64	0.76
1:E:626:THR:HG1	1:E:666:HIS:HD1	1.30	0.76
1:B:359:VAL:O	3:B:801:AGS:O2B	2.04	0.76
1:C:381:LEU:CB	1:C:427:MET:CE	2.58	0.76
1:B:434:ASP:CG	1:B:436:ALA:HB3	2.10	0.75
3:A:801:AGS:O3B	1:B:484:ARG:NH2	2.20	0.75
1:D:682:THR:CG2	1:D:702:MET:CG	2.63	0.75
1:B:435:PRO:C	1:B:437:SER:N	2.45	0.75
1:E:272:ARG:O	1:E:275:ARG:NH1	2.18	0.75
1:C:360:GLY:N	3:C:801:AGS:H8	2.02	0.75
1:F:681:ILE:HG23	1:F:682:THR:N	1.99	0.75
1:E:293:LEU:HD11	1:E:456:LEU:HD11	1.67	0.75
1:C:683:MET:O	1:C:684:ALA:C	2.28	0.74
1:E:541:ARG:O	1:E:541:ARG:NH1	2.19	0.74
1:D:357:PRO:HG3	1:D:472:ASN:HD22	1.53	0.74
1:E:421:LEU:HD22	1:E:469:THR:HG23	1.69	0.74
1:C:678:SER:HB3	1:C:715:ILE:HD12	1.69	0.74
1:C:399:GLY:HA3	1:D:396:THR:HA	1.69	0.74
1:B:534:TYR:HE1	1:B:581:PRO:HA	1.52	0.73
1:F:440:LEU:HD21	1:F:480:PRO:HB2	1.69	0.73
1:E:480:PRO:O	1:E:484:ARG:NH2	2.22	0.73
1:C:498:LYS:C	1:C:501:ILE:HD12	1.97	0.73
1:B:667:VAL:O	1:B:674:LYS:NZ	2.20	0.73
1:A:759:VAL:HG21	1:A:765:VAL:HG23	1.70	0.73
1:A:385:ARG:HH22	1:B:434:ASP:N	1.85	0.72
1:B:679:ALA:O	1:B:682:THR:OG1	2.07	0.72
1:E:619:GLY:HA3	1:E:662:ASP:HB2	1.71	0.72
1:C:667:VAL:CG2	1:C:674:LYS:CE	2.58	0.72
1:C:541:ARG:NH2	1:D:484:ARG:HG2	2.04	0.72
1:E:612:ILE:HG12	1:E:667:VAL:HG12	1.71	0.72
1:B:432:ARG:HD2	1:B:432:ARG:C	2.14	0.72
1:C:381:LEU:HB3	1:C:427:MET:HE2	1.67	0.72
1:F:493:TYR:OH	5:F:801:ADP:N7	2.23	0.72
1:A:496:MET:SD	1:A:499:GLN:NE2	2.63	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:VAL:HG23	1:A:764:GLU:HB2	1.72	0.71
1:C:679:ALA:HB2	4:C:802:4KZ:C24	2.20	0.71
1:F:409:MET:HE1	1:F:415:ILE:HA	1.72	0.71
1:D:375:LYS:HB2	1:D:417:PRO:HB3	1.72	0.71
1:A:311:THR:HA	1:A:314:VAL:HG12	1.71	0.71
1:D:311:THR:HA	1:D:314:VAL:HG12	1.72	0.71
1:D:558:TRP:HD1	1:E:338:LEU:HD11	1.55	0.71
1:C:381:LEU:HD13	1:C:427:MET:HE1	1.72	0.71
1:B:391:ARG:NH2	1:B:441:GLU:OE2	2.24	0.71
1:F:264:THR:O	1:F:268:LYS:NZ	2.24	0.70
1:B:431:TRP:CE3	1:B:431:TRP:HA	2.26	0.70
1:A:385:ARG:HA	1:A:435:PRO:HG3	1.74	0.70
1:E:394:ARG:NH1	1:E:457:ASP:OD1	2.25	0.70
1:F:275:ARG:HG3	1:F:283:ALA:HB2	1.72	0.70
1:B:434:ASP:OD2	1:B:436:ALA:CA	2.40	0.70
1:E:374:ARG:HH22	1:E:418:VAL:HB	1.57	0.70
1:D:316:ASP:O	1:D:505:TYR:OH	2.09	0.70
1:C:381:LEU:HB3	1:C:427:MET:HE1	1.68	0.69
1:D:306:LEU:O	1:D:337:GLN:NE2	2.25	0.69
1:C:501:ILE:HD12	1:C:501:ILE:H	1.57	0.69
1:C:379:ILE:CG2	1:C:381:LEU:HG	2.22	0.69
1:F:292:TRP:O	1:F:296:VAL:N	2.26	0.69
1:D:358:GLY:O	5:D:801:ADP:H5'2	1.92	0.69
1:E:394:ARG:HG3	1:E:396:THR:HG23	1.73	0.69
1:D:368:ILE:O	1:D:371:SER:OG	2.08	0.69
1:D:250:ARG:NH2	1:D:274:GLU:OE2	2.26	0.69
1:D:304:GLU:OE1	1:D:374:ARG:NH2	2.25	0.69
1:D:498:LYS:HA	1:D:501:ILE:HG22	1.73	0.69
1:E:574:ILE:HG23	1:E:578:LEU:HD13	1.74	0.69
1:C:501:ILE:HD12	1:C:501:ILE:N	2.07	0.69
1:A:262:VAL:HG13	1:A:458:VAL:HG11	1.75	0.69
1:A:528:LEU:HA	1:A:531:ILE:HD12	1.74	0.69
1:C:545:ARG:NH1	1:D:485:MET:O	2.26	0.68
1:A:678:SER:HB2	1:A:715:ILE:HG12	1.74	0.68
1:F:672:THR:OG1	1:F:674:LYS:NZ	2.26	0.68
1:E:286:ALA:HA	1:E:289:TYR:HB3	1.75	0.68
1:C:501:ILE:HG22	3:C:801:AGS:N1	2.07	0.68
1:C:681:ILE:HD11	1:C:712:VAL:HG13	1.75	0.68
1:F:498:LYS:NZ	1:F:539:GLY:O	2.27	0.68
1:D:719:LYS:HD2	1:D:746:LEU:HD23	1.76	0.67
1:E:682:THR:HA	1:E:702:MET:HE3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:LYS:NZ	1:C:472:ASN:OD1	2.23	0.67
1:C:422:ASP:O	1:C:423:GLU:HG2	1.94	0.67
1:A:429:SER:HA	1:A:434:ASP:OD1	1.94	0.67
1:A:430:ASP:OD2	1:B:432:ARG:HB2	1.94	0.67
1:D:503:ARG:NH2	1:D:522:VAL:O	2.27	0.67
1:B:430:ASP:OD2	1:C:433:GLY:N	2.28	0.67
1:F:276:MET:HE3	1:F:284:THR:HG22	1.77	0.67
1:F:362:THR:OG1	5:F:801:ADP:O1A	2.12	0.67
1:E:374:ARG:HH12	1:E:418:VAL:H	1.43	0.67
1:A:430:ASP:OD2	1:B:432:ARG:CB	2.43	0.67
1:B:654:PRO:HB2	1:B:657:PHE:HB3	1.77	0.67
1:D:526:ALA:HB1	1:D:574:ILE:HD11	1.76	0.67
1:B:366:ARG:HH12	1:C:447:GLN:HE22	1.39	0.67
1:F:272:ARG:HE	1:F:275:ARG:HH22	1.40	0.67
1:A:250:ARG:NH2	1:A:271:ASP:OD1	2.25	0.66
1:E:385:ARG:NH2	1:E:426:LYS:O	2.28	0.66
1:C:589:GLU:OE1	1:C:590:THR:N	2.28	0.66
1:C:703:THR:OG1	1:C:721:LYS:NZ	2.29	0.66
1:A:432:ARG:CG	2:S:7:UNK:CB	2.74	0.66
1:B:502:ALA:HA	1:B:506:LEU:HB2	1.76	0.66
1:C:360:GLY:HA3	3:C:801:AGS:C8	2.20	0.66
1:B:385:ARG:HD3	1:B:428:SER:HG	1.57	0.66
1:D:665:VAL:HG11	1:D:683:MET:HE3	1.78	0.66
1:C:440:LEU:HB3	1:C:484:ARG:HH21	1.61	0.66
1:D:682:THR:HG23	1:D:702:MET:HG3	1.78	0.66
1:E:288:THR:O	1:E:455:TYR:OH	2.13	0.66
1:A:676:GLY:HA3	4:A:802:4KZ:C14	2.26	0.66
1:B:541:ARG:NH2	3:B:801:AGS:S1G	2.69	0.66
1:A:545:ARG:NH1	1:B:347:LYS:NZ	2.43	0.65
1:A:678:SER:CB	1:A:715:ILE:HG12	2.26	0.65
1:D:700:ILE:HG13	1:D:732:LYS:HB2	1.77	0.65
1:D:596:THR:HG21	1:E:709:ARG:HD3	1.78	0.65
1:E:258:MET:HB2	1:E:263:LYS:HE3	1.78	0.65
1:F:250:ARG:NH1	1:F:270:LEU:O	2.27	0.65
1:B:434:ASP:OD2	1:B:436:ALA:N	2.29	0.65
1:C:390:ILE:HG22	1:C:391:ARG:HG3	1.79	0.65
1:A:388:ALA:O	1:B:394:ARG:NH2	2.22	0.65
1:C:391:ARG:NH1	1:C:441:GLU:OE1	2.29	0.65
1:D:366:ARG:HD2	1:D:378:ARG:HH21	1.60	0.64
1:E:516:MET:SD	1:E:519:ARG:NH2	2.71	0.64
1:C:678:SER:CB	1:C:715:ILE:HD12	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:250:ARG:NH2	1:F:274:GLU:OE2	2.29	0.64
1:F:681:ILE:HD11	1:F:765:VAL:HG21	1.79	0.64
1:C:410:LYS:O	1:C:410:LYS:NZ	2.24	0.64
1:E:393:HIS:ND1	1:E:401:MET:O	2.29	0.64
1:C:385:ARG:HD3	1:C:428:SER:HB3	1.78	0.64
1:F:264:THR:OG1	1:F:268:LYS:NZ	2.31	0.64
1:A:431:TRP:HZ3	2:S:7:UNK:CB	2.10	0.64
1:C:320:TYR:O	3:C:801:AGS:N6	2.30	0.64
1:A:543:LEU:C	1:A:543:LEU:HD23	2.23	0.64
1:B:390:ILE:HD12	1:B:390:ILE:H	1.63	0.64
1:E:626:THR:OG1	1:E:666:HIS:ND1	2.24	0.64
1:D:336:ARG:HG2	1:D:344:VAL:HA	1.80	0.64
1:D:617:VAL:HG21	1:E:645:ARG:HB3	1.79	0.64
1:E:360:GLY:H	1:E:540:VAL:HG22	1.60	0.64
1:D:676:GLY:C	1:D:677:PRO:CD	2.69	0.64
1:E:557:PHE:O	1:E:561:GLY:N	2.25	0.64
1:E:616:ALA:HB3	1:E:693:ARG:HH12	1.62	0.64
1:C:304:GLU:OE1	1:C:345:ARG:NH2	2.31	0.63
1:E:374:ARG:NH1	1:E:416:ASN:O	2.31	0.63
1:E:404:LYS:HA	1:E:407:HIS:HB2	1.80	0.63
1:C:448:ASN:ND2	1:C:462:LEU:O	2.31	0.63
1:F:250:ARG:NH2	1:F:271:ASP:OD1	2.31	0.63
1:F:372:MET:SD	1:F:374:ARG:NH1	2.72	0.63
1:B:435:PRO:HG2	1:B:436:ALA:N	2.13	0.63
1:D:321:GLY:O	1:D:326:LYS:NZ	2.31	0.63
1:E:534:TYR:O	1:E:582:ARG:NH2	2.32	0.63
1:A:275:ARG:NH2	1:A:282:GLU:OE2	2.32	0.63
1:B:453:ASP:OD1	1:B:454:HIS:N	2.31	0.63
1:B:529:ARG:NH1	1:B:533:GLU:OE1	2.32	0.63
1:F:681:ILE:CG2	1:F:704:GLY:N	2.62	0.63
1:B:345:ARG:HH22	1:B:349:PRO:C	2.06	0.63
1:A:305:VAL:HG22	1:A:307:ASP:H	1.62	0.63
1:A:339:THR:O	1:A:340:GLN:NE2	2.25	0.63
1:B:372:MET:SD	1:B:374:ARG:NH1	2.71	0.63
1:D:360:GLY:HA2	5:D:801:ADP:H5'1	1.79	0.63
1:A:389:GLU:O	1:A:404:LYS:N	2.32	0.63
1:E:390:ILE:HG23	1:E:405:LEU:HB2	1.80	0.63
1:A:360:GLY:CA	3:A:801:AGS:H8	2.29	0.63
1:C:580:ILE:HD11	1:D:741:ALA:HB1	1.81	0.63
1:F:681:ILE:HG22	1:F:704:GLY:H	1.64	0.63
1:C:681:ILE:HD11	1:C:704:GLY:HA3	1.72	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:675:ASP:OD1	1:F:676:GLY:N	2.32	0.62
1:B:589:GLU:OE1	1:B:590:THR:N	2.32	0.62
1:D:693:ARG:HB2	1:D:774:PRO:HB3	1.81	0.62
1:E:353:LEU:HB3	1:E:470:THR:HG23	1.81	0.62
1:E:427:MET:HE3	1:E:435:PRO:HG2	1.81	0.62
1:A:332:TYR:OH	1:A:345:ARG:NH1	2.32	0.62
1:D:379:ILE:HD11	1:D:408:ALA:HB2	1.82	0.62
1:C:501:ILE:CG2	3:C:801:AGS:C2	2.77	0.62
1:D:682:THR:HG23	1:D:702:MET:HG2	1.69	0.62
1:E:494:THR:H	1:E:497:GLU:HB2	1.64	0.62
1:F:681:ILE:HG21	1:F:704:GLY:N	2.13	0.62
1:A:378:ARG:NH1	1:A:380:SER:OG	2.33	0.62
1:A:412:VAL:HG21	1:A:417:PRO:HB3	1.80	0.62
1:D:361:LYS:HE2	5:D:801:ADP:O1B	1.99	0.62
1:D:392:GLY:HA3	1:D:402:PRO:HA	1.81	0.62
1:D:575:PRO:O	1:D:579:GLY:N	2.32	0.62
1:A:354:VAL:O	1:A:490:ILE:N	2.31	0.62
1:B:529:ARG:HH21	1:B:575:PRO:HG3	1.64	0.62
1:A:545:ARG:NH1	1:B:347:LYS:HZ3	1.96	0.62
1:B:412:VAL:HG21	1:B:417:PRO:HB3	1.81	0.62
1:B:429:SER:HA	1:B:434:ASP:HB3	1.82	0.62
1:C:402:PRO:O	1:D:394:ARG:NH2	2.32	0.62
1:A:709:ARG:NE	1:F:613:GLU:OE1	2.32	0.61
1:C:386:ASP:OD1	1:C:386:ASP:N	2.32	0.61
1:A:451:PHE:O	1:A:460:TYR:N	2.32	0.61
1:A:678:SER:O	1:A:704:GLY:O	2.19	0.61
1:B:316:ASP:O	1:B:505:TYR:OH	2.19	0.61
1:C:321:GLY:O	1:C:326:LYS:NZ	2.31	0.61
1:A:276:MET:HG3	1:A:283:ALA:HB2	1.81	0.61
1:A:714:PRO:HB3	1:A:738:ASP:HB3	1.82	0.61
1:C:297:PRO:O	1:C:460:TYR:OH	2.17	0.61
1:C:377:HIS:CE1	1:C:408:ALA:HA	2.36	0.61
3:C:801:AGS:O1B	3:C:801:AGS:O2A	2.17	0.61
1:E:402:PRO:HB3	1:E:455:TYR:CG	2.35	0.61
1:C:516:MET:SD	1:C:519:ARG:NH2	2.72	0.61
1:F:381:LEU:HD13	1:F:424:ILE:HD13	1.82	0.61
1:F:473:THR:HG22	1:F:475:GLN:H	1.66	0.61
1:E:328:ARG:CZ	1:E:489:GLU:H	2.14	0.61
1:A:705:GLU:HB3	1:A:713:MET:HB2	1.83	0.61
1:E:322:LEU:HD23	1:E:325:VAL:HG11	1.83	0.61
1:E:336:ARG:O	1:E:340:GLN:NE2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:ILE:HD12	1:B:404:LYS:HG2	1.83	0.60
1:F:589:GLU:O	1:F:590:THR:N	2.34	0.60
1:F:375:LYS:HD2	1:F:412:VAL:HG13	1.83	0.60
1:D:314:VAL:HG11	1:D:371:SER:HA	1.83	0.60
1:A:501:ILE:HD11	3:A:801:AGS:C6	2.32	0.60
1:A:718:VAL:HG13	1:A:722:LEU:HD13	1.82	0.60
1:D:498:LYS:HB3	1:D:531:ILE:HD13	1.82	0.60
1:A:345:ARG:HG3	1:A:464:LYS:HA	1.84	0.60
1:F:682:THR:HA	1:F:702:MET:SD	2.42	0.60
1:E:322:LEU:HB3	1:E:325:VAL:HB	1.82	0.60
1:E:573:ASP:O	1:E:576:THR:OG1	2.11	0.60
1:A:331:GLU:OE2	1:F:552:ARG:NE	2.35	0.60
1:C:506:LEU:HD22	1:C:544:GLU:HB3	1.84	0.60
1:F:251:LYS:NZ	1:F:255:GLU:OE1	2.34	0.60
1:A:362:THR:OG1	3:A:801:AGS:O1A	2.20	0.59
1:B:431:TRP:CE3	1:B:431:TRP:CA	2.85	0.59
1:E:358:GLY:O	1:E:541:ARG:N	2.34	0.59
1:B:435:PRO:C	1:B:438:ALA:H	2.08	0.59
1:F:280:SER:OG	1:F:284:THR:N	2.35	0.59
1:D:677:PRO:HB2	1:D:705:GLU:HG2	1.84	0.59
1:C:377:HIS:ND1	1:C:408:ALA:HA	2.17	0.59
1:F:352:VAL:HG22	1:F:469:THR:HB	1.83	0.59
1:D:257:GLY:HA2	1:D:298:TRP:HB2	1.84	0.59
1:C:677:PRO:O	1:C:705:GLU:HB2	2.01	0.59
1:B:381:LEU:HB3	1:B:427:MET:HE1	1.84	0.59
1:D:320:TYR:N	5:D:801:ADP:HN62	2.01	0.59
1:C:529:ARG:NH2	1:C:533:GLU:OE2	2.32	0.59
1:D:320:TYR:H	5:D:801:ADP:HN62	1.51	0.59
1:B:599:GLY:N	1:B:610:LEU:O	2.34	0.59
1:B:345:ARG:NH2	1:B:349:PRO:O	2.25	0.59
1:A:339:THR:HG22	1:A:344:VAL:HG22	1.85	0.58
1:A:385:ARG:NH2	1:B:434:ASP:N	2.35	0.58
1:D:584:ARG:HH22	1:D:587:LYS:HG2	1.67	0.58
1:A:425:ASP:HB2	1:A:476:THR:HB	1.85	0.58
1:D:653:LEU:HD22	1:D:691:LEU:HB2	1.85	0.58
1:E:582:ARG:HG3	1:E:583:TYR:CD1	2.34	0.58
1:A:621:GLY:N	1:A:662:ASP:OD1	2.36	0.58
1:A:503:ARG:NH2	1:A:522:VAL:O	2.33	0.58
1:A:601:ALA:HB2	4:A:802:4KZ:C25	2.33	0.58
1:C:503:ARG:O	1:C:503:ARG:HD3	2.02	0.58
1:D:302:ASP:H	1:D:416:ASN:HD21	1.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:273:LEU:HD22	1:E:286:ALA:HB1	1.85	0.58
1:E:312:ARG:HB2	1:E:330:LEU:HD21	1.85	0.58
1:C:302:ASP:HB2	1:C:414:VAL:HG11	1.86	0.58
1:C:390:ILE:HD13	1:C:435:PRO:HB3	1.84	0.58
1:A:336:ARG:HH21	1:A:345:ARG:HB2	1.67	0.58
1:A:709:ARG:HD3	1:F:596:THR:HG21	1.86	0.58
1:C:667:VAL:CG2	1:C:674:LYS:HE3	2.30	0.58
1:F:364:LEU:O	1:F:368:ILE:N	2.27	0.58
1:D:363:SER:HA	1:D:366:ARG:HH21	1.68	0.58
1:B:385:ARG:O	1:B:385:ARG:HG2	2.04	0.58
1:D:541:ARG:NH2	1:E:482:LEU:O	2.37	0.58
1:D:681:ILE:HD12	1:D:703:THR:O	2.02	0.58
1:D:719:LYS:HE3	1:D:747:PRO:HD3	1.85	0.58
1:B:409:MET:HA	1:B:412:VAL:HG12	1.86	0.58
1:A:268:LYS:O	1:A:272:ARG:N	2.35	0.57
1:A:320:TYR:H	3:A:801:AGS:HN62	1.52	0.57
1:F:681:ILE:CG2	1:F:704:GLY:H	2.17	0.57
1:D:361:LYS:HE2	5:D:801:ADP:PB	2.43	0.57
1:E:502:ALA:HA	1:E:506:LEU:HB2	1.85	0.57
1:B:350:ILE:HG23	1:B:467:PHE:HB2	1.86	0.57
1:E:526:ALA:HB1	1:E:574:ILE:HD11	1.87	0.57
1:A:699:ASP:N	1:A:699:ASP:OD1	2.37	0.57
1:A:537:GLU:OE1	1:A:538:ALA:N	2.37	0.57
1:F:428:SER:OG	1:F:430:ASP:OD2	2.23	0.57
1:F:681:ILE:CG2	1:F:682:THR:N	2.67	0.57
1:F:742:GLN:HG2	1:E:580:ILE:HD11	1.86	0.57
1:D:345:ARG:NH1	1:D:462:LEU:O	2.38	0.57
1:B:625:LEU:HB2	1:B:634:LYS:HE2	1.85	0.57
1:F:354:VAL:O	1:F:490:ILE:N	2.35	0.57
1:E:384:VAL:HG13	1:E:389:GLU:HG2	1.86	0.57
1:E:714:PRO:HG3	1:E:738:ASP:HB3	1.86	0.57
1:A:544:GLU:OE1	1:B:347:LYS:HG2	2.04	0.57
1:B:584:ARG:NH2	1:C:738:ASP:O	2.29	0.57
1:C:272:ARG:NH1	1:C:282:GLU:OE1	2.38	0.57
1:A:524:ASP:O	1:A:528:LEU:N	2.34	0.57
1:C:610:LEU:HD12	4:C:802:4KZ:C26	2.35	0.57
1:F:451:PHE:HE2	1:F:462:LEU:HD12	1.68	0.57
1:F:412:VAL:HG12	1:F:414:VAL:H	1.70	0.57
1:E:369:ALA:HA	1:E:372:MET:HG2	1.87	0.57
1:F:715:ILE:H	1:F:739:ASN:HD21	1.53	0.56
1:D:677:PRO:HG2	1:D:705:GLU:OE2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:556:LYS:O	1:E:560:GLU:N	2.38	0.56
1:A:678:SER:HB3	1:A:715:ILE:CD1	2.35	0.56
1:A:534:TYR:CE1	1:A:581:PRO:HA	2.38	0.56
1:B:421:LEU:HB2	1:B:469:THR:HG22	1.87	0.56
1:C:281:PRO:O	1:C:284:THR:OG1	2.22	0.56
1:C:304:GLU:CD	1:C:336:ARG:HH22	2.13	0.56
1:C:378:ARG:HH22	1:C:422:ASP:CG	2.12	0.56
1:E:509:LYS:O	1:E:512:ARG:NH1	2.38	0.56
1:C:423:GLU:OE2	1:D:440:LEU:HD12	2.05	0.56
1:B:391:ARG:HD3	1:B:454:HIS:HE1	1.69	0.56
1:C:501:ILE:CD1	1:C:501:ILE:H	2.14	0.56
1:F:432:ARG:HH21	1:E:432:ARG:HE	1.52	0.56
1:A:614:VAL:HG23	1:A:690:ALA:HB2	1.88	0.56
1:B:435:PRO:CG	1:B:436:ALA:N	2.68	0.56
1:C:422:ASP:C	1:C:423:GLU:HG2	2.30	0.56
1:E:263:LYS:HD3	1:E:266:ALA:HB3	1.86	0.56
1:E:325:VAL:HA	1:E:328:ARG:HH21	1.71	0.56
1:A:318:ASP:OD2	1:A:370:ARG:NH2	2.38	0.56
1:D:304:GLU:HG3	1:D:306:LEU:HD11	1.86	0.56
1:E:675:ASP:OD1	1:E:676:GLY:N	2.30	0.56
1:A:431:TRP:CZ3	2:S:7:UNK:CB	2.89	0.56
1:C:681:ILE:HD12	1:C:704:GLY:N	2.19	0.56
1:C:681:ILE:HD11	1:C:712:VAL:CG1	2.34	0.56
1:B:328:ARG:NH1	1:B:331:GLU:OE1	2.38	0.56
1:E:421:LEU:HD23	1:E:424:ILE:HG21	1.88	0.56
1:E:379:ILE:HD11	1:E:408:ALA:HB2	1.88	0.56
1:C:359:VAL:HG23	1:C:493:TYR:CE2	2.41	0.55
1:C:675:ASP:O	4:C:802:4KZ:C10	2.54	0.55
1:D:623:LEU:HD12	1:D:663:LEU:HB2	1.87	0.55
1:B:388:ALA:HB1	1:C:394:ARG:HE	1.72	0.55
1:C:423:GLU:OE1	1:D:440:LEU:HD11	2.04	0.55
1:F:320:TYR:OH	1:F:504:GLN:NE2	2.39	0.55
1:F:423:GLU:OE2	1:F:472:ASN:N	2.39	0.55
1:F:541:ARG:NH2	5:F:801:ADP:O2B	2.39	0.55
1:D:665:VAL:HG11	1:D:683:MET:CE	2.36	0.55
1:F:654:PRO:HB2	1:F:657:PHE:HB3	1.88	0.55
1:F:722:LEU:HD22	1:F:733:ILE:HD13	1.88	0.55
1:C:384:VAL:CG1	1:C:427:MET:HE2	2.37	0.55
1:D:676:GLY:CA	4:D:802:4KZ:C16	2.85	0.55
1:E:315:LEU:HB3	1:E:326:LYS:HZ2	1.71	0.55
1:B:431:TRP:C	1:B:431:TRP:HE3	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398:ILE:HD11	2:S:8:UNK:CB	2.37	0.55
1:F:285:VAL:HG12	1:F:398:ILE:HA	1.89	0.55
1:E:439:MET:HB3	1:E:443:LEU:HD13	1.88	0.55
1:E:522:VAL:HG12	1:E:569:ILE:HD12	1.88	0.55
1:A:586:ASP:N	1:A:586:ASP:OD1	2.39	0.55
1:C:304:GLU:HG3	1:C:336:ARG:HH12	1.70	0.55
1:C:501:ILE:HG22	3:C:801:AGS:H2	1.87	0.55
1:D:558:TRP:CD1	1:E:338:LEU:HD11	2.39	0.55
1:A:545:ARG:HH12	1:B:347:LYS:HZ3	1.53	0.55
1:C:498:LYS:NZ	1:C:539:GLY:O	2.40	0.55
1:C:256:VAL:O	1:C:258:MET:HB2	2.06	0.55
1:D:627:GLY:O	1:D:674:LYS:NZ	2.39	0.55
1:D:681:ILE:HG13	1:D:704:GLY:C	2.32	0.55
1:E:257:GLY:HA2	1:E:259:PRO:HD3	1.89	0.55
1:B:501:ILE:HD11	3:B:801:AGS:C6	2.37	0.54
1:D:382:GLY:HA2	1:D:426:LYS:HB2	1.88	0.54
1:D:412:VAL:HG21	1:D:417:PRO:HG3	1.90	0.54
1:D:675:ASP:OD1	1:D:676:GLY:N	2.41	0.54
1:A:423:GLU:HB3	1:A:426:LYS:HG2	1.89	0.54
1:B:633:MET:HE1	1:B:667:VAL:HG21	1.88	0.54
1:C:685:THR:O	1:C:689:SER:N	2.34	0.54
1:E:603:THR:HG23	1:E:605:VAL:HG12	1.90	0.54
1:C:401:MET:HG3	1:D:394:ARG:NH2	2.23	0.54
1:D:737:LYS:N	1:D:759:VAL:O	2.39	0.54
1:E:332:TYR:OH	1:E:336:ARG:NH2	2.41	0.54
1:B:382:GLY:HA2	1:B:426:LYS:HB2	1.90	0.54
1:C:680:GLY:CA	1:C:706:VAL:HG12	2.35	0.54
1:F:526:ALA:HB1	1:F:574:ILE:HD11	1.89	0.54
1:D:324:ASP:O	1:D:328:ARG:NH2	2.41	0.54
1:B:614:VAL:HG22	1:B:665:VAL:HG22	1.89	0.54
1:C:250:ARG:O	1:C:254:GLU:N	2.36	0.54
1:E:702:MET:HB3	1:E:734:VAL:HB	1.90	0.54
1:A:380:SER:OG	1:B:441:GLU:OE1	2.24	0.54
1:A:570:ASP:OD1	1:A:571:ALA:N	2.38	0.54
1:C:389:GLU:O	1:C:404:LYS:N	2.35	0.54
1:C:453:ASP:OD2	1:C:456:LEU:N	2.41	0.54
1:B:289:TYR:CE2	1:B:395:ARG:HD2	2.43	0.53
1:B:299:SER:HA	1:B:415:ILE:HD13	1.90	0.53
1:C:257:GLY:HA2	1:C:298:TRP:HB2	1.89	0.53
1:C:678:SER:O	1:C:704:GLY:O	2.25	0.53
1:F:343:ASP:HA	1:F:346:ASN:HD21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:489:GLU:OE1	1:F:489:GLU:N	2.41	0.53
1:E:380:SER:O	1:E:384:VAL:HG23	2.08	0.53
1:E:498:LYS:NZ	1:E:539:GLY:H	2.06	0.53
1:B:393:HIS:HD2	1:C:396:THR:HG21	1.73	0.53
1:B:550:ILE:HD11	1:B:578:LEU:HD11	1.90	0.53
1:C:412:VAL:HG21	1:C:417:PRO:HG3	1.89	0.53
1:D:318:ASP:O	1:D:319:HIS:ND1	2.41	0.53
1:E:310:HIS:NE2	1:E:371:SER:O	2.41	0.53
1:A:265:LYS:O	1:A:269:GLU:HG2	2.09	0.53
1:F:526:ALA:HA	1:F:571:ALA:HB2	1.90	0.53
1:E:265:LYS:HB2	1:E:458:VAL:HG21	1.89	0.53
1:C:715:ILE:H	1:C:739:ASN:ND2	2.03	0.53
1:F:392:GLY:N	1:F:453:ASP:OD1	2.42	0.53
1:E:407:HIS:O	1:E:411:GLN:HG2	2.08	0.53
1:D:427:MET:HB3	1:D:435:PRO:HG2	1.90	0.53
1:D:678:SER:CB	4:D:802:4KZ:O31	2.56	0.53
1:C:379:ILE:HG22	1:C:379:ILE:O	2.08	0.53
1:F:527:ILE:O	1:F:531:ILE:HG12	2.09	0.53
1:E:392:GLY:C	1:E:454:HIS:HB2	2.33	0.53
1:B:431:TRP:CE3	1:B:431:TRP:C	2.87	0.53
1:F:357:PRO:O	1:F:541:ARG:NH2	2.42	0.53
1:C:501:ILE:HG21	3:C:801:AGS:N1	2.23	0.53
1:D:320:TYR:H	5:D:801:ADP:N6	2.06	0.53
1:E:351:LEU:O	1:E:469:THR:HB	2.09	0.53
1:E:386:ASP:HA	1:E:432:ARG:HB2	1.91	0.53
1:A:479:ARG:HD3	1:A:482:LEU:HD23	1.91	0.53
1:A:613:GLU:OE2	1:B:707:SER:OG	2.27	0.53
1:E:506:LEU:HD11	1:E:540:VAL:HG12	1.90	0.53
1:B:417:PRO:HD2	1:B:465:VAL:HG23	1.91	0.52
1:C:497:GLU:O	1:C:501:ILE:HG13	2.09	0.52
1:D:682:THR:HG22	1:D:702:MET:SD	2.49	0.52
1:C:569:ILE:HG23	1:C:573:ASP:HB2	1.91	0.52
1:D:553:LYS:NZ	1:E:331:GLU:OE2	2.41	0.52
1:B:679:ALA:O	1:B:680:GLY:C	2.50	0.52
1:F:597:ALA:HB1	1:F:682:THR:HG22	1.90	0.52
1:A:602:TRP:HA	1:A:607:GLY:HA2	1.92	0.52
1:A:648:THR:HG21	1:A:655:GLU:HA	1.91	0.52
1:B:392:GLY:O	1:B:454:HIS:HB2	2.10	0.52
1:A:428:SER:HA	1:B:431:TRP:CH2	2.44	0.52
1:A:505:TYR:HB3	3:A:801:AGS:H2	1.92	0.52
1:B:435:PRO:O	1:B:437:SER:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:801:AGS:O2B	3:B:801:AGS:O2A	2.25	0.52
3:B:801:AGS:O1B	3:B:801:AGS:O2G	2.23	0.52
1:D:584:ARG:NH2	1:D:585:PRO:O	2.41	0.52
1:E:443:LEU:HB3	1:E:484:ARG:HH12	1.74	0.52
1:E:520:ILE:HD11	1:E:550:ILE:HG22	1.91	0.52
1:C:392:GLY:O	1:C:454:HIS:HB2	2.10	0.52
1:B:250:ARG:HH11	1:B:270:LEU:HD22	1.75	0.52
1:B:537:GLU:OE2	1:B:538:ALA:N	2.43	0.52
1:C:657:PHE:O	1:C:661:VAL:HG12	2.10	0.52
1:F:280:SER:HG	1:F:284:THR:H	1.57	0.52
1:A:429:SER:CA	1:A:434:ASP:OD1	2.58	0.52
1:B:499:GLN:HE22	1:B:524:ASP:HB3	1.74	0.52
1:B:599:GLY:O	1:B:610:LEU:N	2.42	0.52
1:C:382:GLY:CA	1:C:423:GLU:CD	2.82	0.52
1:C:432:ARG:HG2	1:D:432:ARG:HG3	1.92	0.52
1:E:301:ALA:HB2	1:E:415:ILE:HG12	1.90	0.52
1:E:376:PHE:HD1	1:E:418:VAL:HG13	1.73	0.52
1:A:359:VAL:HG23	1:A:493:TYR:CZ	2.44	0.52
1:A:695:PRO:HD3	1:A:774:PRO:HA	1.92	0.52
1:B:435:PRO:HG2	1:B:436:ALA:H	1.73	0.52
1:A:357:PRO:O	3:A:801:AGS:O2B	2.28	0.51
1:B:520:ILE:HD11	1:B:569:ILE:HD11	1.92	0.51
1:E:291:ASP:O	1:E:294:THR:OG1	2.26	0.51
1:C:494:THR:HG23	1:C:497:GLU:H	1.74	0.51
1:D:356:PRO:O	1:D:359:VAL:HG12	2.10	0.51
1:A:250:ARG:O	1:A:254:GLU:N	2.40	0.51
1:A:545:ARG:HH11	1:B:347:LYS:HZ1	1.58	0.51
1:B:722:LEU:HD21	1:B:733:ILE:HG21	1.93	0.51
1:C:573:ASP:O	1:C:576:THR:OG1	2.28	0.51
1:D:335:VAL:HG12	1:D:343:ASP:HB3	1.91	0.51
1:A:744:GLU:O	1:A:748:LYS:NZ	2.44	0.51
1:C:503:ARG:HD3	1:C:503:ARG:C	2.36	0.51
1:F:266:ALA:O	1:F:270:LEU:N	2.39	0.51
1:D:257:GLY:HA3	1:D:258:MET:HB2	1.91	0.51
1:E:646:ALA:O	1:E:647:HIS:ND1	2.43	0.51
1:C:660:LYS:HB3	1:C:780:VAL:HG21	1.93	0.51
1:D:680:GLY:HA3	1:D:706:VAL:HG12	1.91	0.51
1:A:358:GLY:HA3	1:A:539:GLY:HA3	1.92	0.51
1:F:570:ASP:OD1	1:F:571:ALA:N	2.37	0.51
1:D:387:GLU:OE2	1:D:391:ARG:NH2	2.43	0.51
1:A:366:ARG:HH22	1:B:447:GLN:HE22	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:531:ILE:O	1:C:535:THR:OG1	2.29	0.51
1:F:600:LEU:HD21	1:F:725:ALA:HB2	1.93	0.51
1:F:689:SER:OG	1:F:694:ARG:O	2.21	0.51
1:C:310:HIS:O	1:C:314:VAL:HG23	2.10	0.51
1:C:378:ARG:NH1	1:C:422:ASP:CG	2.54	0.51
1:E:534:TYR:HB3	1:E:582:ARG:HH12	1.75	0.51
1:E:654:PRO:HB2	1:E:657:PHE:HB3	1.92	0.51
1:F:474:LEU:HA	1:F:477:ILE:HD12	1.92	0.51
1:D:322:LEU:HB3	1:D:325:VAL:HB	1.92	0.51
1:E:337:GLN:HA	1:E:340:GLN:HE21	1.76	0.51
1:C:603:THR:HG23	4:C:802:4KZ:N1	2.26	0.51
1:F:449:ASN:ND2	1:F:462:LEU:O	2.44	0.51
1:F:713:MET:HB3	1:F:714:PRO:HD2	1.93	0.51
1:B:288:THR:HG21	1:C:272:ARG:HE	1.76	0.50
1:C:415:ILE:HD13	1:C:464:LYS:HD2	1.93	0.50
1:C:663:LEU:HD21	1:C:691:LEU:HD21	1.93	0.50
1:C:705:GLU:N	1:C:715:ILE:HD11	2.26	0.50
3:C:801:AGS:O3G	3:C:801:AGS:O2B	2.29	0.50
1:F:527:ILE:HG22	1:F:531:ILE:HG12	1.92	0.50
1:E:285:VAL:O	1:E:289:TYR:N	2.33	0.50
1:E:328:ARG:NH2	1:E:489:GLU:O	2.39	0.50
1:A:589:GLU:C	1:A:590:THR:HA	2.37	0.50
1:C:288:THR:HG21	1:D:272:ARG:HH21	1.75	0.50
1:C:600:LEU:HD13	1:C:721:LYS:HB3	1.94	0.50
1:C:612:ILE:HG12	1:C:667:VAL:HG12	1.94	0.50
1:D:501:ILE:HD11	5:D:801:ADP:C6	2.47	0.50
1:E:715:ILE:HG12	1:E:739:ASN:ND2	2.26	0.50
1:A:541:ARG:HD2	1:B:483:ASP:OD2	2.09	0.50
1:C:564:GLU:N	1:C:564:GLU:OE1	2.44	0.50
1:E:285:VAL:HG12	1:E:289:TYR:HB2	1.93	0.50
1:E:746:LEU:HD23	1:E:751:LEU:HD22	1.93	0.50
1:B:381:LEU:HD13	1:B:427:MET:HE1	1.93	0.50
1:A:552:ARG:HB3	1:B:331:GLU:HB3	1.94	0.50
1:B:388:ALA:O	1:C:394:ARG:NH2	2.45	0.50
1:F:724:ALA:HA	1:F:727:GLN:HE21	1.76	0.50
1:D:664:HIS:CD2	1:E:708:LEU:HD11	2.46	0.50
1:D:494:THR:OG1	1:D:495:ASN:N	2.45	0.50
1:E:523:THR:OG1	1:E:569:ILE:O	2.14	0.50
1:A:360:GLY:HA3	3:A:801:AGS:C8	2.38	0.50
1:B:439:MET:O	1:B:442:VAL:N	2.45	0.50
1:F:262:VAL:HG21	1:F:298:TRP:CZ2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:HIS:HD2	1:D:364:LEU:HD23	1.77	0.50
1:A:245:ASP:O	1:A:249:LEU:N	2.45	0.50
1:A:391:ARG:NH2	1:A:438:ALA:O	2.45	0.50
1:A:603:THR:HG23	1:A:605:VAL:HG12	1.94	0.50
1:B:453:ASP:OD1	1:B:455:TYR:N	2.36	0.50
1:B:674:LYS:HA	4:B:802:4KZ:O8	2.12	0.50
1:E:527:ILE:O	1:E:531:ILE:HG13	2.11	0.50
1:E:737:LYS:N	1:E:759:VAL:O	2.45	0.50
1:E:537:GLU:HG2	1:E:605:VAL:HG22	1.93	0.49
1:B:366:ARG:HH12	1:C:447:GLN:NE2	2.09	0.49
1:C:662:ASP:OD2	1:D:645:ARG:NH2	2.45	0.49
1:D:332:TYR:OH	1:D:336:ARG:NH1	2.45	0.49
1:B:289:TYR:HE2	1:B:395:ARG:HD2	1.76	0.49
1:C:384:VAL:HG11	1:C:427:MET:HE2	1.94	0.49
1:C:422:ASP:O	1:C:423:GLU:CG	2.60	0.49
1:E:421:LEU:HD13	1:E:469:THR:HA	1.94	0.49
1:A:258:MET:HG3	1:A:262:VAL:HB	1.94	0.49
1:F:354:VAL:HA	1:F:471:ALA:O	2.13	0.49
1:F:625:LEU:HB3	1:F:629:LEU:HD12	1.92	0.49
1:A:389:GLU:OE2	1:B:394:ARG:NE	2.46	0.49
1:C:715:ILE:N	1:C:739:ASN:HD21	2.06	0.49
1:E:629:LEU:HD21	1:E:667:VAL:HG21	1.94	0.49
1:B:714:PRO:HB3	1:B:738:ASP:HB2	1.94	0.49
1:D:434:ASP:OD1	1:D:437:SER:N	2.42	0.49
1:E:746:LEU:HD12	1:E:747:PRO:HD2	1.93	0.49
1:B:625:LEU:HB3	1:B:629:LEU:HD12	1.94	0.49
1:C:418:VAL:HG12	1:C:466:PHE:HB3	1.95	0.49
1:A:627:GLY:N	1:B:635:GLU:OE1	2.46	0.49
1:B:442:VAL:HG12	1:B:443:LEU:HD23	1.94	0.49
1:C:384:VAL:CG1	1:C:427:MET:HG2	2.42	0.49
1:C:681:ILE:HD12	1:C:703:THR:C	2.38	0.49
1:F:507:TRP:HZ2	1:F:521:GLU:HA	1.77	0.49
1:D:371:SER:OG	1:D:372:MET:SD	2.71	0.49
1:D:474:LEU:HD22	1:D:482:LEU:HD21	1.95	0.49
1:D:550:ILE:HG12	1:D:578:LEU:HD21	1.93	0.49
1:D:682:THR:HG22	1:D:702:MET:CG	2.42	0.49
1:B:586:ASP:OD1	1:B:586:ASP:N	2.43	0.49
1:E:416:ASN:HA	1:E:464:LYS:O	2.13	0.49
1:A:328:ARG:NH1	1:A:331:GLU:OE2	2.46	0.49
1:A:436:ALA:HB1	1:A:478:PRO:HG2	1.93	0.49
1:A:747:PRO:O	1:A:750:VAL:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:PRO:O	1:B:460:TYR:OH	2.27	0.49
1:F:301:ALA:HA	1:F:416:ASN:ND2	2.28	0.49
1:D:318:ASP:OD2	1:D:367:SER:HB2	2.13	0.49
1:D:510:GLN:O	1:D:514:SER:N	2.42	0.49
1:D:594:VAL:HG11	1:D:776:MET:SD	2.52	0.49
1:B:601:ALA:HB2	4:B:802:4KZ:C25	2.43	0.48
1:B:643:TYR:OH	1:B:651:TYR:OH	2.19	0.48
1:C:700:ILE:HG12	1:C:732:LYS:HB2	1.95	0.48
1:F:326:LYS:HA	1:F:329:ILE:HD12	1.94	0.48
1:D:677:PRO:O	1:D:705:GLU:HG2	2.13	0.48
1:D:701:ALA:HB2	1:D:730:ILE:HD13	1.95	0.48
1:D:720:GLU:H	1:D:720:GLU:CD	2.21	0.48
1:A:434:ASP:HB2	1:A:437:SER:HB3	1.95	0.48
1:C:319:HIS:CE1	1:C:364:LEU:HD22	2.48	0.48
1:D:352:VAL:HA	1:D:469:THR:HB	1.95	0.48
1:A:614:VAL:HG12	1:A:665:VAL:HG22	1.95	0.48
1:B:325:VAL:HG11	1:B:364:LEU:HD21	1.93	0.48
1:C:295:GLU:HB3	1:C:410:LYS:HD3	1.94	0.48
1:C:682:THR:HA	1:C:702:MET:SD	2.53	0.48
1:E:279:GLY:HA3	1:E:280:SER:HA	1.56	0.48
1:E:352:VAL:HG12	1:E:486:GLU:H	1.77	0.48
1:A:393:HIS:HD2	1:B:396:THR:HG21	1.79	0.48
1:A:529:ARG:NE	1:A:533:GLU:OE1	2.33	0.48
1:B:372:MET:HG3	1:B:374:ARG:HG2	1.95	0.48
1:B:431:TRP:HA	1:B:431:TRP:HE3	1.77	0.48
1:B:439:MET:HB2	1:B:481:LEU:HD11	1.95	0.48
1:B:627:GLY:N	1:C:635:GLU:OE1	2.47	0.48
1:D:515:GLY:HA2	1:E:339:THR:HG21	1.95	0.48
1:D:620:SER:N	1:D:662:ASP:OD1	2.46	0.48
1:E:258:MET:HB3	1:E:262:VAL:HG13	1.96	0.48
1:F:618:PRO:HG3	1:F:779:VAL:HG13	1.96	0.48
1:F:633:MET:O	1:F:636:SER:OG	2.26	0.48
1:E:381:LEU:HA	1:E:384:VAL:CG2	2.43	0.48
1:E:402:PRO:HD3	1:E:455:TYR:CE1	2.49	0.48
1:E:614:VAL:HG12	1:E:665:VAL:HA	1.96	0.48
1:A:378:ARG:NH2	1:B:441:GLU:OE1	2.35	0.48
1:F:385:ARG:HA	1:F:427:MET:HA	1.96	0.48
1:D:264:THR:HA	1:D:267:LEU:HB3	1.95	0.48
1:E:575:PRO:O	1:E:579:GLY:HA2	2.14	0.48
1:D:253:ILE:O	1:D:263:LYS:NZ	2.26	0.48
1:E:256:VAL:HG22	1:E:298:TRP:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:438:ALA:O	1:F:442:VAL:HG23	2.14	0.48
1:B:384:VAL:HG11	1:B:389:GLU:HG3	1.95	0.48
1:B:613:GLU:OE2	1:C:709:ARG:NE	2.46	0.48
1:E:602:TRP:CD1	1:E:717:GLY:HA3	2.49	0.48
1:C:533:GLU:HB3	1:C:581:PRO:HB3	1.96	0.47
1:C:545:ARG:NH1	1:D:485:MET:H	2.11	0.47
1:C:676:GLY:CA	4:C:802:4KZ:C17	2.91	0.47
1:F:394:ARG:HG2	1:F:454:HIS:HB3	1.96	0.47
1:F:726:HIS:ND1	1:F:750:VAL:HG23	2.28	0.47
1:E:296:VAL:HG13	1:E:409:MET:HB3	1.96	0.47
1:E:600:LEU:HD13	1:E:703:THR:HG23	1.96	0.47
1:E:695:PRO:HG2	1:E:771:LEU:HD12	1.96	0.47
1:A:356:PRO:O	1:A:359:VAL:HG12	2.14	0.47
3:B:801:AGS:S1G	1:C:484:ARG:NH1	2.87	0.47
1:F:423:GLU:HA	1:F:471:ALA:HA	1.97	0.47
1:F:681:ILE:HG23	1:F:682:THR:H	1.75	0.47
1:F:724:ALA:HA	1:F:727:GLN:NE2	2.28	0.47
1:D:332:TYR:CZ	1:D:336:ARG:HD2	2.49	0.47
1:E:479:ARG:HA	1:E:482:LEU:HB3	1.96	0.47
1:E:479:ARG:N	1:E:480:PRO:HD2	2.29	0.47
1:C:309:ASN:OD1	1:C:309:ASN:N	2.47	0.47
1:D:300:LYS:O	1:D:415:ILE:HG12	2.14	0.47
1:E:349:PRO:HA	1:E:484:ARG:HB3	1.96	0.47
1:C:304:GLU:OE1	1:C:304:GLU:N	2.36	0.47
1:F:773:GLU:OE1	1:F:775:THR:OG1	2.31	0.47
1:B:360:GLY:H	3:B:801:AGS:H2	1.79	0.47
1:B:391:ARG:HB3	1:B:454:HIS:CE1	2.50	0.47
1:C:439:MET:O	1:C:442:VAL:N	2.48	0.47
1:F:679:ALA:HB2	4:F:802:4KZ:C23	2.44	0.47
1:D:361:LYS:HE2	5:D:801:ADP:O3B	2.14	0.47
1:D:598:GLN:HE21	1:D:730:ILE:HD11	1.78	0.47
1:E:427:MET:HE1	1:E:436:ALA:HB2	1.96	0.47
1:A:432:ARG:HG3	2:S:7:UNK:CB	2.43	0.47
1:B:342:LEU:HG	1:B:343:ASP:H	1.79	0.47
1:F:322:LEU:HB3	1:F:325:VAL:HB	1.96	0.47
1:D:386:ASP:OD1	1:D:386:ASP:N	2.48	0.47
1:D:676:GLY:HA2	4:D:802:4KZ:C16	2.45	0.47
1:E:301:ALA:HA	1:E:414:VAL:HG13	1.95	0.47
1:E:715:ILE:H	1:E:739:ASN:HD21	1.61	0.47
1:A:408:ALA:O	1:A:412:VAL:HG12	2.15	0.47
1:A:430:ASP:N	1:A:434:ASP:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:705:GLU:O	1:B:713:MET:N	2.48	0.47
1:C:246:LEU:O	1:C:250:ARG:N	2.48	0.47
1:D:353:LEU:N	1:D:469:THR:O	2.47	0.47
1:D:374:ARG:HG2	1:D:417:PRO:HA	1.97	0.47
1:D:495:ASN:O	1:D:499:GLN:N	2.40	0.47
1:E:703:THR:HG21	1:E:721:LYS:HD3	1.96	0.47
1:E:678:SER:O	1:E:704:GLY:O	2.33	0.47
1:C:289:TYR:CE1	1:C:456:LEU:HA	2.50	0.47
1:C:384:VAL:HG13	1:C:427:MET:HG2	1.97	0.47
1:C:501:ILE:HB	1:C:506:LEU:HD12	1.97	0.47
1:D:722:LEU:HD13	1:D:746:LEU:HD11	1.97	0.47
1:E:359:VAL:HA	1:E:540:VAL:H	1.80	0.47
1:E:681:ILE:HA	1:E:684:ALA:HB3	1.97	0.47
1:C:275:ARG:NH1	1:C:275:ARG:HA	2.30	0.47
1:D:320:TYR:N	5:D:801:ADP:N6	2.63	0.47
1:C:678:SER:HA	1:C:704:GLY:C	2.40	0.46
1:F:658:TYR:CE2	1:F:659:ASN:HB2	2.50	0.46
1:C:612:ILE:HG12	1:C:667:VAL:CG1	2.45	0.46
1:D:613:GLU:OE1	1:E:709:ARG:HG3	2.15	0.46
1:D:746:LEU:HD12	1:D:751:LEU:HD23	1.96	0.46
1:A:278:GLN:O	1:A:280:SER:OG	2.32	0.46
1:A:354:VAL:HG21	1:A:474:LEU:HD21	1.97	0.46
1:A:474:LEU:HD12	1:A:482:LEU:HD13	1.98	0.46
1:C:257:GLY:CA	1:C:298:TRP:HB2	2.46	0.46
1:F:395:ARG:HG3	1:F:455:TYR:HE1	1.81	0.46
1:E:343:ASP:H	1:E:346:ASN:ND2	2.12	0.46
1:A:516:MET:HB3	1:A:516:MET:HE3	1.86	0.46
1:B:385:ARG:HB2	1:B:428:SER:HB3	1.97	0.46
1:C:616:ALA:HB1	1:C:661:VAL:HG21	1.98	0.46
1:F:379:ILE:HD11	1:F:408:ALA:HB2	1.95	0.46
1:D:321:GLY:HA2	1:D:323:LYS:NZ	2.31	0.46
1:D:613:GLU:OE2	1:E:707:SER:HB3	2.15	0.46
1:A:351:LEU:HD23	1:A:351:LEU:HA	1.81	0.46
1:B:354:VAL:HA	1:B:471:ALA:O	2.16	0.46
1:C:545:ARG:NH1	1:D:483:ASP:O	2.49	0.46
1:D:364:LEU:O	1:D:368:ILE:N	2.27	0.46
1:D:592:PRO:HA	1:D:698:MET:HG2	1.96	0.46
1:E:378:ARG:HH21	1:E:422:ASP:CG	2.23	0.46
1:A:391:ARG:HD3	1:A:454:HIS:CE1	2.51	0.46
1:A:429:SER:CA	1:A:434:ASP:CG	2.83	0.46
1:A:452:THR:HA	1:A:459:PRO:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:801:AGS:O1B	3:A:801:AGS:O2A	2.34	0.46
1:C:376:PHE:HD1	1:C:418:VAL:HG23	1.79	0.46
1:C:536:ARG:O	1:C:605:VAL:HG13	2.16	0.46
1:F:723:LEU:HD23	1:F:723:LEU:HA	1.75	0.46
1:D:682:THR:HG22	1:D:702:MET:HG2	1.90	0.46
1:A:253:ILE:HD12	1:A:270:LEU:HD22	1.97	0.46
1:C:352:VAL:HA	1:C:469:THR:HB	1.98	0.46
1:C:381:LEU:HD22	1:C:427:MET:HE2	1.98	0.46
1:C:552:ARG:HH12	1:D:486:GLU:CD	2.23	0.46
1:E:390:ILE:HD13	1:E:404:LYS:HB2	1.98	0.46
1:C:521:GLU:OE1	1:C:522:VAL:N	2.47	0.46
1:C:555:ALA:O	1:C:559:LEU:N	2.32	0.46
1:F:531:ILE:O	1:F:535:THR:HB	2.16	0.46
1:F:669:ASP:OD1	1:F:670:GLY:N	2.49	0.46
1:F:746:LEU:HD13	1:F:751:LEU:HD21	1.98	0.46
1:E:700:ILE:HG13	1:E:732:LYS:HB2	1.97	0.46
1:B:431:TRP:CA	1:B:431:TRP:HE3	2.28	0.46
1:C:304:GLU:OE2	1:C:306:LEU:HD21	2.16	0.46
1:F:272:ARG:NE	1:F:275:ARG:HH22	2.10	0.46
1:A:429:SER:HB3	1:A:434:ASP:OD2	2.16	0.45
1:A:678:SER:HB3	1:A:715:ILE:HG12	1.98	0.45
1:B:435:PRO:CG	1:B:436:ALA:H	2.29	0.45
1:D:678:SER:HB3	4:D:802:4KZ:O31	2.16	0.45
1:B:435:PRO:O	1:B:437:SER:CA	2.63	0.45
1:F:601:ALA:HB1	4:F:802:4KZ:C3	2.46	0.45
1:D:621:GLY:N	1:D:662:ASP:OD1	2.28	0.45
1:D:631:GLU:O	1:D:635:GLU:HG3	2.17	0.45
1:E:435:PRO:O	1:E:439:MET:HG2	2.16	0.45
1:A:601:ALA:CB	4:A:802:4KZ:C25	2.94	0.45
1:B:262:VAL:HA	1:B:265:LYS:HB3	1.98	0.45
1:F:279:GLY:HA3	1:F:280:SER:HA	1.52	0.45
1:F:462:LEU:HD23	1:F:462:LEU:HA	1.80	0.45
1:F:659:ASN:C	1:F:660:LYS:HD2	2.41	0.45
1:E:290:LEU:HA	1:E:293:LEU:HD12	1.98	0.45
1:E:543:LEU:HD23	1:E:546:GLU:HB3	1.98	0.45
1:F:381:LEU:HB3	1:F:422:ASP:O	2.16	0.45
1:E:380:SER:HA	1:E:422:ASP:HB3	1.98	0.45
1:B:257:GLY:HA3	1:B:258:MET:HG3	1.98	0.45
1:B:296:VAL:HG11	1:B:456:LEU:HD11	1.98	0.45
1:B:503:ARG:HH22	1:B:522:VAL:HG23	1.81	0.45
1:C:586:ASP:OD1	1:C:586:ASP:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:250:ARG:HG3	1:F:270:LEU:HD21	1.99	0.45
1:D:342:LEU:HD22	1:D:346:ASN:HD22	1.81	0.45
1:E:358:GLY:C	1:E:539:GLY:HA3	2.42	0.45
1:A:596:THR:HA	1:A:612:ILE:O	2.16	0.45
1:B:336:ARG:NH1	1:B:344:VAL:HG13	2.31	0.45
1:C:251:LYS:HA	1:C:254:GLU:HB2	1.97	0.45
1:C:284:THR:O	1:C:288:THR:HG23	2.16	0.45
1:C:381:LEU:CB	1:C:427:MET:HE1	2.39	0.45
1:F:387:GLU:HG2	1:F:433:GLY:HA3	1.99	0.45
1:D:359:VAL:O	5:D:801:ADP:O3A	2.34	0.45
1:E:381:LEU:HA	1:E:384:VAL:HG23	1.99	0.45
1:A:333:LEU:HD21	1:A:372:MET:SD	2.57	0.45
1:A:610:LEU:HD12	4:A:802:4KZ:C25	2.47	0.45
1:B:534:TYR:CE1	1:B:581:PRO:HA	2.42	0.45
1:F:614:VAL:HG12	1:F:665:VAL:HA	1.99	0.45
4:D:802:4KZ:C22	4:D:802:4KZ:O30	2.65	0.45
1:E:584:ARG:HE	1:E:585:PRO:HD2	1.82	0.45
1:A:264:THR:HA	1:A:267:LEU:HD12	1.99	0.45
1:B:262:VAL:O	1:B:266:ALA:N	2.40	0.45
1:A:679:ALA:HB1	1:A:682:THR:CG2	2.47	0.45
1:A:737:LYS:N	1:A:759:VAL:O	2.50	0.45
1:B:424:ILE:O	1:B:427:MET:HG2	2.16	0.45
1:F:292:TRP:HZ2	1:F:407:HIS:HE1	1.65	0.45
1:F:364:LEU:HA	1:F:367:SER:HB3	1.99	0.45
1:F:630:GLY:N	1:F:674:LYS:O	2.45	0.45
1:D:361:LYS:N	5:D:801:ADP:O1A	2.45	0.45
1:D:766:LEU:HD23	1:D:766:LEU:HA	1.83	0.45
1:B:541:ARG:NH1	3:B:801:AGS:O5'	2.50	0.44
1:B:625:LEU:HD12	1:B:634:LYS:HG2	1.99	0.44
1:C:614:VAL:HG22	1:C:665:VAL:HG22	1.99	0.44
1:D:507:TRP:HZ2	1:D:521:GLU:HA	1.82	0.44
1:D:584:ARG:HG2	1:D:585:PRO:HD2	1.99	0.44
1:E:389:GLU:HG3	1:E:390:ILE:H	1.82	0.44
1:E:474:LEU:HA	1:E:477:ILE:HD13	1.99	0.44
1:E:760:GLU:N	1:E:760:GLU:OE1	2.51	0.44
1:A:536:ARG:HG3	1:A:583:TYR:CD1	2.53	0.44
1:B:381:LEU:HD13	1:B:427:MET:CE	2.47	0.44
1:F:427:MET:HG3	1:F:428:SER:H	1.83	0.44
1:F:345:ARG:NH2	1:F:464:LYS:HA	2.32	0.44
1:F:451:PHE:O	1:F:459:PRO:HA	2.18	0.44
1:F:713:MET:HB3	1:F:713:MET:HE2	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:449:ASN:OD1	1:D:450:THR:HG23	2.18	0.44
1:E:699:ASP:OD1	1:E:700:ILE:HD12	2.17	0.44
1:B:700:ILE:HG12	1:B:768:TYR:HE2	1.81	0.44
1:C:545:ARG:NH2	1:D:483:ASP:HA	2.32	0.44
1:D:292:TRP:O	1:D:296:VAL:HG12	2.18	0.44
1:D:594:VAL:HA	1:D:695:PRO:HA	1.99	0.44
1:E:440:LEU:HD21	1:E:480:PRO:HB2	1.99	0.44
1:A:345:ARG:CZ	1:A:374:ARG:HH22	2.29	0.44
1:C:245:ASP:O	1:C:249:LEU:N	2.42	0.44
1:C:323:LYS:O	1:C:327:GLU:HG2	2.17	0.44
1:C:540:VAL:O	1:C:541:ARG:C	2.55	0.44
1:E:384:VAL:HG22	1:E:389:GLU:HG2	1.98	0.44
1:E:543:LEU:HA	1:E:546:GLU:HB3	2.00	0.44
1:A:250:ARG:HA	1:A:253:ILE:HB	2.00	0.44
3:A:801:AGS:O1B	3:A:801:AGS:O2G	2.34	0.44
1:B:541:ARG:NH1	3:B:801:AGS:O3A	2.51	0.44
1:B:589:GLU:HA	1:B:590:THR:N	2.32	0.44
1:F:306:LEU:HD22	1:F:337:GLN:HB2	1.98	0.44
1:F:423:GLU:HG2	1:F:426:LYS:HZ1	1.83	0.44
1:D:674:LYS:HG2	4:D:802:4KZ:N1	2.33	0.44
1:A:285:VAL:HA	1:A:288:THR:HG22	2.00	0.44
1:A:420:LEU:HD12	1:A:468:ILE:O	2.18	0.44
1:A:462:LEU:C	1:A:464:LYS:H	2.26	0.44
1:B:262:VAL:HG23	1:B:458:VAL:HG11	1.98	0.44
1:B:593:GLN:O	1:B:696:ALA:N	2.46	0.44
1:B:626:THR:HB	1:C:635:GLU:HB3	2.00	0.44
1:C:271:ASP:HA	1:C:274:GLU:HG3	1.99	0.44
1:F:527:ILE:O	1:F:531:ILE:N	2.45	0.44
1:E:328:ARG:NH1	1:E:489:GLU:H	2.16	0.44
1:E:443:LEU:HB3	1:E:484:ARG:NH1	2.33	0.44
1:E:601:ALA:HB2	4:E:801:4KZ:C28	2.45	0.44
1:B:296:VAL:HG23	1:B:298:TRP:NE1	2.33	0.44
1:B:394:ARG:HG3	1:B:395:ARG:N	2.33	0.44
1:B:420:LEU:HD12	1:B:468:ILE:O	2.16	0.44
1:B:610:LEU:HD12	4:B:802:4KZ:C25	2.45	0.44
1:D:665:VAL:CG1	1:D:683:MET:HE3	2.46	0.44
1:E:246:LEU:HD21	1:E:274:GLU:HG2	1.99	0.44
1:E:611:THR:O	1:E:668:PRO:HD2	2.18	0.44
1:C:378:ARG:HB2	1:C:420:LEU:HB3	2.00	0.43
1:C:386:ASP:C	1:C:435:PRO:HG3	2.42	0.43
1:C:495:ASN:OD1	1:C:727:GLN:NE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:ARG:HG2	1:D:463:SER:O	2.18	0.43
1:D:569:ILE:HG23	1:D:573:ASP:HB3	1.99	0.43
1:E:357:PRO:HG3	1:E:605:VAL:HA	1.99	0.43
1:C:407:HIS:O	1:C:411:GLN:HG2	2.18	0.43
1:C:423:GLU:O	1:C:423:GLU:HG3	2.18	0.43
1:C:425:ASP:HB2	1:C:476:THR:HG23	2.00	0.43
1:F:635:GLU:OE1	1:E:626:THR:HA	2.18	0.43
1:E:406:ILE:O	1:E:410:LYS:N	2.51	0.43
1:A:699:ASP:OD1	1:A:700:ILE:HD12	2.19	0.43
1:B:645:ARG:HG2	1:B:657:PHE:CZ	2.54	0.43
1:D:300:LYS:O	1:D:414:VAL:HB	2.18	0.43
1:E:743:LEU:HD23	1:E:743:LEU:HA	1.80	0.43
1:A:376:PHE:CG	1:A:377:HIS:N	2.86	0.43
1:A:401:MET:HE1	1:B:395:ARG:HD3	1.99	0.43
1:D:259:PRO:HB2	1:D:262:VAL:HG12	1.99	0.43
1:D:321:GLY:HA2	1:D:323:LYS:HZ2	1.84	0.43
1:D:678:SER:N	4:D:802:4KZ:O30	2.45	0.43
1:E:368:ILE:HG22	1:E:372:MET:HE3	2.00	0.43
1:A:260:GLU:H	1:A:260:GLU:CD	2.26	0.43
1:B:354:VAL:HG23	1:B:489:GLU:HA	2.00	0.43
1:F:529:ARG:O	1:F:533:GLU:N	2.43	0.43
1:A:252:LYS:O	1:A:256:VAL:HG22	2.18	0.43
1:F:681:ILE:HB	1:F:704:GLY:O	2.18	0.43
1:E:332:TYR:O	1:E:335:VAL:HG12	2.18	0.43
1:E:546:GLU:C	1:E:548:GLY:H	2.27	0.43
1:B:389:GLU:OE1	1:B:404:LYS:HE2	2.19	0.43
1:B:432:ARG:C	1:B:432:ARG:CD	2.86	0.43
1:F:300:LYS:N	1:F:415:ILE:HG12	2.33	0.43
1:F:597:ALA:CB	1:F:682:THR:CG2	2.93	0.43
1:D:320:TYR:CA	5:D:801:ADP:HN62	2.32	0.43
1:D:415:ILE:C	1:D:417:PRO:HD2	2.43	0.43
1:E:570:ASP:OD1	1:E:571:ALA:N	2.48	0.43
1:A:665:VAL:HG11	1:A:683:MET:HE3	1.99	0.43
1:B:269:GLU:HA	1:B:272:ARG:HB3	1.99	0.43
1:B:444:ASP:CA	1:B:484:ARG:HD3	2.40	0.43
1:C:381:LEU:CD1	1:C:427:MET:HE1	2.45	0.43
1:C:431:TRP:CD1	1:C:431:TRP:H	2.37	0.43
1:D:276:MET:HG3	1:D:280:SER:HB3	2.01	0.43
1:D:381:LEU:HB3	1:D:427:MET:HE1	2.00	0.43
1:E:519:ARG:HH21	1:E:558:TRP:CD1	2.37	0.43
1:A:279:GLY:HA3	1:A:280:SER:HA	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:SER:HB2	1:F:613:GLU:OE2	2.19	0.43
1:C:275:ARG:HA	1:C:275:ARG:CZ	2.49	0.43
1:C:377:HIS:O	1:C:377:HIS:CG	2.70	0.43
1:F:758:LEU:HD23	1:F:758:LEU:HA	1.86	0.43
1:A:597:ALA:HB1	1:A:702:MET:HE3	2.00	0.43
1:B:435:PRO:C	1:B:437:SER:H	2.23	0.43
1:F:501:ILE:HD12	5:F:801:ADP:N1	2.34	0.43
1:D:564:GLU:OE1	1:D:564:GLU:N	2.52	0.43
1:E:509:LYS:HD2	1:E:512:ARG:NH1	2.34	0.43
1:E:698:MET:HE2	1:E:698:MET:HB3	1.87	0.43
1:E:757:LYS:HD3	1:E:768:TYR:CD2	2.53	0.43
1:A:323:LYS:HD2	1:A:323:LYS:HA	1.71	0.42
1:F:718:VAL:O	1:F:722:LEU:HG	2.19	0.42
1:E:548:GLY:O	1:E:552:ARG:N	2.49	0.42
1:A:694:ARG:HA	1:A:774:PRO:HA	2.00	0.42
1:C:262:VAL:O	1:C:266:ALA:N	2.51	0.42
1:F:372:MET:HE2	1:F:372:MET:HB3	1.86	0.42
1:D:455:TYR:C	1:D:456:LEU:HD12	2.44	0.42
1:E:503:ARG:NH2	1:E:522:VAL:O	2.52	0.42
1:A:545:ARG:HH11	1:B:347:LYS:NZ	2.12	0.42
1:C:257:GLY:HA3	1:C:258:MET:HA	1.79	0.42
1:F:374:ARG:HD2	1:F:418:VAL:HG23	2.00	0.42
1:F:479:ARG:HH12	1:F:482:LEU:HD22	1.83	0.42
1:D:442:VAL:HG13	1:D:443:LEU:HD23	2.00	0.42
1:D:452:THR:HG22	1:D:459:PRO:HA	2.01	0.42
1:D:507:TRP:HB3	1:D:508:PRO:HD3	2.00	0.42
1:E:656:ASP:OD1	1:E:656:ASP:N	2.51	0.42
1:A:549:LYS:HE2	1:A:549:LYS:HB3	1.86	0.42
1:C:417:PRO:HD2	1:C:465:VAL:HG23	2.00	0.42
1:C:676:GLY:HA3	4:C:802:4KZ:C17	2.49	0.42
1:F:449:ASN:O	1:F:461:ASP:HA	2.19	0.42
1:D:279:GLY:HA3	1:D:280:SER:HA	1.52	0.42
1:D:765:VAL:HG22	1:D:769:LEU:HD12	2.01	0.42
1:E:342:LEU:HD23	1:E:342:LEU:H	1.85	0.42
1:C:596:THR:HG21	1:D:709:ARG:HD3	2.02	0.42
1:F:356:PRO:O	1:F:359:VAL:HG12	2.19	0.42
1:D:557:PHE:HD2	1:D:567:ARG:HH12	1.67	0.42
1:E:321:GLY:HA2	1:E:323:LYS:NZ	2.34	0.42
1:B:663:LEU:HD12	1:B:691:LEU:HD21	2.01	0.42
1:B:707:SER:HB2	1:B:713:MET:HE2	2.00	0.42
1:C:417:PRO:HG2	1:C:419:ILE:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:596:THR:HG22	1:C:613:GLU:HA	2.02	0.42
1:C:757:LYS:HG3	1:C:759:VAL:HG13	2.02	0.42
1:D:336:ARG:H	1:D:336:ARG:HG3	1.68	0.42
1:A:269:GLU:O	1:A:272:ARG:HB3	2.20	0.42
1:F:246:LEU:H	1:F:246:LEU:HD12	1.85	0.42
1:F:345:ARG:HH22	1:F:465:VAL:H	1.68	0.42
1:F:369:ALA:HB3	1:F:376:PHE:HB2	2.02	0.42
1:F:502:ALA:HB2	1:F:506:LEU:HD12	2.01	0.42
1:D:420:LEU:HD11	1:D:470:THR:HG23	2.00	0.42
1:D:614:VAL:HG22	1:D:665:VAL:HG22	2.02	0.42
1:E:292:TRP:O	1:E:296:VAL:HG23	2.19	0.42
1:E:536:ARG:HH22	1:E:585:PRO:HA	1.85	0.42
1:B:437:SER:HA	1:B:440:LEU:HD12	2.02	0.42
1:D:359:VAL:HG23	1:D:493:TYR:CE2	2.55	0.42
1:E:521:GLU:OE1	1:E:522:VAL:N	2.53	0.42
1:A:354:VAL:HA	1:A:471:ALA:O	2.20	0.42
1:A:396:THR:OG1	1:A:397:TYR:N	2.52	0.42
1:A:545:ARG:NH1	1:A:545:ARG:HG3	2.35	0.42
1:A:678:SER:O	1:A:704:GLY:N	2.40	0.42
1:C:313:GLN:H	1:C:313:GLN:HG2	1.64	0.42
1:C:360:GLY:H	3:C:801:AGS:H8	1.83	0.42
1:F:444:ASP:CG	1:F:447:GLN:H	2.27	0.42
1:D:628:GLN:NE2	1:E:632:VAL:HG22	2.35	0.42
1:E:711:LYS:HB3	1:E:711:LYS:HE2	1.76	0.42
1:A:429:SER:C	1:A:434:ASP:OD1	2.63	0.42
1:C:556:LYS:HE2	1:C:556:LYS:HB3	1.89	0.42
1:C:681:ILE:CD1	1:C:704:GLY:CA	2.56	0.42
1:F:265:LYS:HA	1:F:265:LYS:HD2	1.87	0.42
1:F:314:VAL:HA	1:F:317:GLU:HB2	2.02	0.42
1:F:343:ASP:HA	1:F:346:ASN:ND2	2.35	0.42
1:F:494:THR:HG23	1:F:497:GLU:OE2	2.20	0.42
1:F:599:GLY:N	1:F:610:LEU:O	2.45	0.42
1:D:520:ILE:HD11	1:D:569:ILE:HD11	2.01	0.42
1:D:625:LEU:HD22	1:D:634:LYS:HG2	2.01	0.42
1:E:434:ASP:OD2	1:E:437:SER:N	2.46	0.42
1:E:506:LEU:HD23	1:E:506:LEU:HA	1.83	0.42
1:A:245:ASP:HA	1:A:248:ALA:HB3	2.02	0.41
1:A:412:VAL:HG11	1:A:417:PRO:HG3	2.02	0.41
1:A:691:LEU:HD23	1:A:691:LEU:HA	1.91	0.41
1:A:693:ARG:HH11	1:A:776:MET:HG2	1.84	0.41
1:B:259:PRO:HB2	1:B:262:VAL:HG12	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:GLU:OE1	1:B:404:LYS:HB2	2.20	0.41
1:B:394:ARG:HG2	1:B:396:THR:HG22	2.02	0.41
1:D:338:LEU:HA	1:D:338:LEU:HD12	1.81	0.41
1:D:416:ASN:HA	1:D:464:LYS:O	2.20	0.41
1:E:437:SER:HA	1:E:440:LEU:HG	2.02	0.41
1:A:440:LEU:HD21	1:A:480:PRO:HB2	2.01	0.41
1:F:667:VAL:O	1:F:674:LYS:HE2	2.20	0.41
1:E:296:VAL:HG11	1:E:460:TYR:OH	2.20	0.41
1:A:390:ILE:H	1:A:390:ILE:HD12	1.85	0.41
1:B:302:ASP:OD2	1:B:414:VAL:HG11	2.19	0.41
1:B:349:PRO:HB2	1:B:351:LEU:HD12	2.01	0.41
1:F:641:LEU:HD11	1:F:657:PHE:HE2	1.85	0.41
1:D:644:LEU:HD23	1:D:644:LEU:HA	1.78	0.41
1:D:695:PRO:HD3	1:D:775:THR:HG23	2.02	0.41
1:A:301:ALA:HB2	1:A:415:ILE:HD11	2.03	0.41
1:A:421:LEU:HD12	1:A:469:THR:HG22	2.01	0.41
1:A:523:THR:H	1:A:526:ALA:HB3	1.86	0.41
1:B:707:SER:OG	1:B:708:LEU:N	2.51	0.41
1:C:497:GLU:O	1:C:501:ILE:CD1	2.68	0.41
1:F:358:GLY:HA3	1:F:539:GLY:HA3	2.03	0.41
1:F:401:MET:HE3	1:F:407:HIS:CE1	2.55	0.41
1:F:507:TRP:CE2	1:F:522:VAL:HG12	2.55	0.41
1:E:669:ASP:OD1	1:E:672:THR:HG22	2.20	0.41
1:A:676:GLY:HA3	4:A:802:4KZ:C13	2.50	0.41
1:B:552:ARG:HB3	1:C:331:GLU:HB3	2.03	0.41
1:C:324:ASP:O	1:C:328:ARG:HG2	2.19	0.41
1:C:610:LEU:HD23	1:C:610:LEU:HA	1.81	0.41
1:E:631:GLU:O	1:E:635:GLU:HG3	2.21	0.41
1:E:663:LEU:HD23	1:E:663:LEU:HA	1.84	0.41
1:A:719:LYS:HA	1:A:746:LEU:HD21	2.02	0.41
1:B:253:ILE:HG22	1:B:263:LYS:HE2	2.03	0.41
1:B:473:THR:OG1	1:B:474:LEU:N	2.54	0.41
1:B:669:ASP:O	1:B:674:LYS:NZ	2.49	0.41
1:C:401:MET:HG3	1:D:394:ARG:HH21	1.84	0.41
1:C:449:ASN:HB3	1:C:463:SER:OG	2.21	0.41
1:F:643:TYR:OH	1:F:651:TYR:OH	2.27	0.41
1:F:681:ILE:CG2	1:F:682:THR:H	2.33	0.41
1:D:298:TRP:O	1:D:300:LYS:HG3	2.20	0.41
1:D:534:TYR:CZ	1:D:578:LEU:HB3	2.55	0.41
1:A:275:ARG:NH1	1:A:276:MET:HB2	2.36	0.41
1:A:479:ARG:N	1:A:480:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:VAL:HG13	1:B:487:VAL:HA	2.01	0.41
1:B:754:LEU:HD23	1:B:754:LEU:HA	1.88	0.41
1:C:289:TYR:OH	1:C:457:ASP:OD1	2.34	0.41
1:C:499:GLN:OE1	1:C:528:LEU:HD21	2.21	0.41
1:C:630:GLY:HA3	1:C:675:ASP:OD2	2.20	0.41
1:F:257:GLY:HA3	1:F:258:MET:HA	1.64	0.41
1:F:292:TRP:CD1	1:F:410:LYS:HD3	2.56	0.41
1:D:409:MET:HE1	1:D:415:ILE:HA	2.02	0.41
1:D:617:VAL:HG21	1:E:645:ARG:HE	1.86	0.41
1:D:669:ASP:HB2	1:D:672:THR:HG23	2.03	0.41
1:D:746:LEU:HB2	1:D:751:LEU:HD21	2.01	0.41
1:E:633:MET:HE3	1:E:679:ALA:HB3	2.02	0.41
1:B:498:LYS:HA	1:B:501:ILE:HG22	2.02	0.41
1:C:418:VAL:HG23	1:C:418:VAL:O	2.19	0.41
1:F:507:TRP:HE1	1:F:521:GLU:CD	2.28	0.41
1:E:328:ARG:NH2	1:E:489:GLU:H	2.18	0.41
1:E:661:VAL:HG22	1:E:779:VAL:HG11	2.02	0.41
1:A:427:MET:H	1:A:427:MET:HG3	1.70	0.41
1:A:545:ARG:O	1:A:548:GLY:N	2.53	0.41
1:C:589:GLU:C	1:C:590:THR:HA	2.46	0.41
1:C:678:SER:CA	1:C:704:GLY:O	2.68	0.41
1:F:422:ASP:HA	1:F:470:THR:OG1	2.21	0.41
1:F:530:VAL:HA	1:F:534:TYR:HD1	1.86	0.41
1:F:597:ALA:HB1	1:F:682:THR:CG2	2.51	0.41
1:F:610:LEU:HD23	1:F:610:LEU:HA	1.80	0.41
1:D:302:ASP:H	1:D:416:ASN:ND2	2.17	0.41
1:D:394:ARG:HA	1:D:454:HIS:O	2.20	0.41
1:D:415:ILE:HD11	1:D:464:LYS:HE2	2.02	0.41
1:E:315:LEU:HB3	1:E:326:LYS:NZ	2.36	0.41
1:E:324:ASP:OD1	1:E:324:ASP:N	2.43	0.41
1:E:498:LYS:HD3	1:E:501:ILE:CG2	2.50	0.41
1:E:498:LYS:HZ3	1:E:539:GLY:H	1.67	0.41
1:E:741:ALA:HB3	1:E:742:GLN:NE2	2.36	0.41
1:A:407:HIS:O	1:A:411:GLN:HG2	2.21	0.41
1:A:508:PRO:HA	1:A:511:VAL:HG12	2.03	0.41
1:B:273:LEU:HA	1:B:276:MET:HE3	2.02	0.41
1:B:360:GLY:N	3:B:801:AGS:H2	2.36	0.41
1:B:378:ARG:NH1	1:C:447:GLN:HB3	2.36	0.41
1:F:503:ARG:O	1:F:503:ARG:NE	2.42	0.41
1:D:345:ARG:O	1:D:346:ASN:HB2	2.21	0.41
1:D:622:LYS:HB2	1:D:622:LYS:HE3	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:695:PRO:HG2	1:D:771:LEU:HD22	2.03	0.41
1:E:414:VAL:HG12	1:E:416:ASN:OD1	2.21	0.41
1:E:553:LYS:HE3	1:E:553:LYS:HB2	1.92	0.41
1:B:248:ALA:O	1:B:252:LYS:HG3	2.21	0.40
1:B:288:THR:O	1:B:292:TRP:N	2.54	0.40
1:B:697:ARG:HG3	1:B:769:LEU:O	2.20	0.40
1:C:481:LEU:HD23	1:C:481:LEU:HA	1.94	0.40
1:C:536:ARG:HE	1:C:583:TYR:HD1	1.67	0.40
1:F:585:PRO:HB2	1:F:587:LYS:HD3	2.03	0.40
1:F:658:TYR:CZ	1:F:659:ASN:HB2	2.56	0.40
1:E:385:ARG:NE	1:E:428:SER:HB3	2.36	0.40
1:E:715:ILE:N	1:E:739:ASN:HD21	2.18	0.40
1:C:262:VAL:HG13	1:C:458:VAL:HG11	2.03	0.40
1:F:440:LEU:HA	1:F:484:ARG:HH22	1.86	0.40
1:F:505:TYR:CD2	5:F:801:ADP:H2	2.39	0.40
1:D:361:LYS:HE3	1:D:361:LYS:HB2	1.82	0.40
1:B:596:THR:HA	1:B:612:ILE:O	2.22	0.40
1:C:354:VAL:HA	1:C:471:ALA:O	2.21	0.40
1:C:678:SER:HA	1:C:704:GLY:O	2.21	0.40
1:F:390:ILE:HD13	1:F:435:PRO:HA	2.02	0.40
1:E:578:LEU:H	1:E:578:LEU:HD12	1.86	0.40
1:A:360:GLY:N	3:A:801:AGS:H8	2.36	0.40
1:A:713:MET:HE2	1:A:713:MET:HB3	1.85	0.40
1:B:293:LEU:HD23	1:B:456:LEU:HD22	2.02	0.40
1:B:381:LEU:HB3	1:B:427:MET:CE	2.51	0.40
1:B:479:ARG:N	1:B:480:PRO:HD2	2.36	0.40
1:C:319:HIS:CE1	1:C:363:SER:HG	2.37	0.40
1:C:408:ALA:O	1:C:412:VAL:HG22	2.21	0.40
1:F:251:LYS:HA	1:F:251:LYS:HD2	1.94	0.40
1:F:338:LEU:HD23	1:E:515:GLY:HA3	2.03	0.40
1:D:354:VAL:HA	1:D:471:ALA:O	2.20	0.40
1:D:681:ILE:CD1	1:D:703:THR:O	2.68	0.40
1:A:529:ARG:HD2	1:A:571:ALA:HB1	2.03	0.40
1:B:429:SER:HA	1:B:434:ASP:CB	2.49	0.40
1:B:435:PRO:CD	1:B:436:ALA:H	2.33	0.40
1:B:550:ILE:O	1:B:554:GLY:N	2.55	0.40
1:F:344:VAL:HG13	1:F:345:ARG:N	2.37	0.40
1:D:298:TRP:CH2	1:D:458:VAL:HG21	2.57	0.40
1:D:472:ASN:OD1	1:D:472:ASN:N	2.54	0.40
1:E:768:TYR:HB3	1:E:769:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	533/794 (67%)	500 (94%)	33 (6%)	0	100	100
1	B	533/794 (67%)	488 (92%)	41 (8%)	4 (1%)	16	49
1	C	534/794 (67%)	500 (94%)	33 (6%)	1 (0%)	43	72
1	D	533/794 (67%)	483 (91%)	50 (9%)	0	100	100
1	E	533/794 (67%)	478 (90%)	55 (10%)	0	100	100
1	F	533/794 (67%)	490 (92%)	43 (8%)	0	100	100
All	All	3199/4764 (67%)	2939 (92%)	255 (8%)	5 (0%)	44	72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	436	ALA
1	C	677	PRO
1	B	432	ARG
1	B	389	GLU
1	B	390	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	448/666 (67%)	448 (100%)	0	100	100
1	B	448/666 (67%)	444 (99%)	4 (1%)	70	76
1	C	449/666 (67%)	444 (99%)	5 (1%)	65	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	448/666 (67%)	445 (99%)	3 (1%)	76	78
1	E	448/666 (67%)	447 (100%)	1 (0%)	87	85
1	F	448/666 (67%)	446 (100%)	2 (0%)	84	81
All	All	2689/3996 (67%)	2674 (99%)	15 (1%)	76	79

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	431	TRP
1	B	434	ASP
1	B	484	ARG
1	B	485	MET
1	C	378	ARG
1	C	424	ILE
1	C	501	ILE
1	C	675	ASP
1	C	677	PRO
1	F	415	ILE
1	F	682	THR
1	D	596	THR
1	D	682	THR
1	D	683	MET
1	E	424	ILE

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

Mol	Chain	Res	Type
1	A	337	GLN
1	A	454	HIS
1	A	510	GLN
1	B	277	GLN
1	B	340	GLN
1	B	393	HIS
1	B	510	GLN
1	B	638	GLN
1	C	407	HIS
1	C	447	GLN
1	C	454	HIS
1	C	475	GLN
1	C	666	HIS

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Mol	Chain	Res	Type
1	F	278	GLN
1	F	340	GLN
1	F	407	HIS
1	F	411	GLN
1	F	416	ASN
1	F	449	ASN
1	F	504	GLN
1	F	510	GLN
1	F	739	ASN
1	D	337	GLN
1	D	346	ASN
1	D	411	GLN
1	D	454	HIS
1	D	499	GLN
1	D	504	GLN
1	D	628	GLN
1	E	277	GLN
1	E	340	GLN
1	E	411	GLN
1	E	447	GLN
1	E	504	GLN
1	E	739	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](#)

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	4KZ	F	802	1	29,33,33	0.52	0	38,43,43	1.25	5 (13%)
4	4KZ	B	802	1	29,33,33	0.95	3 (10%)	38,43,43	1.73	8 (21%)
3	AGS	A	801	-	32,33,33	0.85	3 (9%)	45,52,52	0.84	1 (2%)
5	ADP	F	801	-	28,29,29	1.43	5 (17%)	43,45,45	1.81	7 (16%)
4	4KZ	D	802	1	29,33,33	0.64	0	38,43,43	1.57	4 (10%)
4	4KZ	E	801	1	29,33,33	0.84	1 (3%)	38,43,43	1.81	5 (13%)
4	4KZ	C	802	1	29,33,33	0.67	0	38,43,43	1.09	3 (7%)
5	ADP	D	801	-	28,29,29	1.43	5 (17%)	43,45,45	1.79	8 (18%)
4	4KZ	A	802	1	29,33,33	0.84	1 (3%)	38,43,43	1.63	3 (7%)
3	AGS	B	801	-	32,33,33	0.88	3 (9%)	45,52,52	0.89	1 (2%)
3	AGS	C	801	-	32,33,33	0.80	3 (9%)	45,52,52	0.80	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	4KZ	F	802	1	-	5/23/28/28	0/3/3/3
4	4KZ	B	802	1	-	6/23/28/28	0/3/3/3
3	AGS	A	801	-	-	3/21/38/38	0/3/3/3
5	ADP	F	801	-	-	2/16/32/32	0/3/3/3
4	4KZ	D	802	1	-	9/23/28/28	0/3/3/3
4	4KZ	E	801	1	-	13/23/28/28	0/3/3/3
4	4KZ	C	802	1	-	0/23/28/28	0/3/3/3
5	ADP	D	801	-	-	3/16/32/32	0/3/3/3
4	4KZ	A	802	1	-	13/23/28/28	0/3/3/3
3	AGS	B	801	-	-	8/21/38/38	0/3/3/3
3	AGS	C	801	-	-	3/21/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	801	ADP	C5-C4	4.61	1.47	1.39
5	F	801	ADP	C5-C4	4.57	1.47	1.39
3	B	801	AGS	PB-O3B	-2.84	1.56	1.59
4	A	802	4KZ	C21-N20	-2.81	1.41	1.46
3	A	801	AGS	PB-O3B	-2.75	1.56	1.59
5	D	801	ADP	C5-C6	2.58	1.48	1.41
4	B	802	4KZ	C21-N20	-2.56	1.41	1.46
5	F	801	ADP	C5-N7	-2.55	1.34	1.39
5	F	801	ADP	C5-C6	2.53	1.48	1.41
5	D	801	ADP	C5-N7	-2.53	1.34	1.39
4	B	802	4KZ	C10-C18	-2.36	1.46	1.52
3	B	801	AGS	PA-O3A	-2.32	1.57	1.59
3	C	801	AGS	PB-O3B	-2.28	1.57	1.59
3	B	801	AGS	PB-O3A	-2.24	1.57	1.59
3	A	801	AGS	PA-O3A	-2.24	1.57	1.59
5	D	801	ADP	C8-N7	2.23	1.36	1.31
3	C	801	AGS	PG-S1G	2.19	1.95	1.90
5	D	801	ADP	C4-N9	-2.16	1.33	1.37
5	F	801	ADP	PA-O3A	2.14	1.61	1.59
5	F	801	ADP	C8-N7	2.12	1.35	1.31
4	B	802	4KZ	C18-N20	-2.06	1.29	1.34
4	E	801	4KZ	C21-N20	-2.06	1.42	1.46
3	A	801	AGS	PG-S1G	2.04	1.95	1.90
3	C	801	AGS	PB-O3A	-2.02	1.57	1.59

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	801	4KZ	C22-C21-N20	-8.34	99.61	110.39
4	B	802	4KZ	C22-C21-N20	-7.67	100.47	110.39
4	A	802	4KZ	C22-C21-N20	-7.01	101.33	110.39
4	D	802	4KZ	C22-C21-N20	-6.06	102.55	110.39
5	F	801	ADP	C5-C4-N3	-5.97	118.50	126.72
5	D	801	ADP	C5-C4-N3	-5.70	118.86	126.72
3	B	801	AGS	PB-O3B-PG	-5.27	113.87	133.17
3	A	801	AGS	PB-O3B-PG	-5.12	114.44	133.17
5	F	801	ADP	N3-C4-N9	4.76	135.26	127.17
3	C	801	AGS	PB-O3B-PG	-4.64	116.20	133.17
5	D	801	ADP	N3-C4-N9	4.44	134.72	127.17
5	F	801	ADP	C4-C5-N7	-3.58	106.49	110.58
5	D	801	ADP	C2-N3-C4	3.56	120.52	111.83
5	F	801	ADP	C2-N3-C4	3.50	120.39	111.83
5	D	801	ADP	C4-C5-N7	-3.45	106.64	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	801	ADP	N3-C2-N1	-3.08	123.92	128.58
4	F	802	4KZ	C6-N1-C2	2.99	120.78	116.93
4	D	802	4KZ	C6-N1-C2	2.90	120.67	116.93
5	F	801	ADP	N3-C2-N1	-2.83	124.30	128.58
4	E	801	4KZ	O19-C18-N20	2.78	127.94	122.96
4	C	802	4KZ	C6-N1-C2	2.73	120.45	116.93
4	B	802	4KZ	O19-C18-N20	2.70	127.79	122.96
5	F	801	ADP	C4-N9-C8	2.68	108.55	105.74
5	F	801	ADP	C5-N7-C8	2.62	107.56	103.45
4	B	802	4KZ	C2-C3-N4	-2.57	118.60	121.97
4	D	802	4KZ	O19-C18-N20	2.52	127.47	122.96
5	D	801	ADP	C4-N9-C8	2.50	108.36	105.74
4	E	801	4KZ	C6-N1-C2	2.49	120.14	116.93
4	F	802	4KZ	C5-N4-C3	2.48	121.19	116.85
4	B	802	4KZ	C6-N1-C2	2.40	120.02	116.93
5	D	801	ADP	C5-N7-C8	2.38	107.18	103.45
4	C	802	4KZ	C7-C2-N1	2.34	120.16	117.42
4	F	802	4KZ	C22-C21-N20	-2.31	107.40	110.39
4	A	802	4KZ	C10-C18-N20	-2.30	111.71	116.63
4	C	802	4KZ	C5-N4-C3	2.28	120.85	116.85
5	D	801	ADP	C3'-C2'-C1'	2.28	105.78	101.46
4	B	802	4KZ	C5-N4-C3	2.24	120.78	116.85
4	F	802	4KZ	C3-C2-N1	-2.23	118.98	121.60
4	A	802	4KZ	C6-N1-C2	2.22	119.79	116.93
4	F	802	4KZ	C6-C5-N4	-2.20	119.22	121.96
4	D	802	4KZ	C5-N4-C3	2.20	120.70	116.85
4	B	802	4KZ	C21-N20-C18	-2.14	117.59	122.99
4	B	802	4KZ	C5-C6-N1	-2.13	119.18	122.19
4	E	801	4KZ	C18-C10-N9	-2.06	105.53	111.11
4	B	802	4KZ	C10-C18-N20	-2.04	112.27	116.63
4	E	801	4KZ	C5-C6-N1	-2.02	119.34	122.19

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	AGS	C5'-O5'-PA-O1A
3	A	801	AGS	C5'-O5'-PA-O2A
3	A	801	AGS	C5'-O5'-PA-O3A
4	A	802	4KZ	O19-C18-N20-C21
4	A	802	4KZ	N20-C21-C22-C23
4	A	802	4KZ	B29-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
4	B	802	4KZ	O19-C18-N20-C21
4	B	802	4KZ	N20-C21-C22-C23
4	B	802	4KZ	B29-C21-C22-C23
4	D	802	4KZ	C3-C2-C7-N9
4	D	802	4KZ	C3-C2-C7-O8
4	D	802	4KZ	O19-C18-N20-C21
4	D	802	4KZ	N20-C21-C22-C23
4	D	802	4KZ	B29-C21-C22-C23
4	E	801	4KZ	C3-C2-C7-N9
4	E	801	4KZ	C3-C2-C7-O8
4	E	801	4KZ	O19-C18-N20-C21
4	E	801	4KZ	N20-C21-C22-C23
4	E	801	4KZ	B29-C21-C22-C23
4	E	801	4KZ	C21-C22-C23-C24
4	E	801	4KZ	C21-C22-C23-C28
4	B	802	4KZ	C10-C18-N20-C21
4	D	802	4KZ	C10-C18-N20-C21
4	E	801	4KZ	N1-C2-C7-N9
4	E	801	4KZ	N1-C2-C7-O8
4	A	802	4KZ	N1-C2-C7-N9
4	D	802	4KZ	N1-C2-C7-O8
4	F	802	4KZ	N1-C2-C7-O8
4	A	802	4KZ	C10-C18-N20-C21
4	A	802	4KZ	N1-C2-C7-O8
4	F	802	4KZ	N1-C2-C7-N9
4	D	802	4KZ	N1-C2-C7-N9
3	B	801	AGS	O4'-C1'-N9-C8
4	F	802	4KZ	C3-C2-C7-O8
4	E	801	4KZ	C10-C18-N20-C21
3	B	801	AGS	O4'-C1'-N9-C4
4	F	802	4KZ	C3-C2-C7-N9
4	A	802	4KZ	C3-C2-C7-O8
4	A	802	4KZ	C3-C2-C7-N9
3	B	801	AGS	PB-O3A-PA-O1A
4	A	802	4KZ	N9-C10-C18-O19
3	B	801	AGS	O4'-C4'-C5'-O5'
4	A	802	4KZ	C11-C10-C18-O19
3	B	801	AGS	C5'-O5'-PA-O1A
5	D	801	ADP	C5'-O5'-PA-O1A
3	B	801	AGS	C3'-C4'-C5'-O5'
4	B	802	4KZ	C21-C22-C23-C24
4	B	802	4KZ	C21-C22-C23-C28

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Mol	Chain	Res	Type	Atoms
5	D	801	ADP	PA-O3A-PB-O1B
3	C	801	AGS	PG-O3B-PB-O1B
3	C	801	AGS	PG-O3B-PB-O2B
3	B	801	AGS	PB-O3A-PA-O2A
3	C	801	AGS	PB-O3A-PA-O2A
4	E	801	4KZ	C10-C11-C12-C17
3	B	801	AGS	C4'-C5'-O5'-PA
4	A	802	4KZ	N9-C10-C18-N20
4	E	801	4KZ	C10-C11-C12-C13
4	A	802	4KZ	C22-C21-N20-C18
4	A	802	4KZ	N9-C10-C11-C12
4	F	802	4KZ	C21-C22-C23-C24
4	D	802	4KZ	C21-C22-C23-C28
4	E	801	4KZ	C18-C10-N9-C7
5	F	801	ADP	PB-O3A-PA-O1A
5	F	801	ADP	PB-O3A-PA-O2A
5	D	801	ADP	O4'-C4'-C5'-O5'

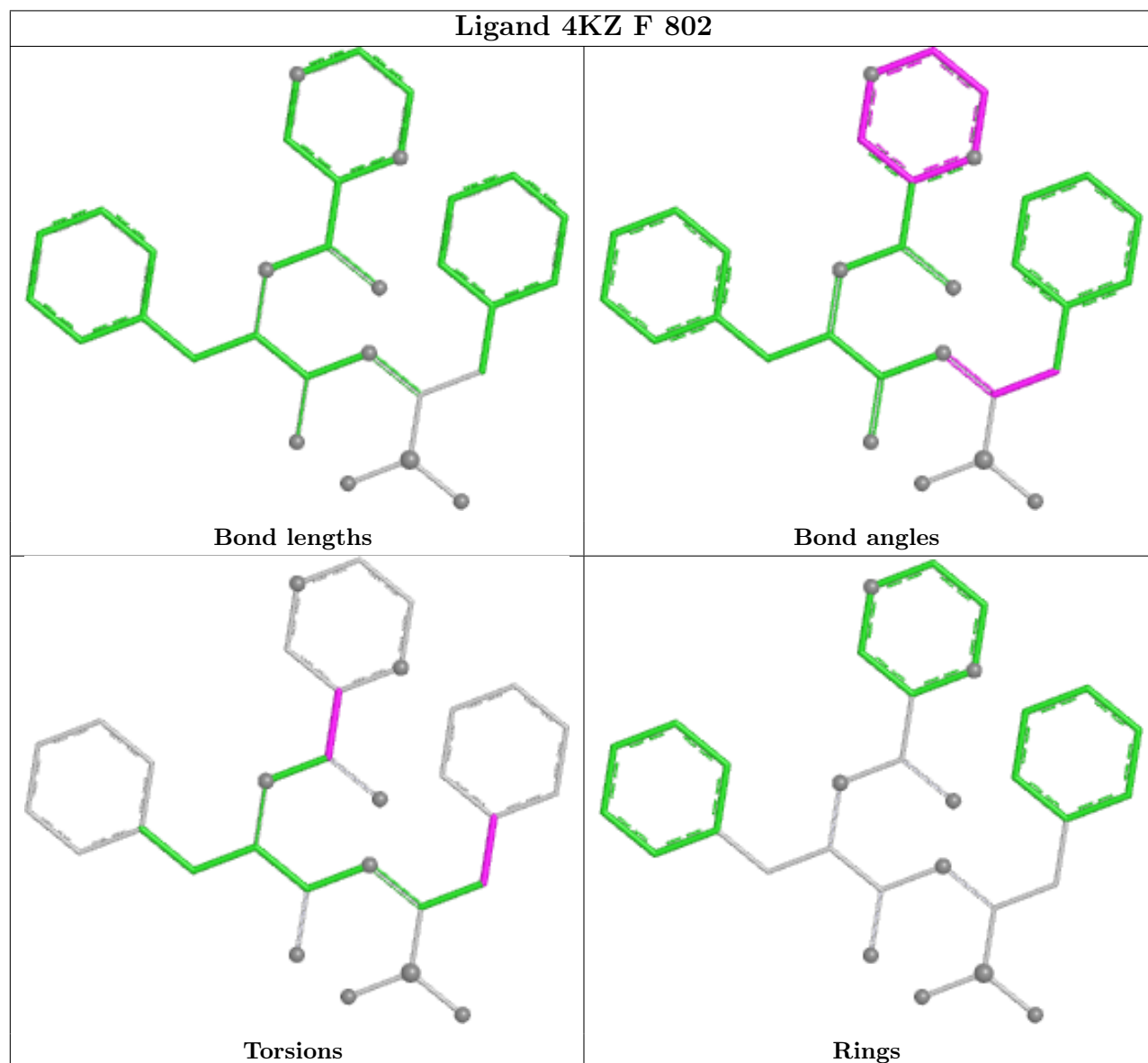
There are no ring outliers.

11 monomers are involved in 89 short contacts:

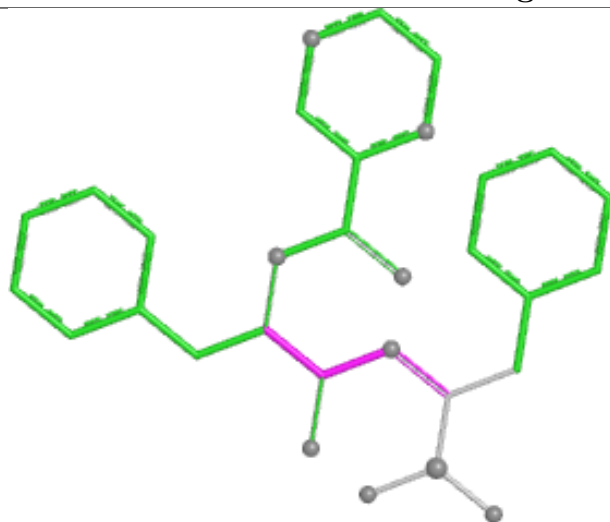
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	802	4KZ	3	0
4	B	802	4KZ	5	0
3	A	801	AGS	13	0
5	F	801	ADP	5	0
4	D	802	4KZ	7	0
4	E	801	4KZ	2	0
4	C	802	4KZ	8	0
5	D	801	ADP	14	0
4	A	802	4KZ	7	0
3	B	801	AGS	10	0
3	C	801	AGS	15	0

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

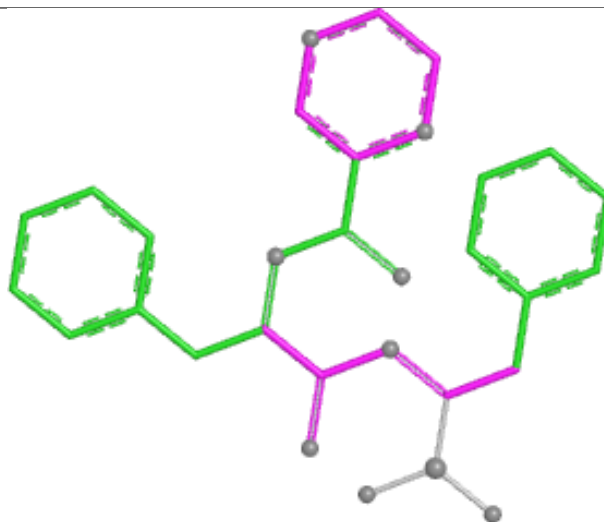
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



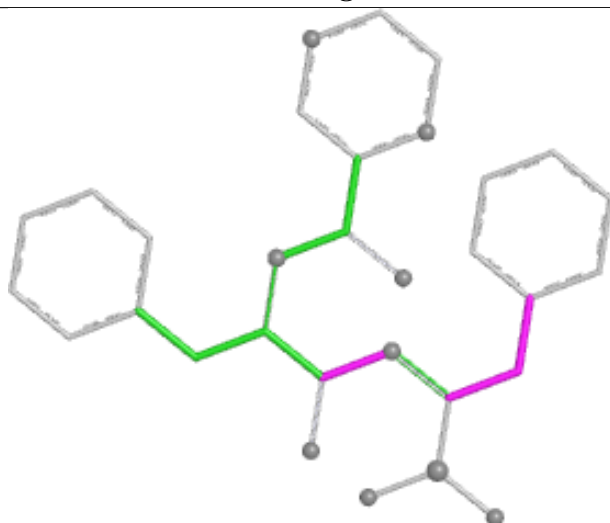
Ligand 4KZ B 802



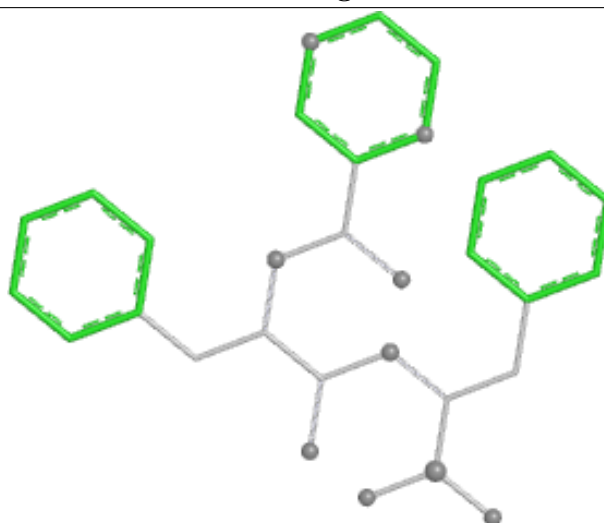
Bond lengths



Bond angles

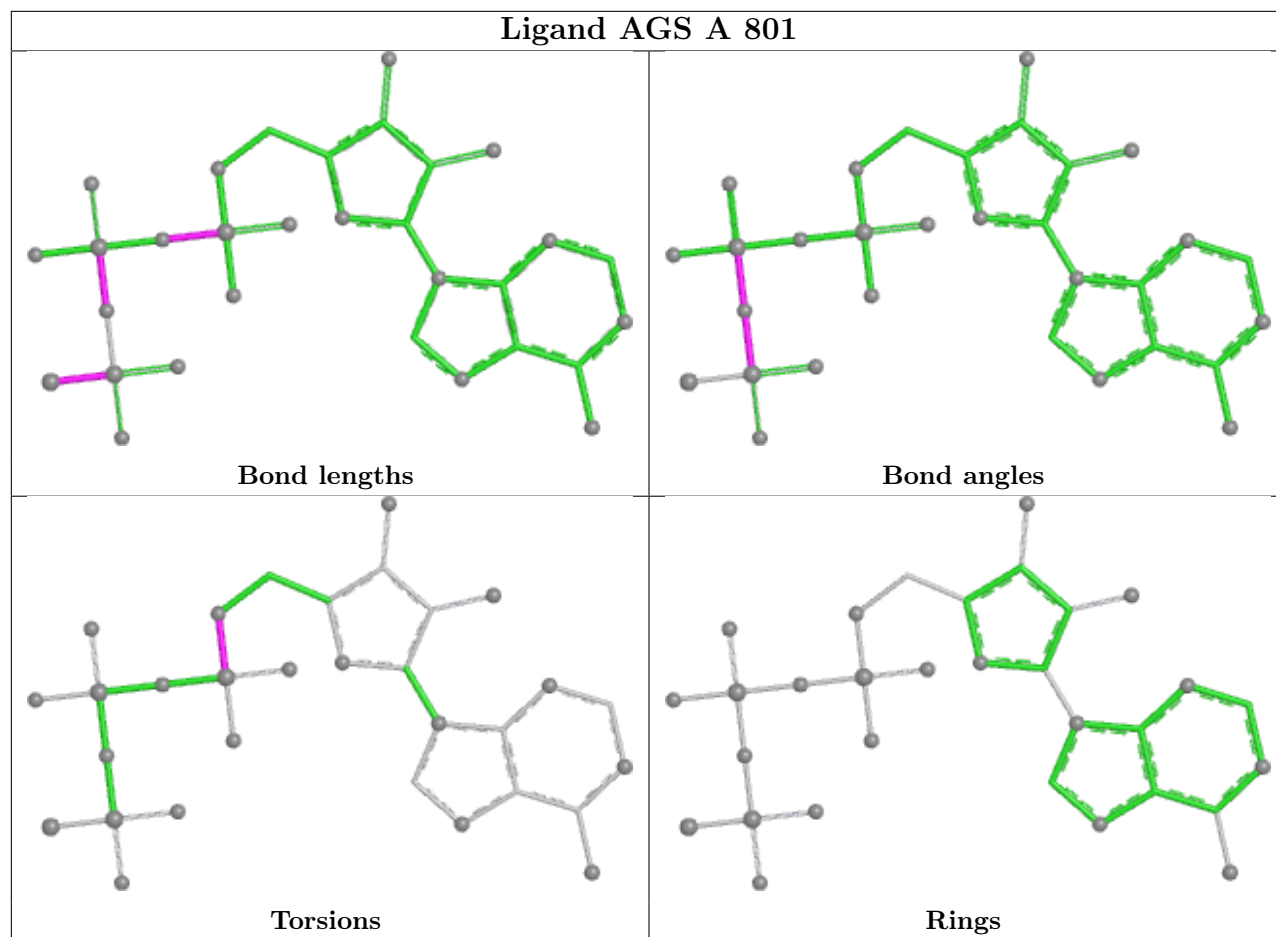


Torsions

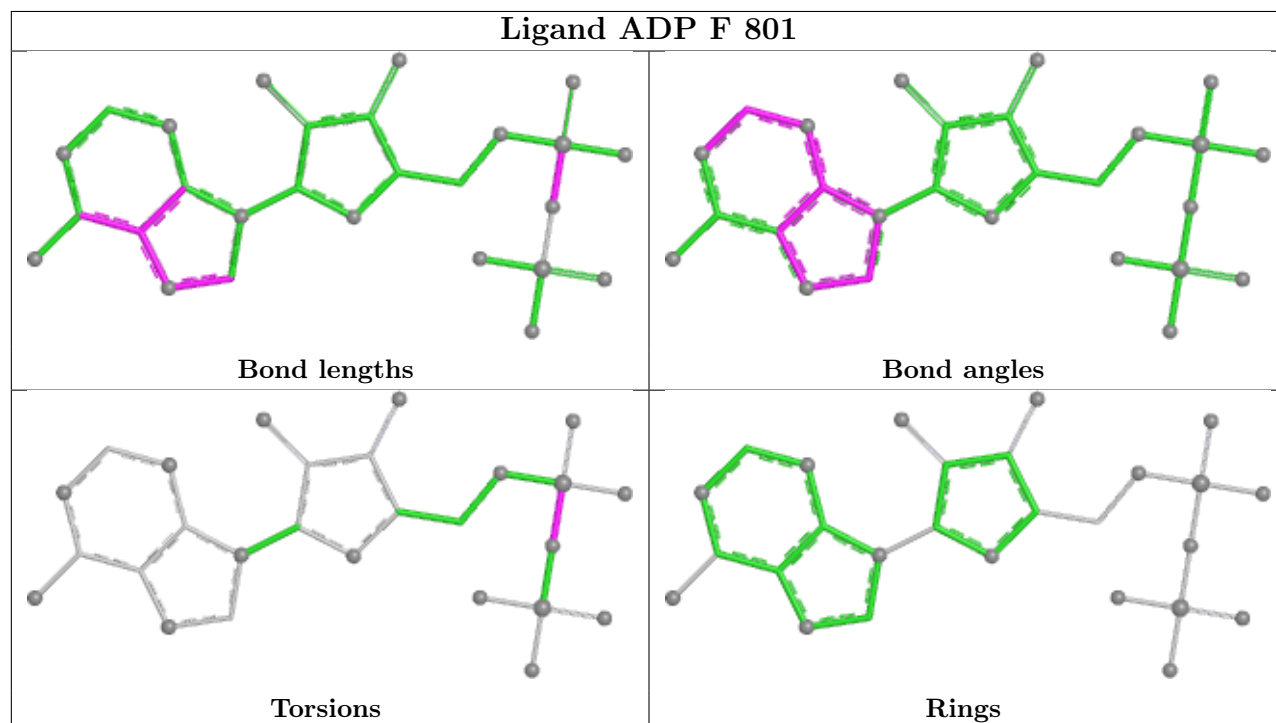


Rings

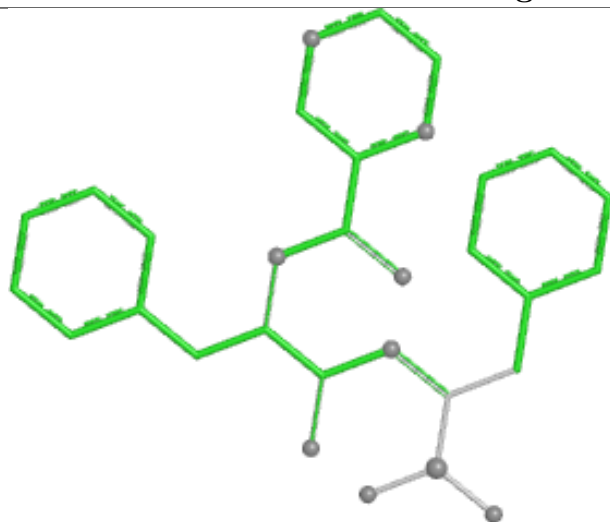
Ligand AGS A 801



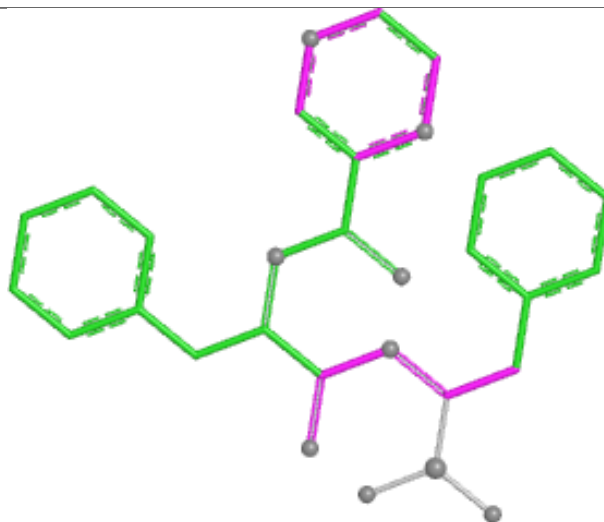
Ligand ADP F 801



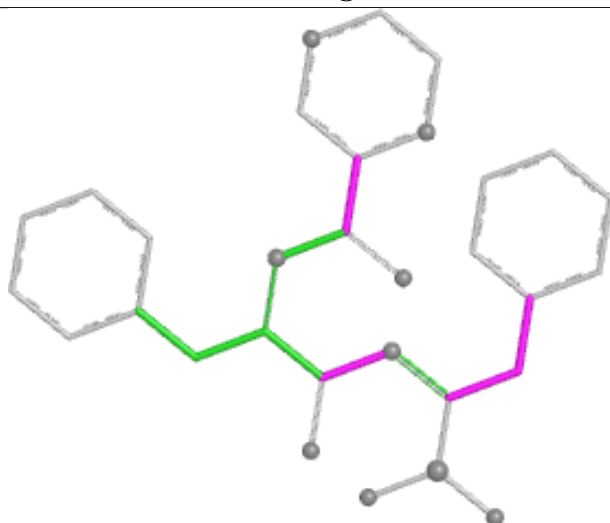
Ligand 4KZ D 802



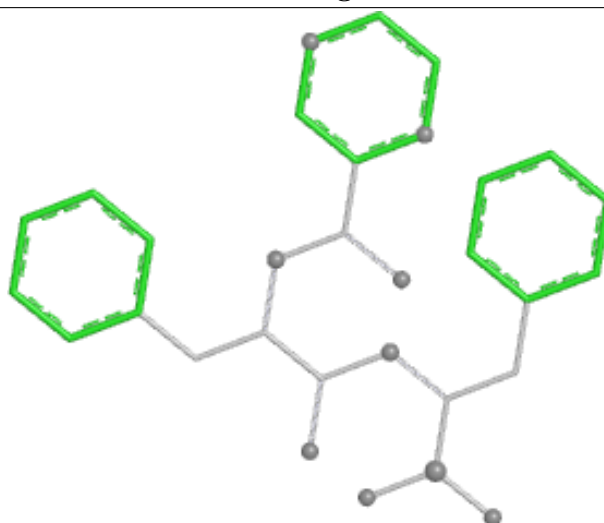
Bond lengths



Bond angles

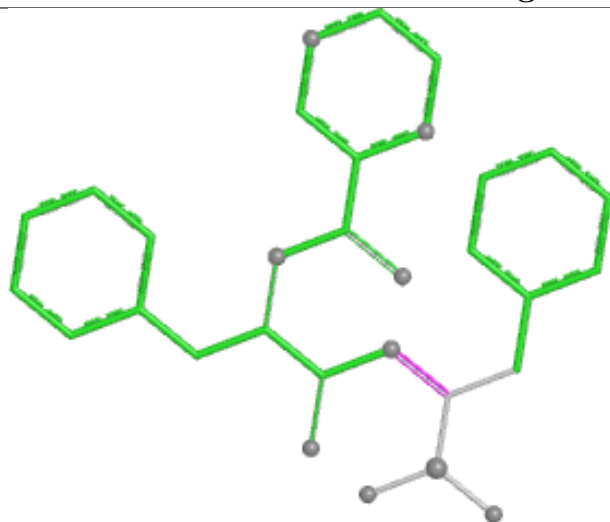


Torsions

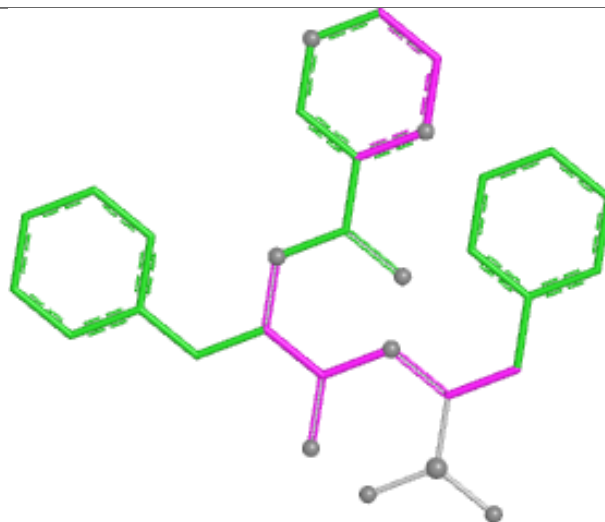


Rings

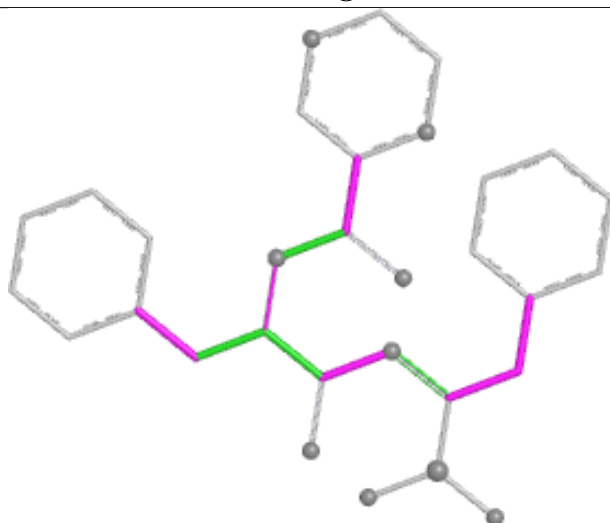
Ligand 4KZ E 801



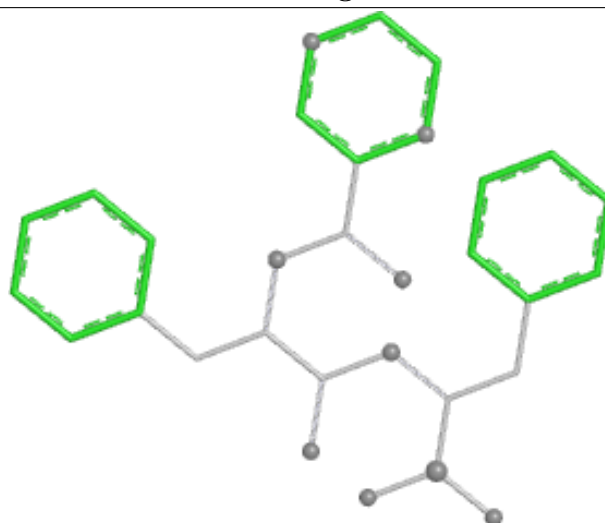
Bond lengths



Bond angles

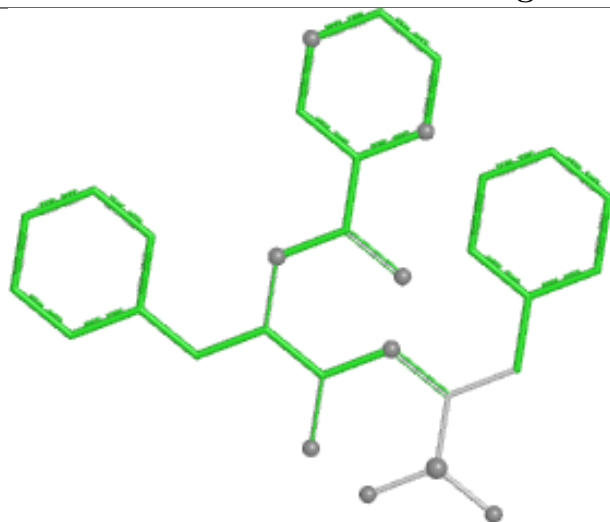


Torsions

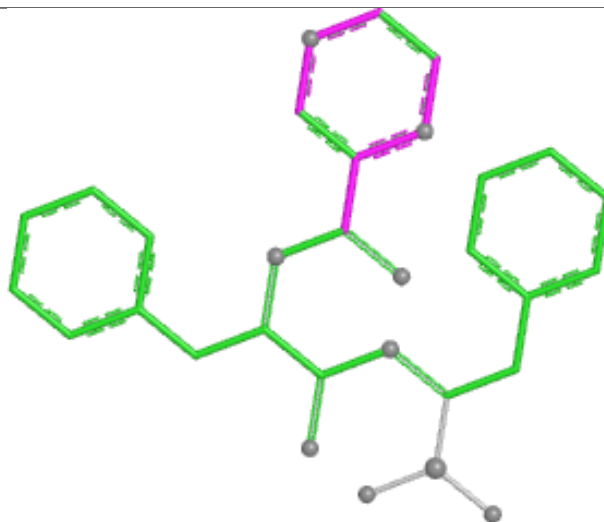


Rings

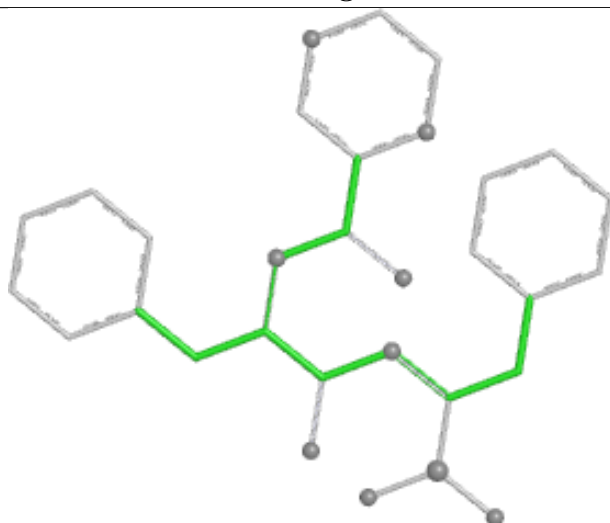
Ligand 4KZ C 802



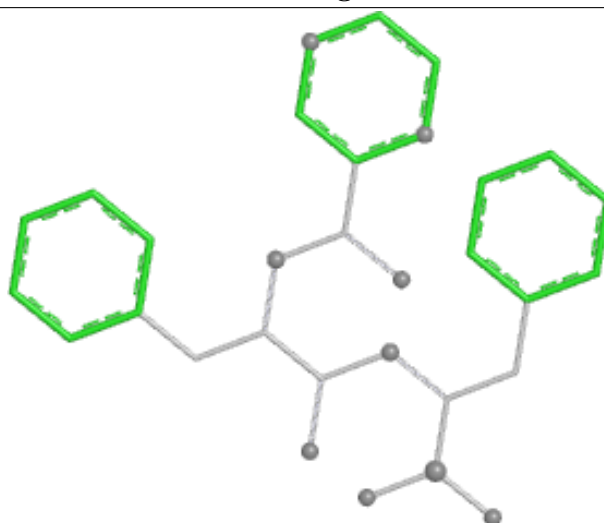
Bond lengths



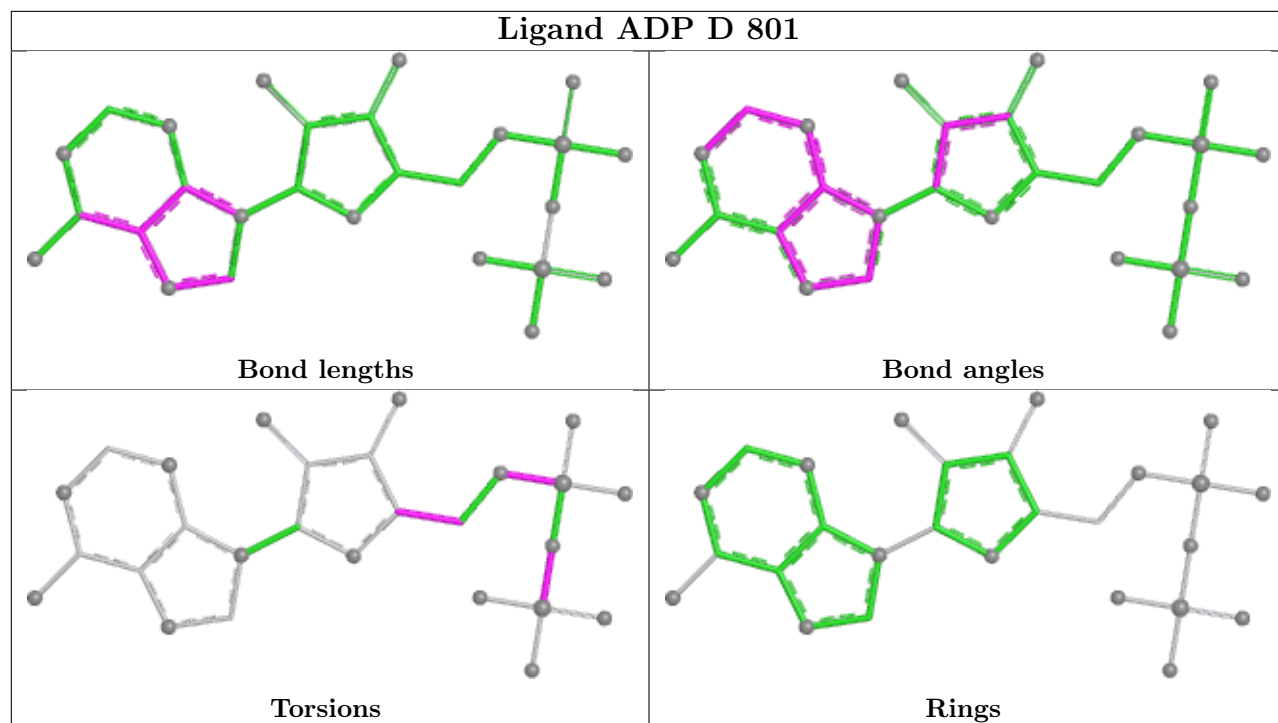
Bond angles



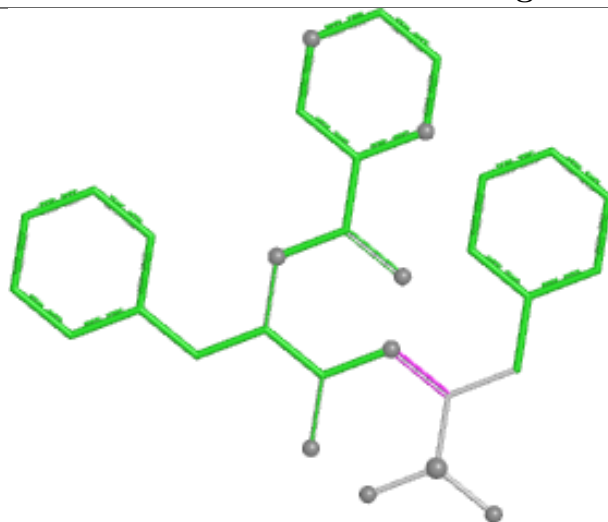
Torsions



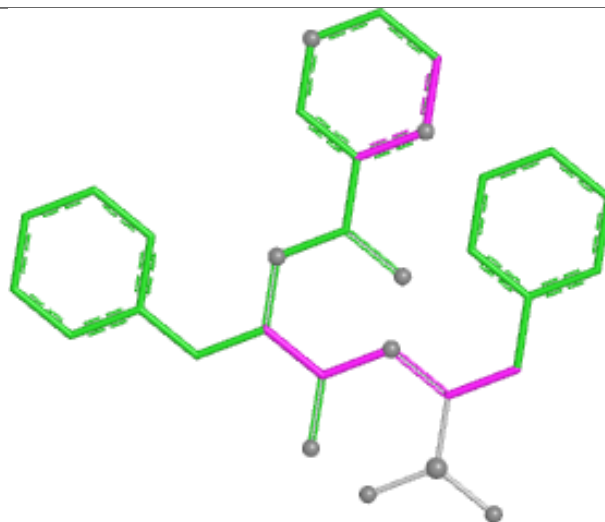
Rings



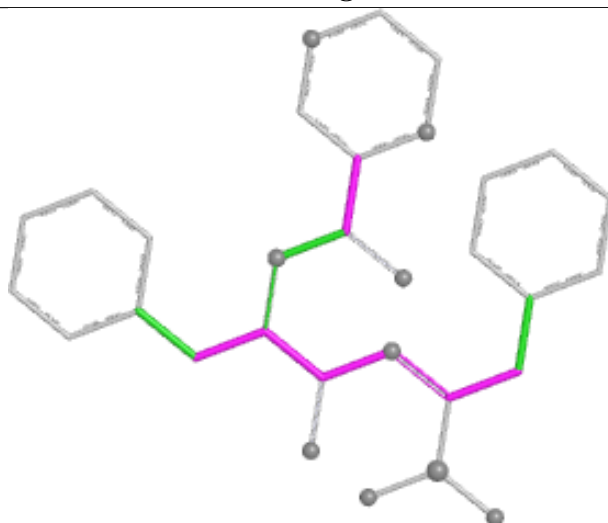
Ligand 4KZ A 802



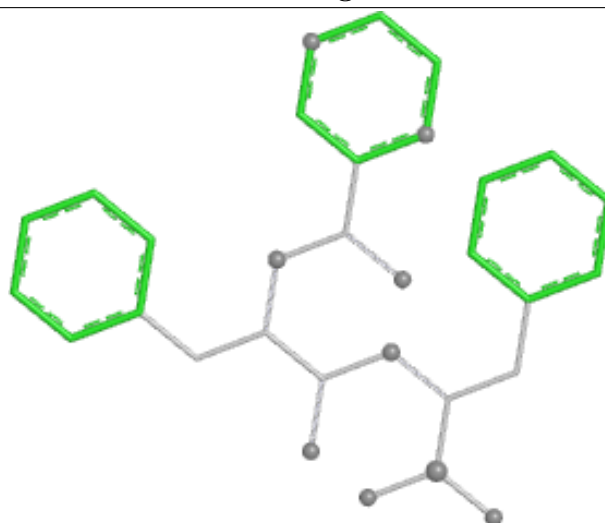
Bond lengths



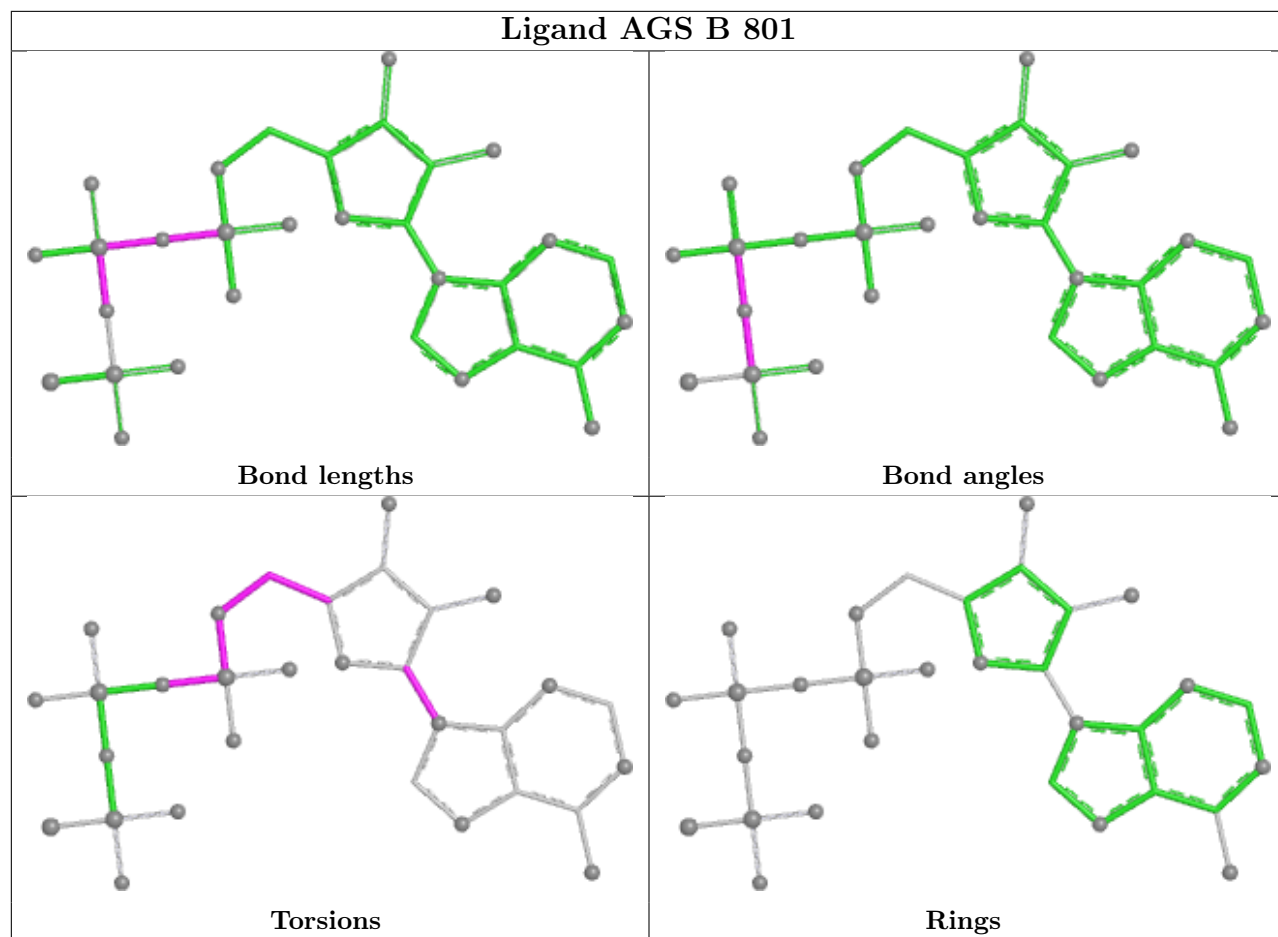
Bond angles

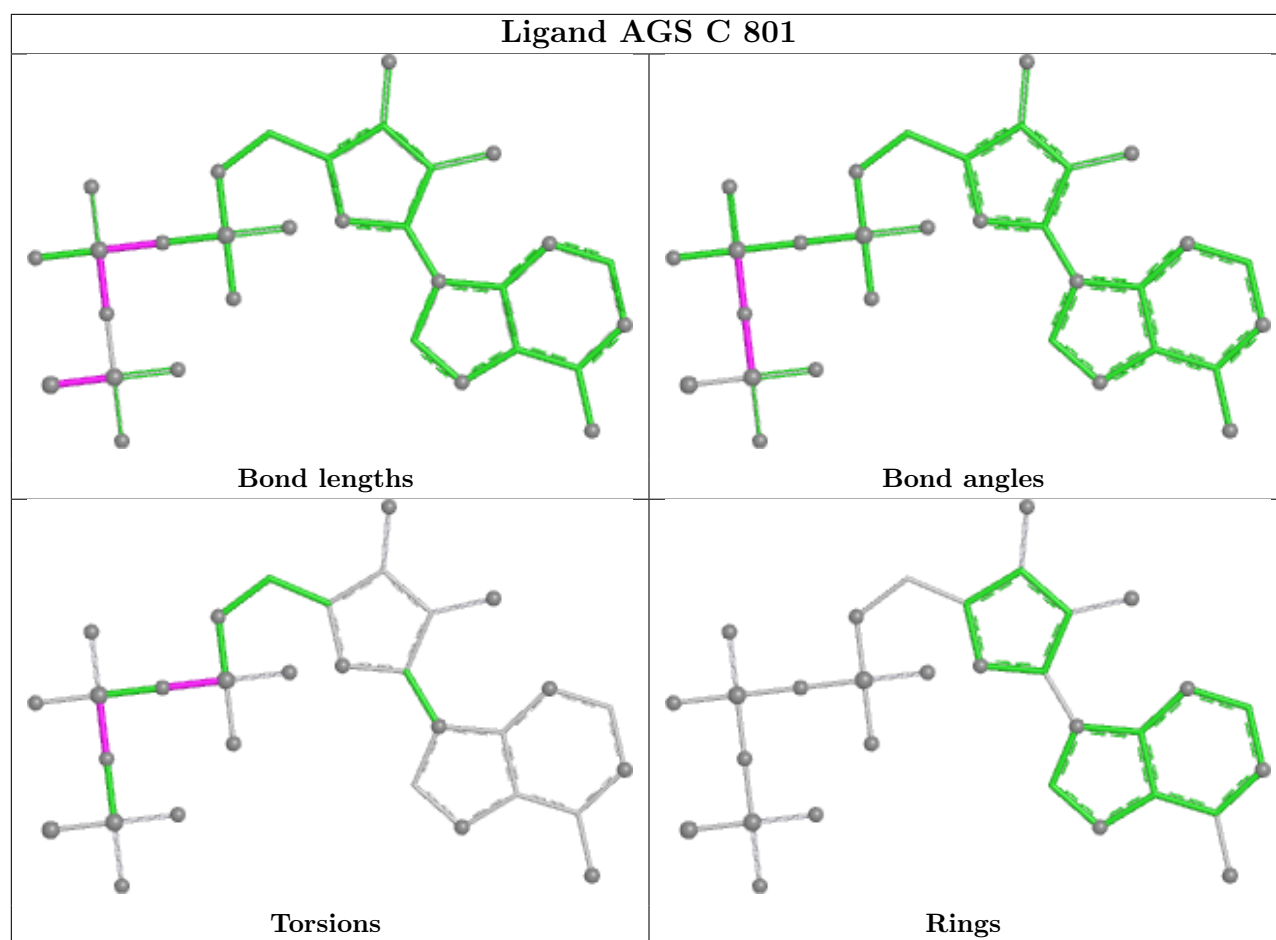


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
1	B	2
1	D	2
1	E	2
1	F	2
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	589:GLU	C	590:THR	N	3.70
1	B	589:GLU	C	590:THR	N	3.68
1	C	589:GLU	C	590:THR	N	3.40
1	D	589:GLU	C	590:THR	N	3.19
1	E	589:GLU	C	590:THR	N	3.07
1	F	589:GLU	C	590:THR	N	2.98
1	F	676:GLY	C	677:PRO	N	1.77
1	D	676:GLY	C	677:PRO	N	1.71
1	A	676:GLY	C	677:PRO	N	1.65
1	B	676:GLY	C	677:PRO	N	1.16
1	A	679:ALA	C	680:GLY	N	1.12
1	E	679:ALA	C	680:GLY	N	1.04

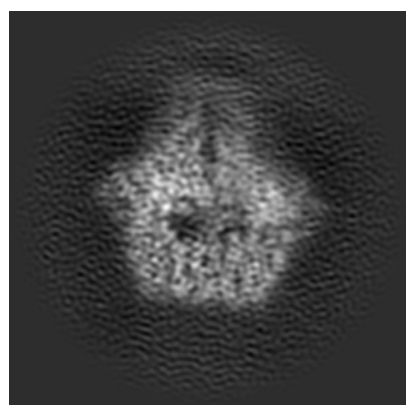
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21870. These allow visual inspection of the internal detail of the map and identification of artifacts.

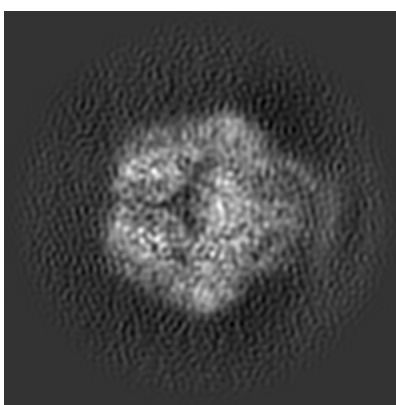
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

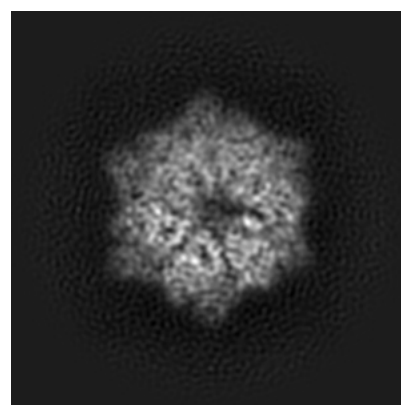
6.1.1 Primary map



X



Y

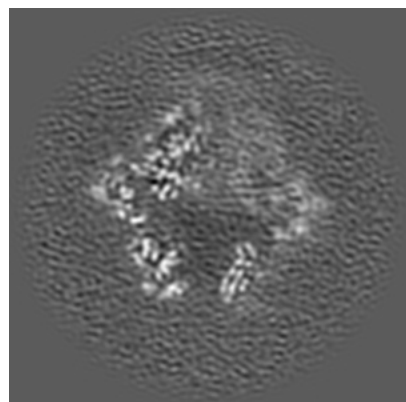


Z

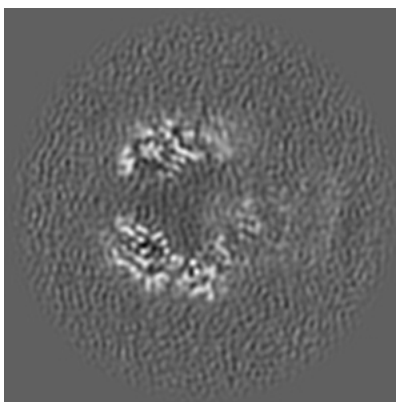
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

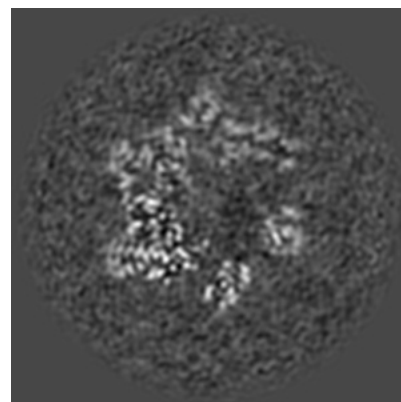
6.2.1 Primary map



X Index: 168



Y Index: 168

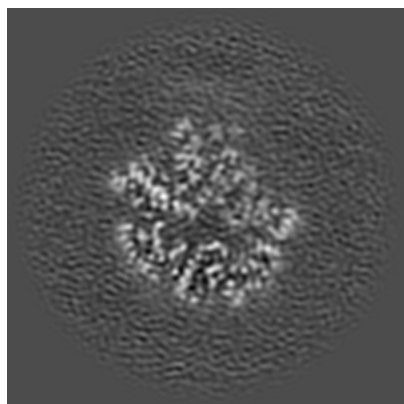


Z Index: 168

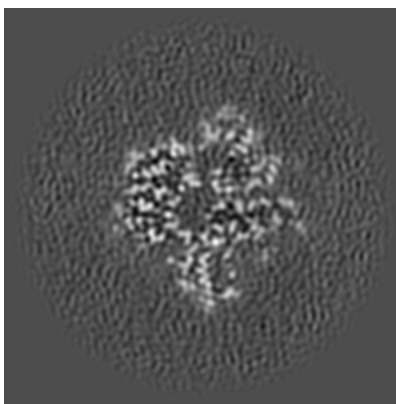
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

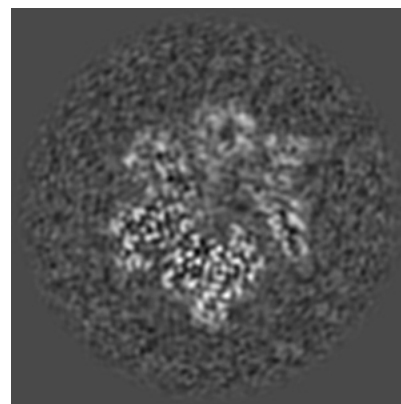
6.3.1 Primary map



X Index: 140



Y Index: 130

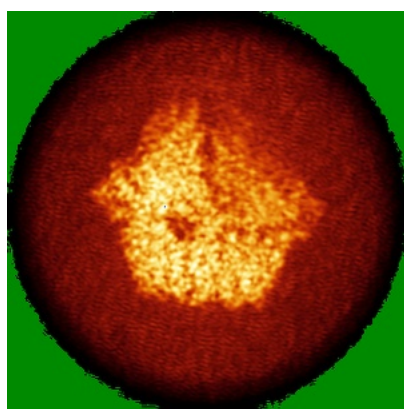


Z Index: 181

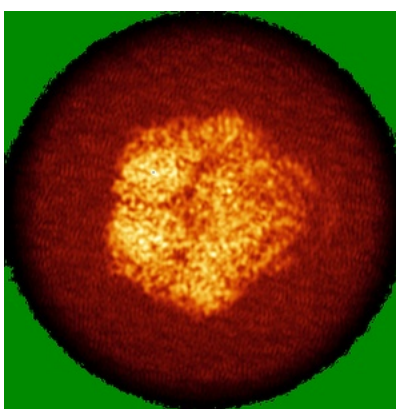
The images above show the largest variance slices of the map in three orthogonal directions.

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

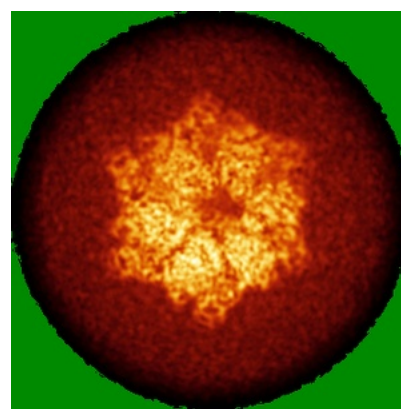
6.4.1 Primary map



X



Y

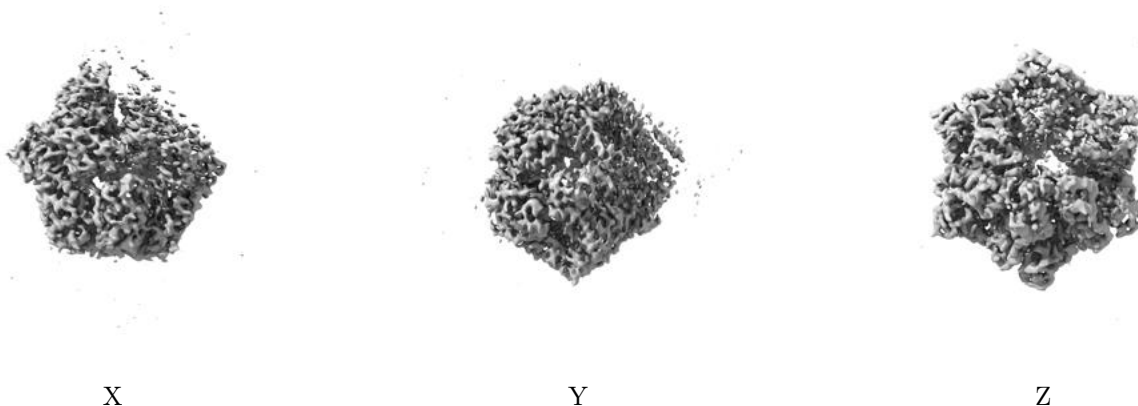


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.32. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

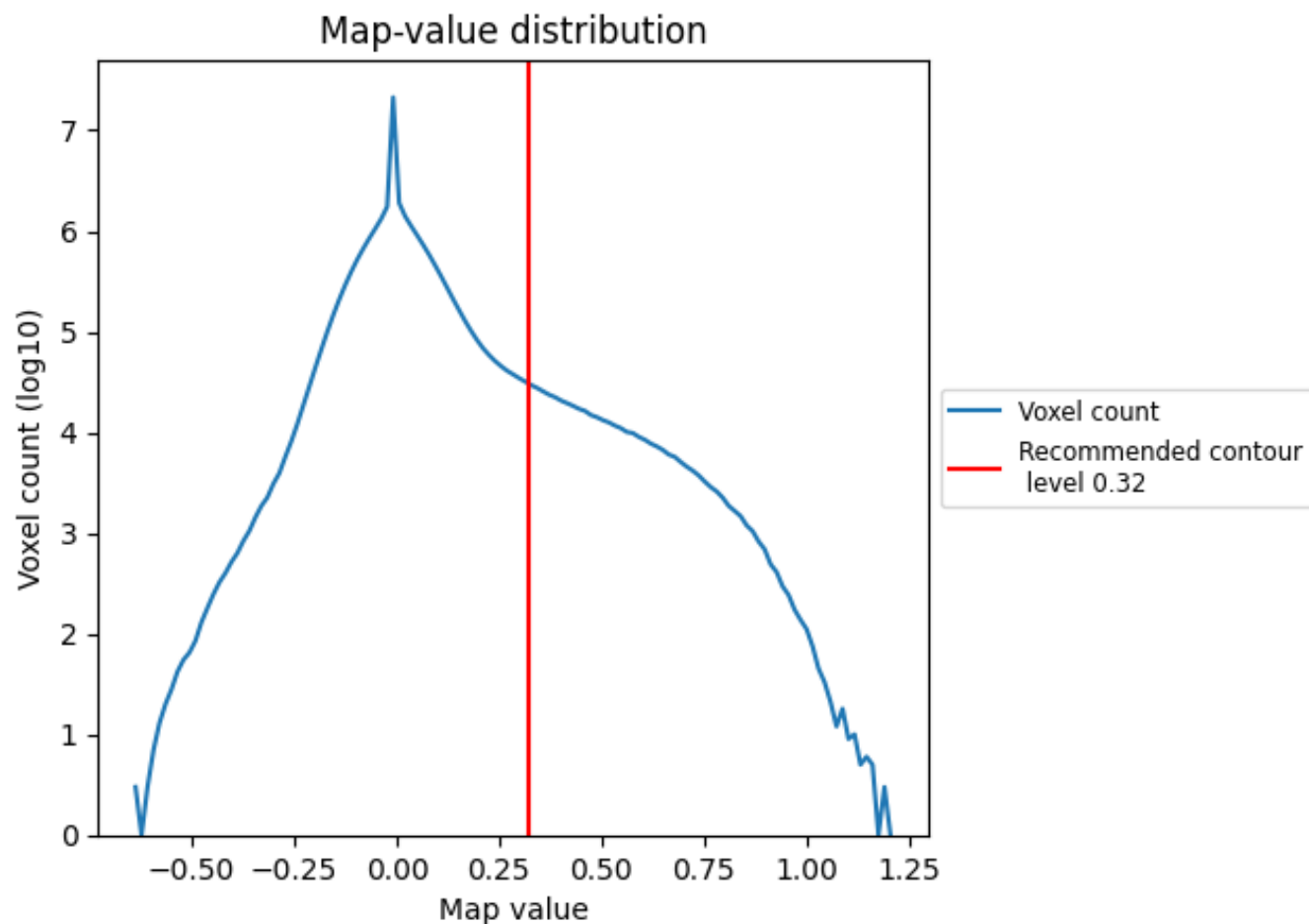
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

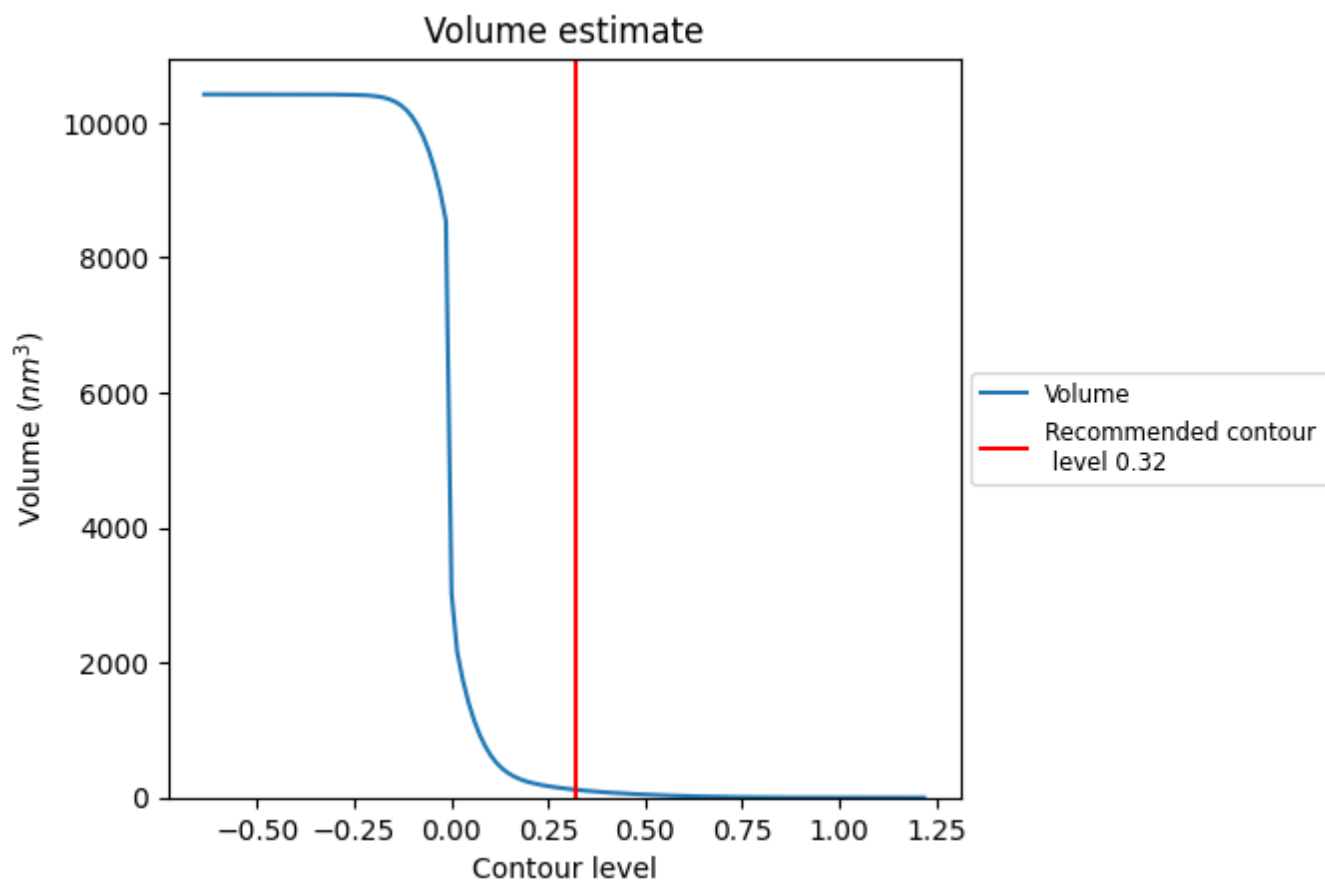
This section contains the results of statistical analysis of the map.

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.

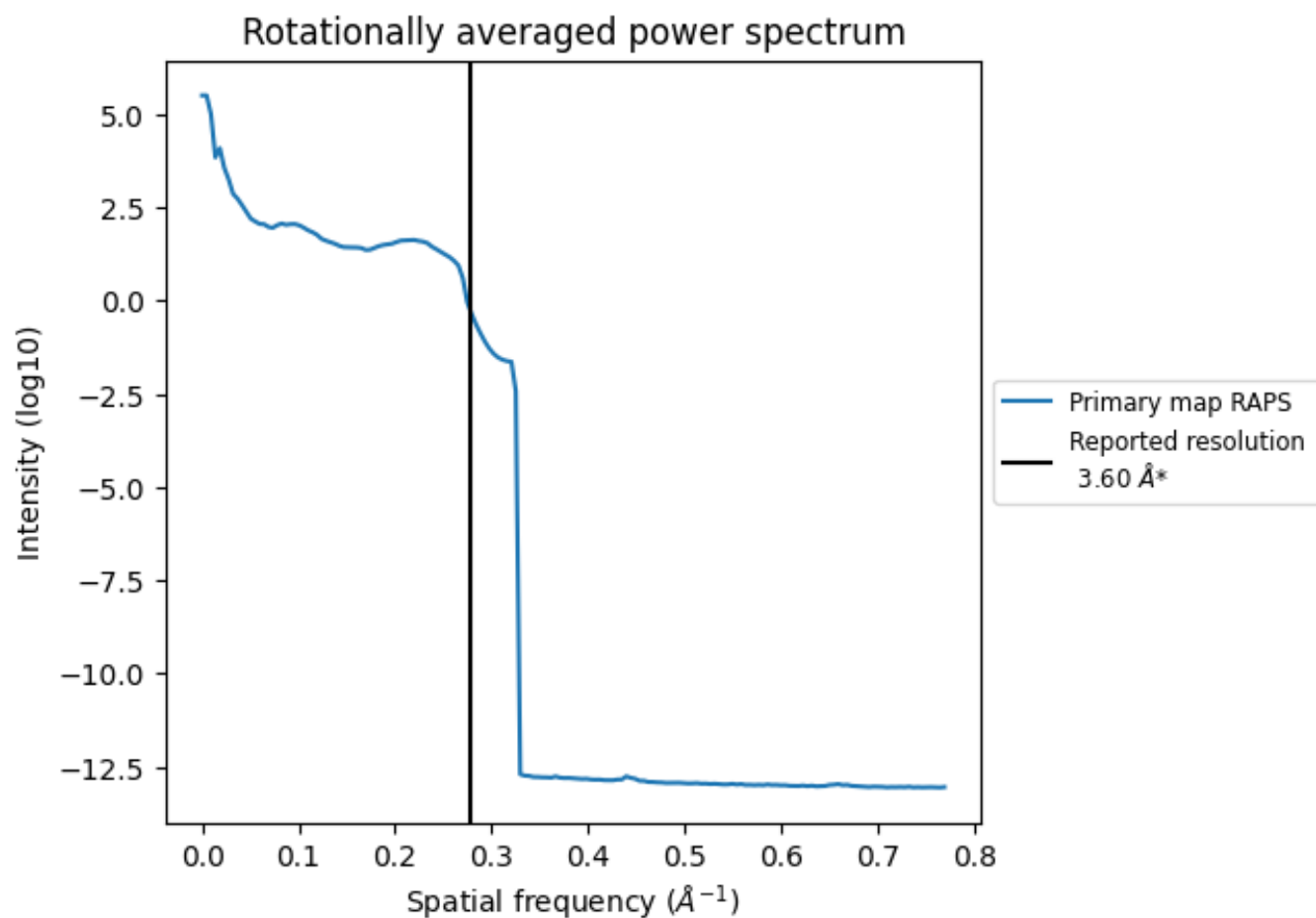
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 117 nm³; this corresponds to an approximate mass of 105 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.

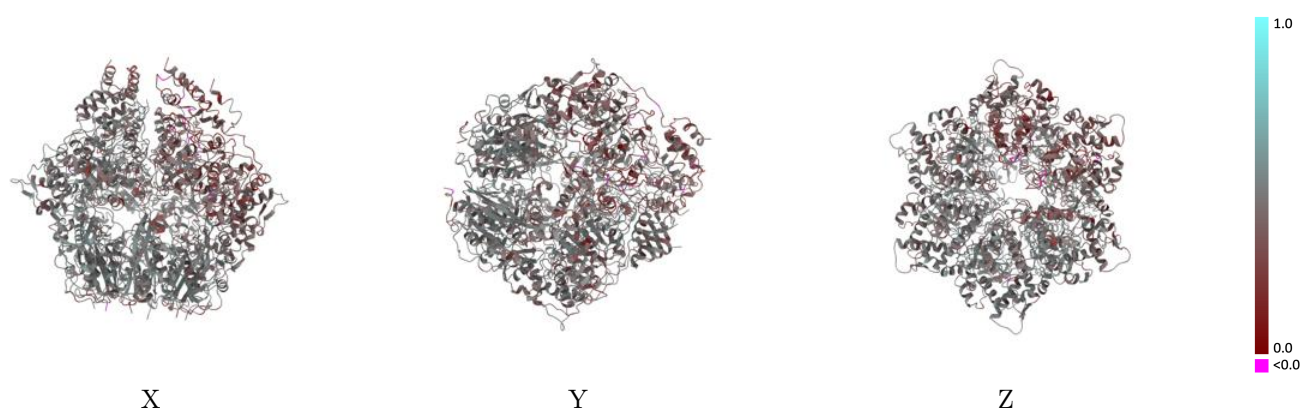
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21870 and PDB model 6WQH. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

This section was not generated.

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

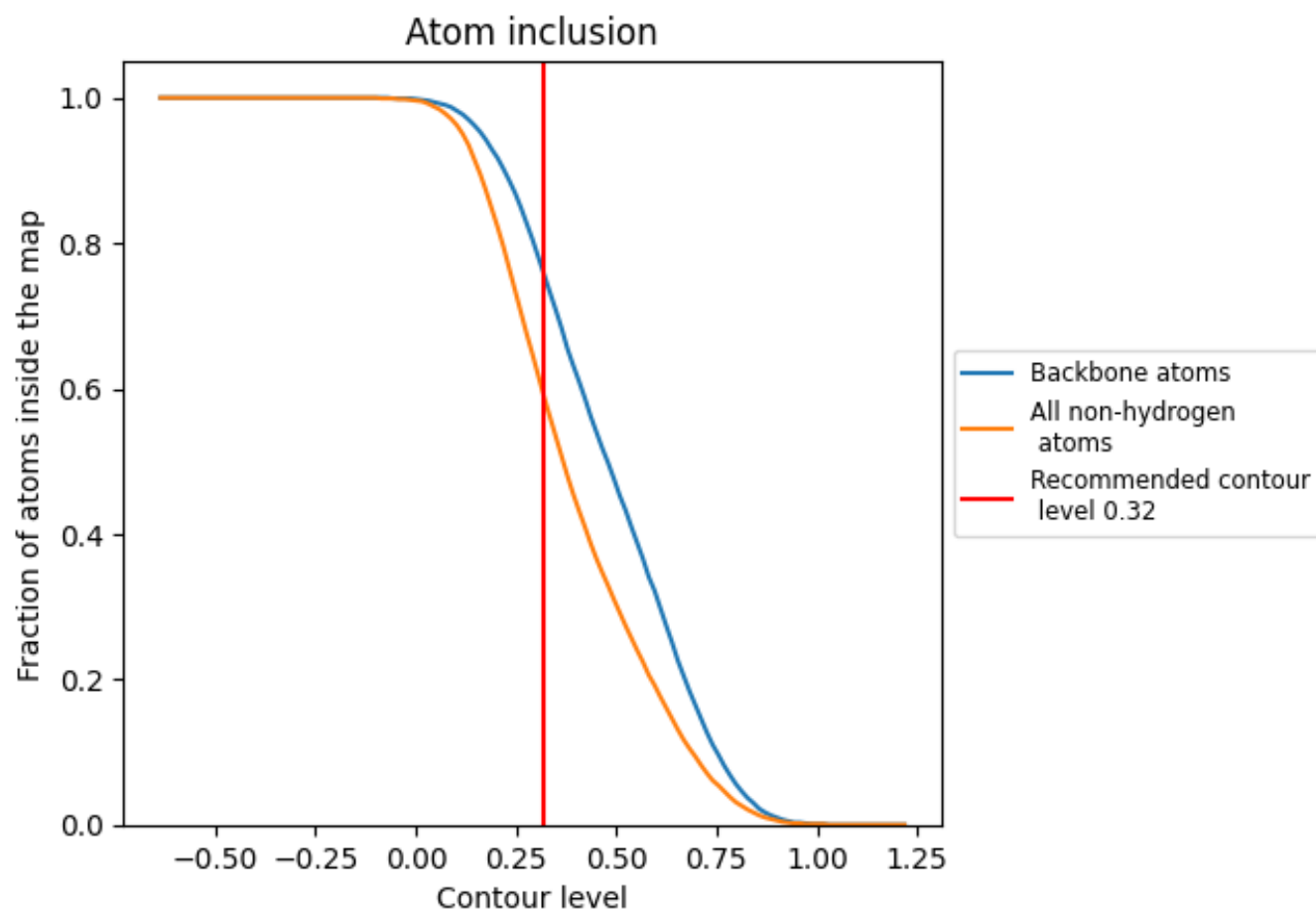


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.32) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5880	0.4310
A	0.6710	0.4560
B	0.7110	0.4680
C	0.6890	0.4620
D	0.5850	0.4330
E	0.4210	0.3730
F	0.4550	0.3930
S	0.4360	0.5310

1.0

0.0

<0.0