



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 09:36 AM UTC

PDB ID : 6OAY / pdb_00006oay
EMDB ID : EMD-20005
Title : Structure of the hyperactive ClpB mutant K476C, bound to casein, post-state
Authors : Rizo, A.R.; Lin, J.-B.; Gates, S.N.; Tse, E.; Bart, S.M.; Castellano, L.M.;
Dimaio, F.; Shorter, J.; Southworth, D.R.
Deposited on : 2019-03-18
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

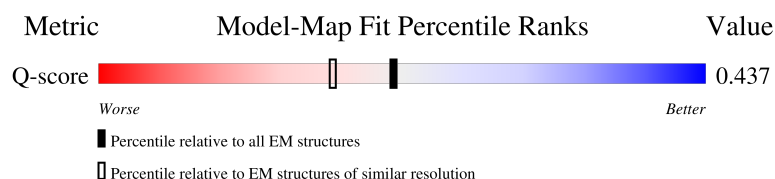
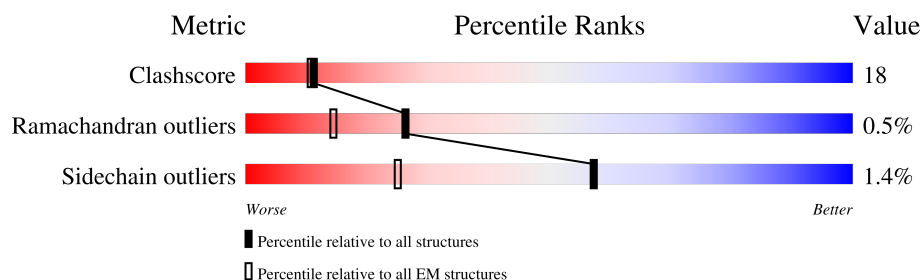
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	867	34% 44% 19% 37%
1	B	867	12% 46% 19% 34%
1	C	867	43% 21% 34%
1	D	867	45% 20% 34%

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Mol	Chain	Length	Quality of chain
1	E	867	44%21%34%
1	F	867	42%46%18%36%
2	P	26	23%81%19%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27261 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.

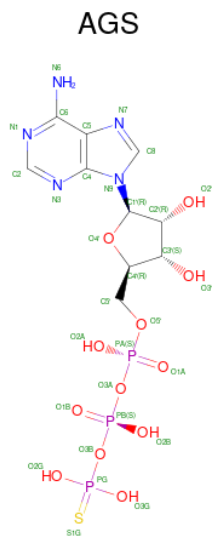
- Molecule 1 is a protein called Hyperactive disaggregase ClpB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	570	Total	C	N	O	S	0	0
			4510	2833	818	844	15		
1	F	558	Total	C	N	O	S	0	0
			4426	2779	806	826	15		
1	E	570	Total	C	N	O	S	0	0
			4510	2833	818	844	15		
1	D	570	Total	C	N	O	S	0	0
			4510	2833	818	844	15		
1	B	570	Total	C	N	O	S	0	0
			4510	2833	818	844	15		
1	A	548	Total	C	N	O	S	0	0
			4340	2726	787	812	15		

- Molecule 2 is a protein called Alpha-S1-casein.

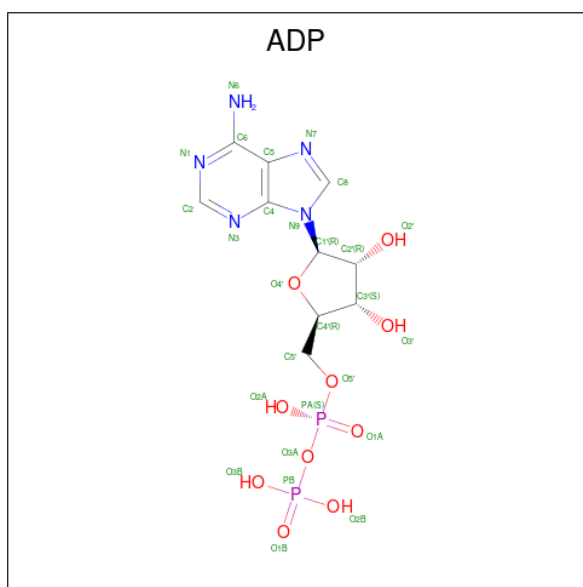
Mol	Chain	Residues	Atoms				AltConf	Trace
2	P	26	Total	C	N	O	0	0
			130	78	26	26		

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

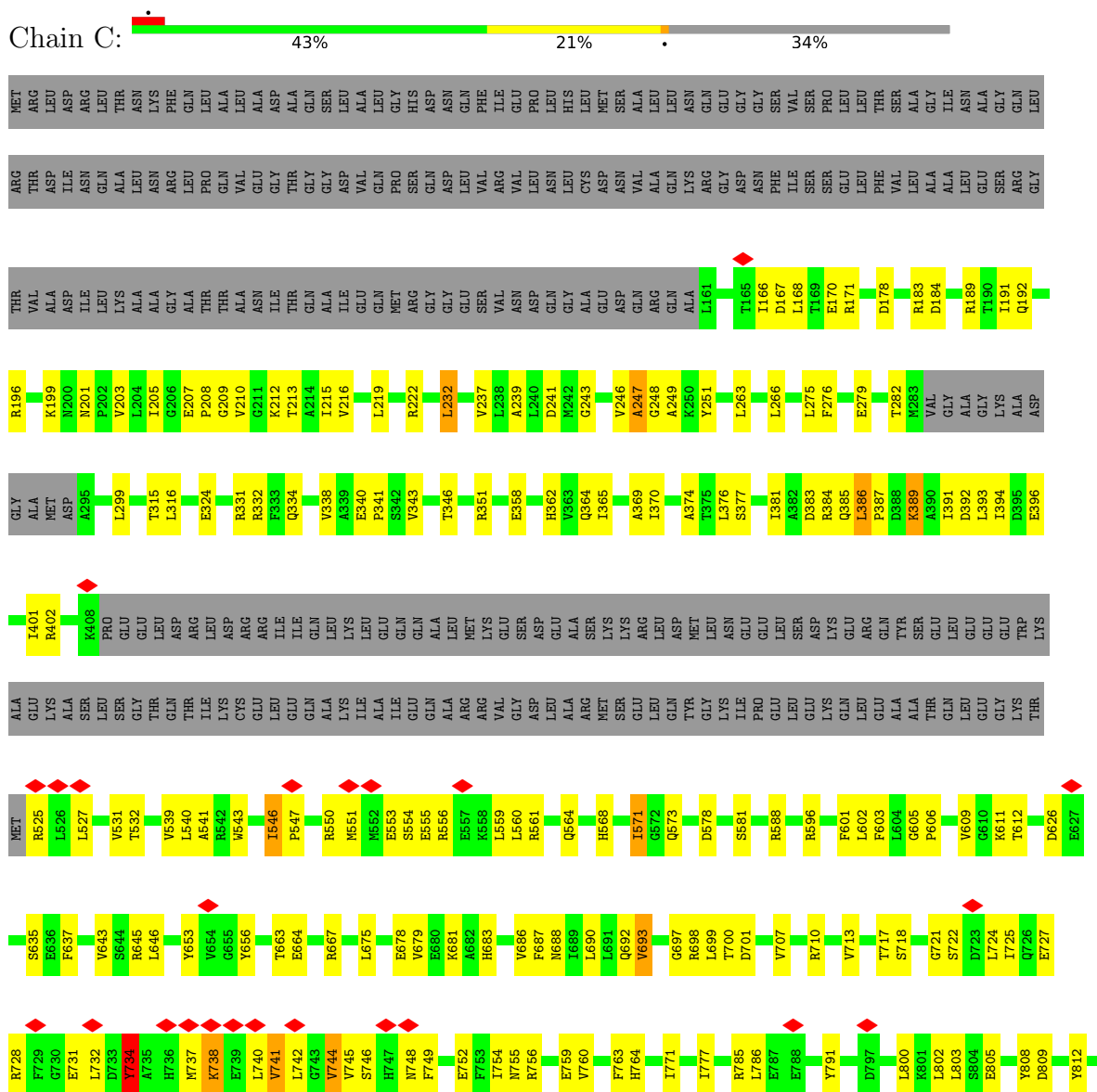


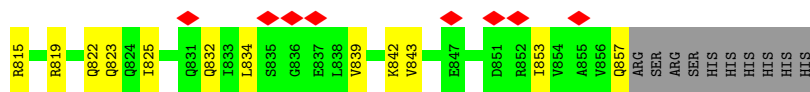
Mol	Chain	Residues	Atoms					AltConf
4	F	1	Total 27	C 10	N 5	O 10	P 2	0
4	B	1	Total 27	C 10	N 5	O 10	P 2	0
4	A	1	Total 27	C 10	N 5	O 10	P 2	0
4	A	1	Total 27	C 10	N 5	O 10	P 2	0

3 Residue-property plots

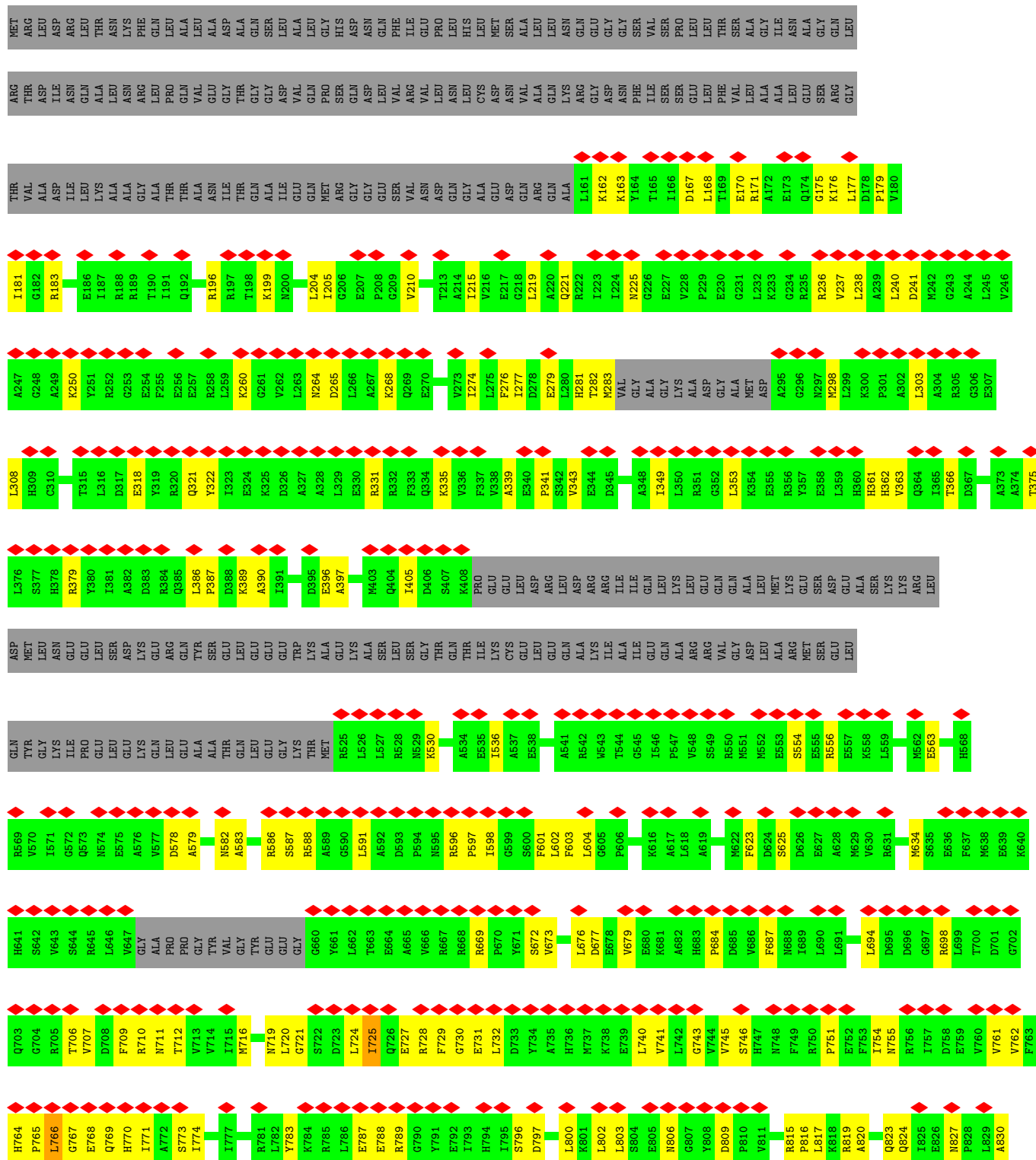
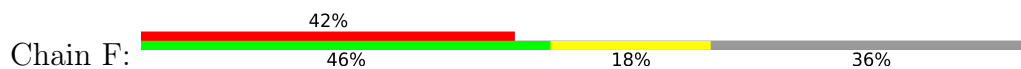
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

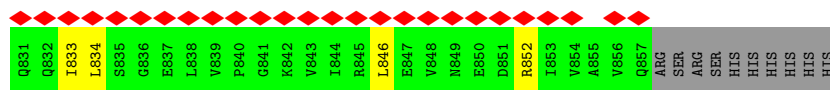
• Molecule 1: Hyperactive disaggregase ClpB





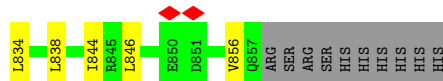
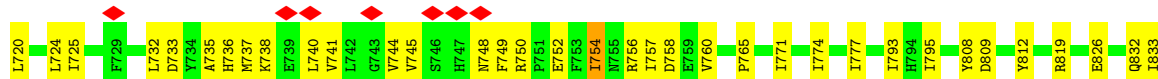
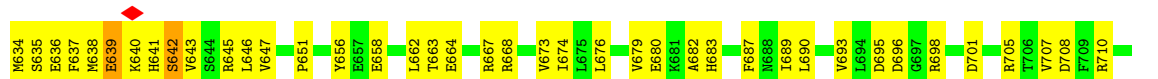
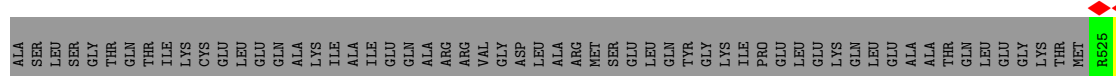
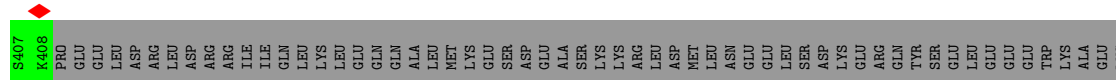
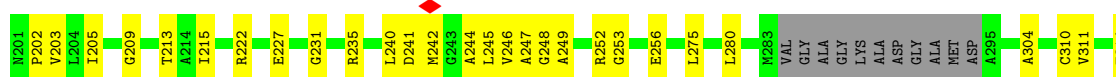
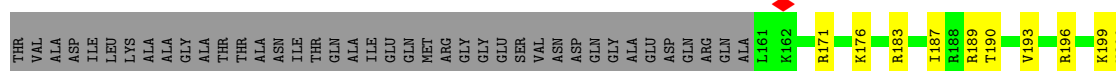
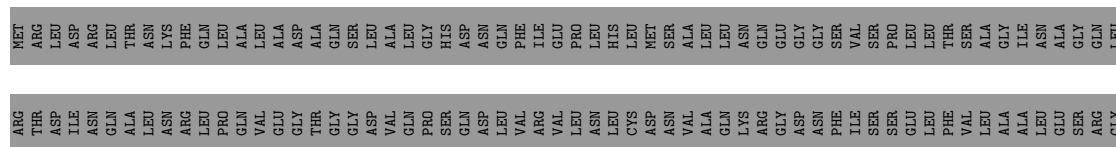
• Molecule 1: Hyperactive disaggregase ClpB





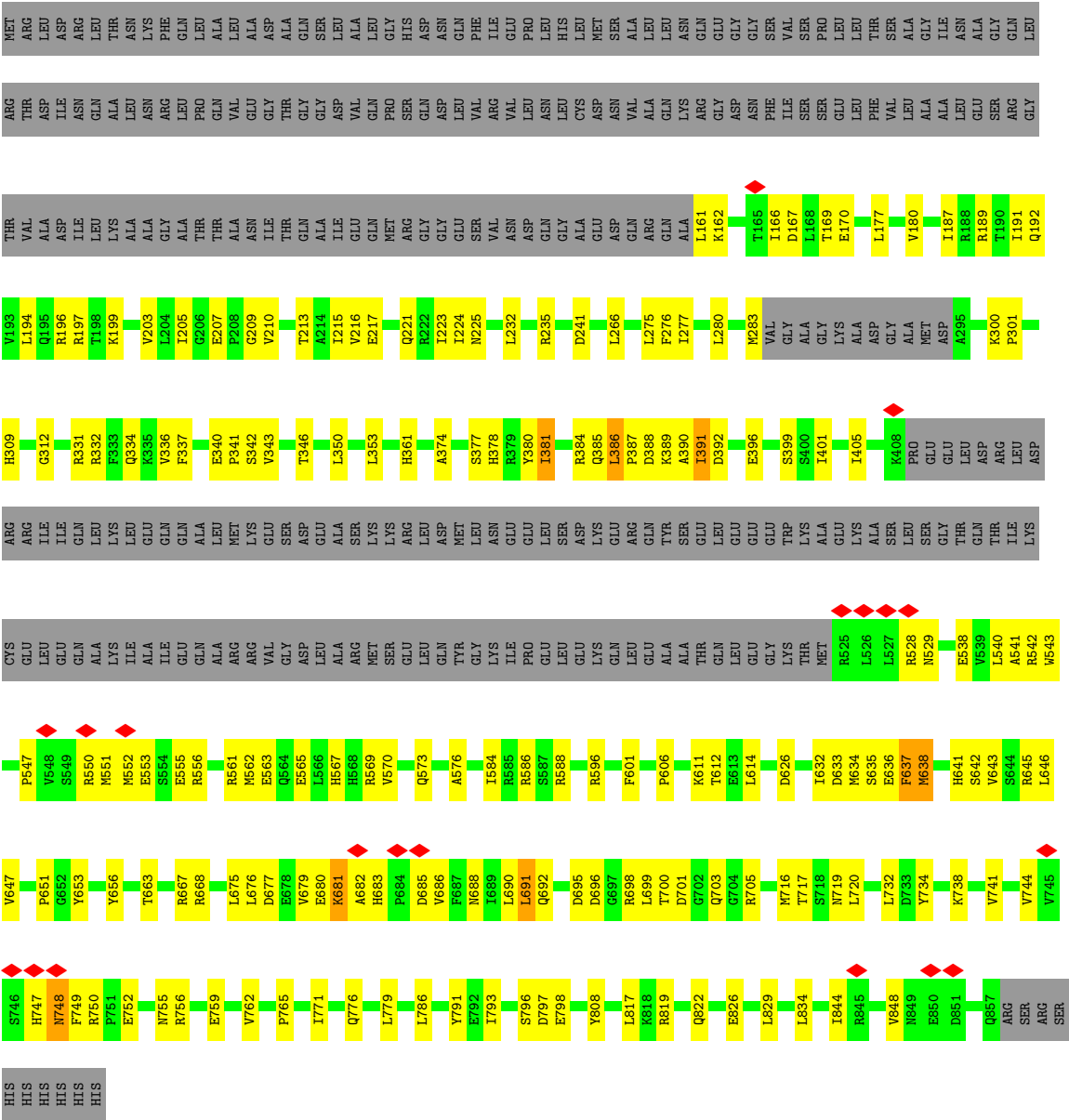
• Molecule 1: Hyperactive disaggregase ClpB

Chain E: 44% 21% 34%

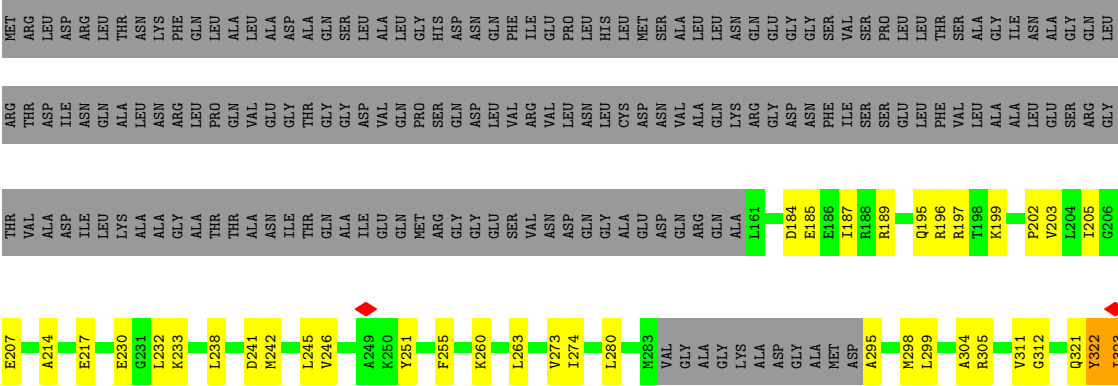


• Molecule 1: Hyperactive disaggregase ClpB

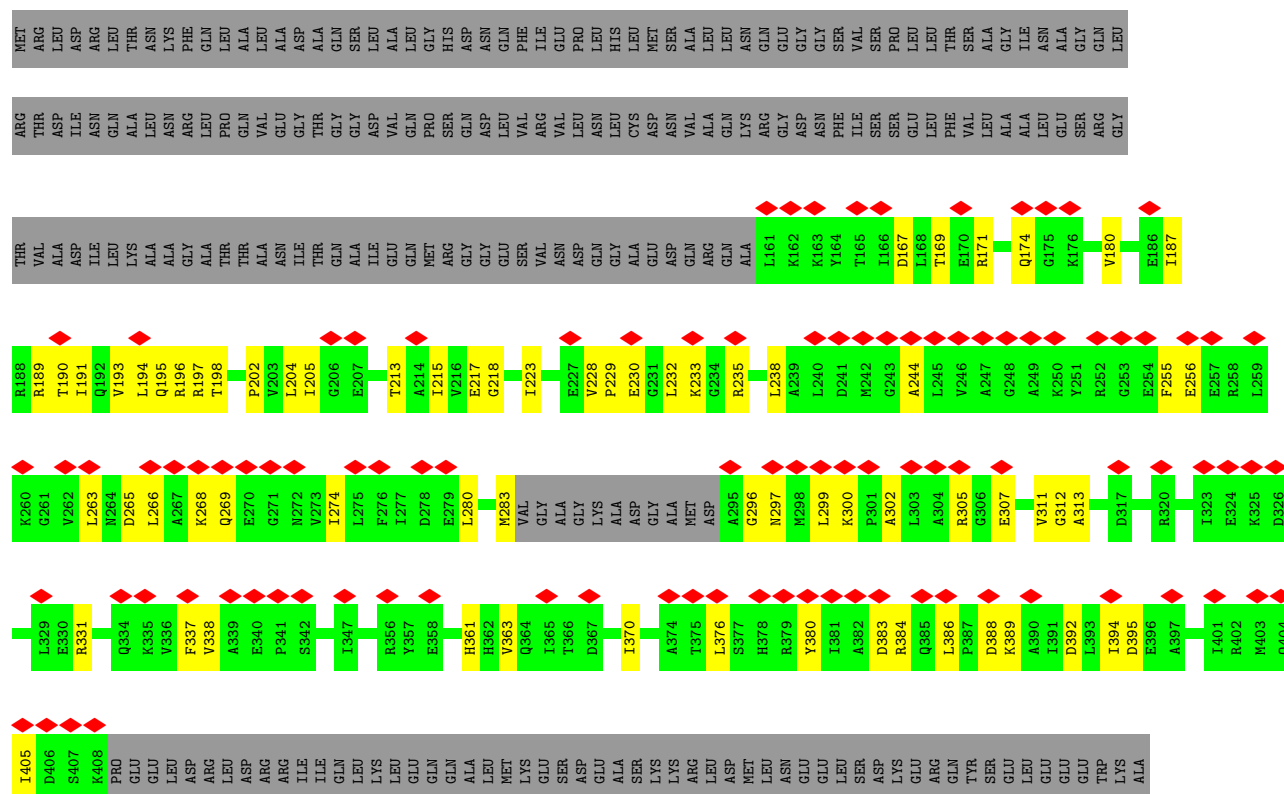
Chain D: 45% 20% 34%



● Molecule 1: Hyperactive disaggregase ClpB



- Molecule 1: Hyperactive disaggregase ClpB



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	213059	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 ($e^-/\text{\AA}^2$)	56	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	0.425	Depositor
Minimum map value	-0.235	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.04	Depositor
Map size ($\text{\AA}$)	264.192, 264.192, 264.192	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.032, 1.032, 1.032	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/4405	0.61	1/5940 (0.0%)
1	B	0.47	0/4576	0.67	1/6172 (0.0%)
1	C	0.63	0/4576	0.73	2/6172 (0.0%)
1	D	0.67	0/4576	0.73	3/6172 (0.0%)
1	E	0.56	0/4576	0.67	0/6172
1	F	0.25	0/4487	0.62	0/6048
All	All	0.50	0/27196	0.67	7/36676 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	321	GLN	N-CA-C	-9.82	100.66	111.36
1	A	793	ILE	N-CA-C	-6.92	104.54	111.88
1	C	324	GLU	N-CA-C	-6.45	104.62	114.16
1	C	734	TYR	CB-CA-C	-5.43	110.30	116.54
1	D	336	VAL	CA-C-N	5.41	131.87	121.54
1	D	336	VAL	C-N-CA	5.41	131.87	121.54
1	D	748	ASN	N-CA-C	5.27	114.56	108.49

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4340	0	4404	117	0
1	B	4510	0	4586	152	0
1	C	4510	0	4586	218	0
1	D	4510	0	4586	269	0
1	E	4510	0	4586	212	0
1	F	4426	0	4515	136	0
2	P	130	0	31	6	0
3	B	31	0	12	2	0
3	C	62	0	24	8	0
3	D	62	0	24	7	0
3	E	62	0	24	9	0
4	A	54	0	24	1	0
4	B	27	0	12	1	0
4	F	27	0	12	0	0
All	All	27261	0	27426	991	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 18.

All (991) 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:737:MET:HE2	1:C:760:VAL:CG1	1.35	1.51
1:D:551:MET:HE3	1:D:556:ARG:CD	1.48	1.43
1:F:802:LEU:CD2	1:F:803:LEU:HD12	1.61	1.29
1:B:322:TYR:OH	1:B:329:LEU:HB3	1.32	1.26
1:D:551:MET:HE3	1:D:556:ARG:CG	1.68	1.22
1:F:724:LEU:O	1:F:725:ILE:HG13	1.40	1.21
1:C:168:LEU:HD12	1:C:237:VAL:CG1	1.70	1.19
1:C:737:MET:CE	1:C:760:VAL:CG1	2.23	1.16
1:E:638:MET:HG2	1:D:685:ASP:CG	1.70	1.15
1:C:724:LEU:CD1	1:C:740:LEU:CD2	2.25	1.15
1:B:654:VAL:HG11	1:A:656:TYR:HB3	1.29	1.14
1:F:802:LEU:HD23	1:F:803:LEU:HD12	1.14	1.14
1:C:737:MET:HE2	1:C:760:VAL:HG11	1.18	1.13
1:C:737:MET:CE	1:C:760:VAL:HG11	1.78	1.13
1:F:802:LEU:HD22	1:F:803:LEU:CD1	1.78	1.13
1:D:637:PHE:HB3	1:D:642:SER:HB3	1.29	1.12
1:E:205:ILE:HG21	1:E:319:TYR:CD1	1.84	1.12
1:C:725:ILE:HG23	1:C:734:TYR:OH	1.45	1.12
1:E:638:MET:HG2	1:D:685:ASP:OD1	1.46	1.11
1:F:802:LEU:CD2	1:F:803:LEU:CD1	2.27	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:551:MET:HG2	1:D:556:ARG:HG3	1.32	1.11
1:C:724:LEU:HD12	1:C:740:LEU:HD21	1.32	1.09
1:E:199:LYS:HG3	1:E:331:ARG:O	1.54	1.08
1:B:185:GLU:O	1:B:189:ARG:HG3	1.52	1.08
1:D:341:PRO:O	1:D:386:LEU:HD13	1.54	1.07
1:C:385:GLN:O	1:C:389:LYS:HE2	1.52	1.07
1:E:634:MET:HA	1:E:637:PHE:CD2	1.89	1.07
1:D:551:MET:CE	1:D:556:ARG:CD	2.33	1.07
1:C:724:LEU:HD12	1:C:740:LEU:CD2	1.84	1.06
1:C:737:MET:HE2	1:C:760:VAL:HG12	1.06	1.05
1:E:634:MET:HA	1:E:637:PHE:HD2	1.18	1.05
1:B:540:LEU:HG	1:B:546:ILE:CD1	1.87	1.05
1:F:732:LEU:H	1:F:766:LEU:HD22	1.22	1.04
1:D:741:VAL:CG2	1:D:749:PHE:CE1	2.41	1.04
1:C:724:LEU:HD11	1:C:740:LEU:HG	1.40	1.03
1:D:680:GLU:OE2	1:D:720:LEU:HD12	1.57	1.03
1:C:724:LEU:HD11	1:C:740:LEU:CG	1.89	1.02
1:D:551:MET:CE	1:D:556:ARG:HD2	1.91	1.01
1:D:551:MET:HE3	1:D:556:ARG:HG2	1.38	1.00
1:D:551:MET:HE3	1:D:556:ARG:HD2	1.42	0.99
1:E:638:MET:O	1:E:639:GLU:O	1.82	0.98
1:D:692:GLN:NE2	1:D:699:LEU:HA	1.79	0.98
1:C:334:GLN:NE2	1:D:543:TRP:CH2	2.32	0.97
1:D:744:VAL:HB	1:D:749:PHE:HB2	1.44	0.97
1:C:168:LEU:CD1	1:C:237:VAL:HG12	1.93	0.97
1:C:724:LEU:HD11	1:C:740:LEU:CD2	1.93	0.96
1:C:541:ALA:HB1	1:C:547:PRO:HG3	1.42	0.96
1:B:540:LEU:HG	1:B:546:ILE:HD11	1.42	0.96
1:F:803:LEU:HG	1:F:806:ASN:ND2	1.80	0.96
1:D:551:MET:HG2	1:D:556:ARG:CG	1.94	0.96
1:E:647:VAL:HG21	1:E:689:ILE:HD12	1.47	0.96
1:C:168:LEU:HD12	1:C:237:VAL:HG12	0.97	0.95
1:D:741:VAL:HG22	1:D:749:PHE:CE1	2.02	0.95
1:F:803:LEU:HG	1:F:806:ASN:HD21	1.30	0.94
1:D:377:SER:O	1:D:389:LYS:HE3	1.66	0.94
1:E:319:TYR:HE1	1:E:335:LYS:HG2	1.31	0.93
1:C:207:GLU:O	1:C:210:VAL:HG23	1.69	0.93
1:D:551:MET:CE	1:D:556:ARG:HG2	1.98	0.93
1:B:654:VAL:CG1	1:A:656:TYR:HB3	1.98	0.92
1:C:724:LEU:CD1	1:C:740:LEU:HG	2.00	0.92
1:C:724:LEU:CD1	1:C:740:LEU:HD23	1.99	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:GLU:HB2	1:D:385:GLN:OE1	1.69	0.92
1:B:322:TYR:HH	1:B:329:LEU:HB3	1.21	0.91
1:D:692:GLN:NE2	1:D:699:LEU:HD12	1.85	0.91
1:C:737:MET:CE	1:C:760:VAL:HG12	1.96	0.90
1:D:166:ILE:HD13	1:D:241:ASP:OD2	1.71	0.89
1:D:551:MET:HE3	1:D:556:ARG:NE	1.86	0.89
1:C:741:VAL:HB	1:C:745:VAL:HG12	1.54	0.89
1:D:551:MET:CE	1:D:556:ARG:CG	2.49	0.89
1:E:638:MET:CG	1:D:685:ASP:CG	2.46	0.89
1:D:346:THR:CG2	1:D:374:ALA:HB1	2.03	0.89
1:D:741:VAL:HG22	1:D:749:PHE:CD1	2.07	0.89
1:B:322:TYR:OH	1:B:329:LEU:CB	2.20	0.89
1:E:638:MET:CG	1:D:685:ASP:OD2	2.21	0.88
1:E:636:GLU:OE1	1:D:647:VAL:HG23	1.73	0.88
1:E:205:ILE:HG21	1:E:319:TYR:HD1	1.36	0.88
1:C:316:LEU:HB2	1:D:668:ARG:CZ	2.04	0.88
1:D:541:ALA:HB2	1:D:547:PRO:HB3	1.53	0.87
1:B:540:LEU:CD2	1:B:546:ILE:CD1	2.53	0.87
1:B:540:LEU:CG	1:B:546:ILE:CD1	2.52	0.87
1:C:543:TRP:HH2	1:B:334:GLN:HE22	1.22	0.86
1:F:724:LEU:O	1:F:725:ILE:CG1	2.21	0.86
1:C:543:TRP:CH2	1:B:334:GLN:NE2	2.43	0.86
1:D:210:VAL:CG2	1:D:385:GLN:HG2	2.06	0.86
1:C:543:TRP:HH2	1:B:334:GLN:NE2	1.74	0.85
1:D:692:GLN:HE21	1:D:699:LEU:CD1	1.90	0.85
1:C:385:GLN:HE21	1:B:331:ARG:HH21	1.17	0.85
1:F:282:THR:HG22	1:E:327:ALA:CB	2.06	0.85
1:E:638:MET:HG2	1:D:685:ASP:OD2	1.76	0.85
1:D:551:MET:SD	1:D:556:ARG:HG2	2.16	0.84
1:C:724:LEU:CD1	1:C:740:LEU:CG	2.54	0.83
1:D:166:ILE:CD1	1:D:241:ASP:OD2	2.26	0.83
1:E:199:LYS:CG	1:E:331:ARG:O	2.26	0.83
1:D:386:LEU:H	1:D:387:PRO:HD2	1.43	0.83
1:E:647:VAL:CG2	1:E:689:ILE:HD12	2.08	0.83
1:E:636:GLU:OE1	1:D:647:VAL:CG2	2.28	0.82
1:C:346:THR:HB	1:C:386:LEU:HD21	1.61	0.82
1:D:683:HIS:N	1:D:748:ASN:HD21	1.78	0.82
1:C:341:PRO:O	1:C:386:LEU:HD13	1.81	0.80
1:B:540:LEU:HD23	1:B:546:ILE:CD1	2.11	0.80
1:C:721:GLY:HA3	1:C:725:ILE:CD1	2.11	0.79
1:C:168:LEU:CD1	1:C:237:VAL:CG1	2.53	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:541:ALA:HB2	1:C:547:PRO:HA	1.64	0.79
1:B:540:LEU:CG	1:B:546:ILE:HD11	2.13	0.79
1:C:346:THR:CG2	1:C:374:ALA:HB1	2.13	0.79
1:E:638:MET:O	1:E:683:HIS:CD2	2.36	0.79
1:F:732:LEU:H	1:F:766:LEU:CD2	1.95	0.78
1:E:325:LYS:HG2	1:E:330:GLU:OE1	1.82	0.78
1:D:346:THR:HG21	1:D:374:ALA:HB1	1.62	0.78
1:E:314:THR:OG1	1:E:319:TYR:HB2	1.83	0.78
1:C:384:ARG:CB	1:C:389:LYS:HB2	2.13	0.78
1:D:637:PHE:CD1	1:D:645:ARG:HD3	2.18	0.78
1:D:207:GLU:CB	1:D:385:GLN:OE1	2.32	0.78
1:D:210:VAL:HG23	1:D:385:GLN:HG2	1.66	0.78
1:F:282:THR:HG22	1:E:327:ALA:HB2	1.64	0.77
1:E:634:MET:CA	1:E:637:PHE:HD2	1.96	0.77
1:D:637:PHE:HB3	1:D:642:SER:CB	2.12	0.77
1:C:207:GLU:HB3	1:C:385:GLN:CD	2.10	0.77
1:C:541:ALA:HB1	1:C:547:PRO:CG	2.14	0.77
1:B:185:GLU:O	1:B:189:ARG:CG	2.33	0.77
1:B:540:LEU:HG	1:B:546:ILE:HD12	1.65	0.77
1:C:346:THR:HB	1:C:386:LEU:CD2	2.15	0.77
1:E:246:VAL:O	1:E:246:VAL:HG12	1.85	0.76
1:E:329:LEU:O	1:E:329:LEU:HD23	1.86	0.76
1:D:643:VAL:HG21	1:D:686:VAL:HA	1.68	0.76
1:D:343:VAL:O	1:D:346:THR:HG22	1.84	0.76
1:E:647:VAL:HG21	1:E:689:ILE:CD1	2.16	0.76
1:F:282:THR:CG2	1:E:327:ALA:CB	2.64	0.76
1:C:343:VAL:O	1:C:346:THR:HG22	1.87	0.75
1:E:199:LYS:HE3	1:E:331:ARG:O	1.86	0.75
1:D:551:MET:CG	1:D:556:ARG:HG3	2.15	0.75
1:C:385:GLN:HE21	1:B:331:ARG:NH2	1.85	0.75
1:B:602:LEU:HD21	1:B:749:PHE:CE2	2.22	0.75
1:C:384:ARG:HB2	1:C:389:LYS:HB2	1.68	0.75
1:C:721:GLY:HA3	1:C:725:ILE:HD11	1.69	0.75
1:D:637:PHE:HD1	1:D:645:ARG:HD3	1.52	0.74
1:D:551:MET:CG	1:D:556:ARG:CG	2.65	0.74
1:E:319:TYR:CE1	1:E:335:LYS:HG2	2.21	0.74
1:D:340:GLU:CD	1:D:385:GLN:HE21	1.95	0.74
1:D:692:GLN:NE2	1:D:699:LEU:CD1	2.51	0.73
1:D:340:GLU:OE2	1:D:386:LEU:HB2	1.87	0.73
1:D:637:PHE:CB	1:D:642:SER:HB3	2.14	0.72
1:E:315:THR:OG1	1:E:318:GLU:HB2	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:THR:HG21	1:C:374:ALA:HB1	1.71	0.72
1:F:816:PRO:HA	1:F:819:ARG:HB2	1.71	0.72
1:C:635:SER:OG	1:B:692:GLN:NE2	2.23	0.72
1:E:641:HIS:ND1	1:D:653:TYR:CE2	2.58	0.72
1:E:638:MET:O	1:E:683:HIS:HD2	1.72	0.72
1:B:540:LEU:HD23	1:B:546:ILE:HD13	1.71	0.72
1:C:386:LEU:HB3	1:C:387:PRO:HD3	1.70	0.71
1:C:334:GLN:NE2	1:D:543:TRP:CZ2	2.57	0.71
1:D:744:VAL:HG11	1:D:749:PHE:HD2	1.56	0.71
1:D:346:THR:HG23	1:D:374:ALA:CB	2.21	0.71
1:F:764:HIS:HB2	1:F:766:LEU:HG	1.72	0.70
1:D:696:ASP:OD1	1:D:696:ASP:O	2.09	0.70
1:D:551:MET:O	1:D:556:ARG:HG3	1.90	0.70
1:E:647:VAL:CG2	1:E:689:ILE:CD1	2.68	0.70
1:B:540:LEU:CG	1:B:546:ILE:HD12	2.20	0.70
1:E:341:PRO:HD2	1:E:387:PRO:HD3	1.73	0.70
1:E:634:MET:SD	1:E:637:PHE:CD2	2.85	0.70
1:D:210:VAL:HG22	1:D:385:GLN:HG2	1.74	0.69
1:B:380:TYR:CD2	1:B:546:ILE:HD13	2.26	0.69
1:D:551:MET:HE2	1:D:556:ARG:HD2	1.71	0.69
1:C:392:ASP:OD2	1:C:393:LEU:N	2.25	0.69
1:E:663:THR:HG23	1:E:707:VAL:HG21	1.74	0.69
1:C:381:ILE:HB	1:C:389:LYS:HD2	1.73	0.69
1:C:724:LEU:HD11	1:C:740:LEU:HD23	1.62	0.68
1:C:207:GLU:HB3	1:C:385:GLN:NE2	2.08	0.68
1:C:316:LEU:HB2	1:D:668:ARG:NH2	2.08	0.68
1:F:281:HIS:CD2	1:E:327:ALA:CB	2.77	0.68
1:E:641:HIS:CD2	2:P:18:UNK:CB	2.76	0.68
1:F:634:MET:SD	1:F:679:VAL:HG13	2.34	0.68
1:B:322:TYR:CE1	1:B:329:LEU:HD23	2.28	0.68
1:C:541:ALA:HB2	1:C:547:PRO:CA	2.24	0.67
1:C:573:GLN:HE21	1:C:764:HIS:H	1.42	0.67
1:D:340:GLU:OE1	1:D:385:GLN:NE2	2.27	0.67
1:E:316:LEU:HD11	1:E:320:ARG:NH2	2.09	0.67
1:F:281:HIS:HD2	1:E:327:ALA:HB2	1.60	0.67
1:E:542:ARG:HH21	1:D:192:GLN:HE22	1.42	0.67
1:C:384:ARG:HB3	1:C:389:LYS:CB	2.24	0.67
1:D:643:VAL:CG2	1:D:686:VAL:HA	2.25	0.67
1:B:540:LEU:CD2	1:B:546:ILE:HD11	2.24	0.67
1:C:386:LEU:HB3	1:C:387:PRO:CD	2.25	0.66
1:A:230:GLU:HA	1:A:233:LYS:HG2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:LYS:CD	1:E:331:ARG:O	2.43	0.66
1:D:680:GLU:OE2	1:D:720:LEU:CD1	2.40	0.66
1:F:177:LEU:HB2	1:F:221:GLN:HE21	1.61	0.66
1:B:654:VAL:HG12	1:A:656:TYR:CD2	2.31	0.66
1:E:720:LEU:HD22	1:E:744:VAL:HG11	1.78	0.66
1:F:732:LEU:O	1:F:766:LEU:CD2	2.44	0.66
1:F:260:LYS:HG2	1:F:264:ASN:HD22	1.61	0.65
1:D:680:GLU:HG2	1:D:720:LEU:HD11	1.79	0.65
1:F:720:LEU:HD23	1:F:745:VAL:HA	1.78	0.65
1:D:750:ARG:HB3	1:D:750:ARG:NH1	2.11	0.65
1:F:281:HIS:HD2	1:E:327:ALA:CB	2.09	0.65
1:A:202:PRO:HG2	1:A:311:VAL:HG13	1.79	0.65
1:E:833:ILE:O	1:D:556:ARG:NH2	2.30	0.65
3:E:901:AGS:O3G	1:D:331:ARG:NH2	2.30	0.64
1:C:384:ARG:HB3	1:C:389:LYS:HB3	1.79	0.64
1:B:728:ARG:HB2	1:B:765:PRO:HG2	1.79	0.64
1:E:647:VAL:CG1	1:E:701:ASP:HA	2.27	0.64
1:E:638:MET:C	1:E:639:GLU:O	2.41	0.64
1:B:688:ASN:HA	1:B:691:LEU:HD13	1.78	0.64
1:C:384:ARG:CB	1:C:389:LYS:CB	2.76	0.64
1:E:199:LYS:CE	1:E:331:ARG:O	2.46	0.64
1:D:747:HIS:O	1:D:748:ASN:OD1	2.15	0.63
1:F:181:ILE:HD12	1:F:349:ILE:HA	1.81	0.63
1:E:641:HIS:ND1	1:D:653:TYR:CZ	2.66	0.63
1:C:396:GLU:HB3	1:B:196:ARG:HD2	1.81	0.63
1:E:323:ILE:HG22	1:E:329:LEU:HD22	1.81	0.63
1:C:166:ILE:HG21	1:C:239:ALA:O	1.98	0.63
3:D:901:AGS:S1G	3:D:901:AGS:O2B	2.57	0.63
1:B:602:LEU:CD2	1:B:749:PHE:CZ	2.82	0.63
1:C:727:GLU:HG3	1:C:728:ARG:HG3	1.80	0.62
1:D:341:PRO:O	1:D:386:LEU:CD1	2.40	0.62
1:D:680:GLU:HG2	1:D:720:LEU:CD1	2.29	0.62
1:D:683:HIS:N	1:D:748:ASN:ND2	2.48	0.62
1:C:698:ARG:HH22	1:D:633:ASP:HB2	1.64	0.62
1:D:695:ASP:HB2	1:D:756:ARG:HG2	1.80	0.62
1:E:315:THR:OG1	1:E:318:GLU:CB	2.47	0.62
1:F:728:ARG:HB3	1:F:768:GLU:H	1.65	0.62
1:D:386:LEU:HB3	1:D:387:PRO:HD3	1.81	0.62
1:D:771:ILE:HG22	1:D:817:LEU:HD22	1.82	0.62
1:F:802:LEU:HD22	1:F:803:LEU:HD13	1.78	0.62
1:E:247:ALA:O	1:E:249:ALA:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:LYS:NZ	1:D:334:GLN:OE1	2.33	0.62
1:C:550:ARG:NH2	1:C:554:SER:O	2.32	0.61
1:E:635:SER:O	1:E:645:ARG:NH1	2.33	0.61
1:D:346:THR:CG2	1:D:374:ALA:CB	2.76	0.61
1:D:386:LEU:H	1:D:387:PRO:CD	2.11	0.61
1:C:183:ARG:NH2	1:C:210:VAL:O	2.33	0.61
1:D:343:VAL:CG2	1:D:378:HIS:CD2	2.83	0.61
1:D:346:THR:HG23	1:D:374:ALA:HB1	1.78	0.61
1:C:192:GLN:OE1	1:D:542:ARG:NH2	2.28	0.61
1:F:563:GLU:HG3	1:F:578:ASP:HA	1.82	0.61
1:E:664:GLU:OE1	1:E:667:ARG:NH1	2.33	0.61
1:D:381:ILE:HD12	1:D:389:LYS:HB3	1.81	0.61
1:E:330:GLU:O	1:E:330:GLU:HG2	2.01	0.61
1:E:834:LEU:C	1:D:556:ARG:HH21	2.09	0.61
1:C:346:THR:HG23	1:C:374:ALA:HB1	1.82	0.61
1:B:380:TYR:CE2	1:B:546:ILE:HG21	2.35	0.61
1:C:209:GLY:O	1:C:387:PRO:HG2	2.01	0.61
1:C:556:ARG:HA	1:C:560:LEU:HD23	1.81	0.61
1:F:362:HIS:HB3	1:F:405:ILE:HG12	1.81	0.61
1:F:603:PHE:HB2	1:F:719:ASN:HA	1.83	0.61
1:A:600:SER:HA	1:A:714:VAL:HG22	1.82	0.61
1:F:623:PHE:O	1:F:669:ARG:NH2	2.34	0.60
1:C:189:ARG:NH1	1:D:396:GLU:OE2	2.34	0.60
1:E:396:GLU:OE1	1:D:189:ARG:NH1	2.34	0.60
1:D:380:TYR:CB	1:D:540:LEU:HD21	2.31	0.60
1:C:679:VAL:HG22	1:C:687:PHE:CE1	2.36	0.60
1:C:741:VAL:HB	1:C:745:VAL:CG1	2.29	0.60
1:E:222:ARG:HG3	1:E:227:GLU:HB3	1.84	0.60
1:B:549:SER:O	1:B:556:ARG:NH1	2.34	0.60
1:B:403:MET:CE	1:A:191:ILE:HB	2.32	0.60
1:D:551:MET:CG	1:D:556:ARG:HG2	2.31	0.60
1:E:698:ARG:HE	1:E:710:ARG:HH12	1.49	0.60
1:A:559:LEU:HD11	1:A:585:ARG:HG3	1.84	0.60
1:D:741:VAL:HG23	1:D:749:PHE:CE1	2.32	0.60
1:B:604:LEU:HD13	1:B:741:VAL:HB	1.83	0.60
1:C:196:ARG:HA	1:D:361:HIS:HE1	1.67	0.59
1:F:586:ARG:HG2	1:F:591:LEU:HD23	1.83	0.59
3:E:901:AGS:O3B	1:D:331:ARG:NH1	2.34	0.59
1:B:812:TYR:OH	1:A:755:ASN:ND2	2.35	0.59
1:E:639:GLU:OE1	1:D:641:HIS:HD2	1.85	0.59
1:C:184:ASP:OD2	1:C:222:ARG:NH1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:664:GLU:OE2	1:C:667:ARG:NH1	2.36	0.59
1:C:365:ILE:HA	1:C:531:VAL:HG12	1.85	0.59
1:F:583:ALA:O	1:F:587:SER:N	2.36	0.59
1:D:343:VAL:HG21	1:D:378:HIS:CD2	2.38	0.59
1:C:546:ILE:HG22	1:C:546:ILE:O	2.02	0.59
1:F:588:ARG:HH12	1:F:711:ASN:HA	1.67	0.59
1:F:732:LEU:N	1:F:766:LEU:HD22	2.06	0.59
1:C:687:PHE:HA	1:C:690:LEU:HD12	1.84	0.59
1:D:342:SER:O	1:D:386:LEU:HD21	2.03	0.59
1:E:366:THR:HG22	1:E:368:PRO:HD2	1.84	0.59
1:C:251:TYR:HA	2:P:5:UNK:HA	1.84	0.58
1:C:351:ARG:HG3	1:C:370:ILE:HD11	1.83	0.58
1:C:756:ARG:NH1	3:D:902:AGS:O2G	2.36	0.58
1:E:241:ASP:HB2	1:E:245:LEU:HG	1.85	0.58
1:A:605:GLY:HA3	1:A:763:PHE:HB2	1.84	0.58
1:F:820:ALA:O	1:F:823:GLN:NE2	2.34	0.58
1:B:815:ARG:NH1	1:A:752:GLU:OE1	2.36	0.58
1:A:628:ALA:H	1:A:629:MET:HE2	1.69	0.58
1:C:168:LEU:CD1	1:C:237:VAL:HG11	2.34	0.58
1:C:697:GLY:HA3	1:C:710:ARG:HG2	1.85	0.58
1:D:166:ILE:HG22	1:D:166:ILE:O	2.03	0.58
1:C:541:ALA:CB	1:C:547:PRO:HG3	2.26	0.58
1:E:602:LEU:HB2	1:E:757:ILE:HD12	1.86	0.58
3:C:901:AGS:S1G	1:B:332:ARG:NH2	2.75	0.58
1:F:199:LYS:HD2	1:F:331:ARG:HG3	1.86	0.58
1:C:606:PRO:HD2	1:C:609:VAL:HG21	1.86	0.58
1:F:554:SER:OG	1:F:556:ARG:NH1	2.36	0.58
1:E:645:ARG:NH2	1:D:700:THR:OG1	2.36	0.58
1:C:688:ASN:HB3	1:D:635:SER:HB2	1.86	0.58
3:C:902:AGS:O2G	3:C:902:AGS:O1B	2.22	0.58
1:F:196:ARG:HH22	1:A:392:ASP:HB2	1.69	0.58
1:E:638:MET:O	1:E:639:GLU:C	2.47	0.58
3:E:902:AGS:O3G	1:D:752:GLU:OE1	2.22	0.58
1:D:561:ARG:NH1	1:D:565:GLU:OE1	2.37	0.58
1:F:386:LEU:HA	1:F:389:LYS:HB2	1.85	0.57
1:B:636:GLU:OE1	1:B:645:ARG:NH2	2.37	0.57
1:A:673:VAL:HG23	1:A:713:VAL:HB	1.85	0.57
1:E:679:VAL:HG22	1:E:687:PHE:HE1	1.69	0.57
1:C:571:ILE:O	3:C:902:AGS:N6	2.36	0.57
1:E:402:ARG:NH1	1:E:406:ASP:OD2	2.37	0.57
1:C:543:TRP:CZ2	1:B:334:GLN:NE2	2.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:ASP:OD1	1:A:196:ARG:NH1	2.37	0.57
1:B:654:VAL:HG12	1:A:656:TYR:CG	2.40	0.57
1:F:167:ASP:OD2	1:F:236:ARG:NH1	2.38	0.57
1:E:638:MET:HG3	1:D:685:ASP:OD2	2.03	0.57
1:E:795:ILE:HG12	1:E:846:LEU:HB2	1.87	0.57
1:D:822:GLN:HA	1:D:826:GLU:HB2	1.87	0.57
1:B:654:VAL:CG1	1:A:656:TYR:CB	2.80	0.57
1:B:664:GLU:HG2	1:B:667:ARG:HH12	1.68	0.57
1:C:343:VAL:HA	1:C:346:THR:HG22	1.84	0.57
1:D:679:VAL:HG11	1:D:716:MET:HB3	1.86	0.57
1:C:191:ILE:HG23	1:C:232:LEU:HG	1.87	0.57
1:E:209:GLY:HA3	1:E:386:LEU:HD13	1.86	0.57
1:D:209:GLY:O	1:D:387:PRO:HG2	2.05	0.57
1:B:777:ILE:HA	1:B:780:LYS:HG2	1.87	0.57
1:A:255:PHE:HE2	1:A:296:GLY:H	1.53	0.57
1:A:588:ARG:NH2	1:A:622:MET:SD	2.76	0.57
1:F:221:GLN:O	1:F:225:ASN:ND2	2.37	0.57
1:D:380:TYR:HB2	1:D:540:LEU:HD21	1.87	0.57
1:B:602:LEU:HD21	1:B:749:PHE:HE2	1.70	0.57
1:C:334:GLN:HE22	1:D:543:TRP:HH2	1.36	0.56
1:C:346:THR:HG23	1:C:374:ALA:CB	2.35	0.56
1:F:803:LEU:CG	1:F:806:ASN:HD21	2.10	0.56
1:B:202:PRO:HG2	1:B:311:VAL:HG13	1.87	0.56
1:B:403:MET:HE1	1:A:191:ILE:HB	1.87	0.56
1:F:728:ARG:NH1	1:F:768:GLU:OE1	2.38	0.56
1:F:265:ASP:O	1:F:268:LYS:NZ	2.38	0.56
1:D:166:ILE:HD11	1:D:241:ASP:OD2	2.06	0.56
1:B:602:LEU:CD2	1:B:749:PHE:CE2	2.88	0.56
1:C:241:ASP:OD2	1:B:260:LYS:NZ	2.39	0.56
1:F:783:TYR:OH	1:F:824:GLN:NE2	2.38	0.56
1:E:205:ILE:CG2	1:E:319:TYR:CD1	2.75	0.56
1:B:602:LEU:HD22	1:B:749:PHE:CZ	2.40	0.56
1:A:190:THR:HG21	1:A:215:ILE:HG21	1.87	0.56
1:A:720:LEU:HD22	1:A:745:VAL:HA	1.87	0.56
1:C:331:ARG:HH11	1:D:388:ASP:HB3	1.70	0.56
1:E:316:LEU:HD11	1:E:320:ARG:CZ	2.36	0.56
1:B:573:GLN:HB3	1:B:576:ALA:HB3	1.87	0.56
1:A:265:ASP:HA	1:A:268:LYS:HD3	1.87	0.56
1:F:698:ARG:HE	1:F:706:THR:HG23	1.70	0.56
1:E:641:HIS:NE2	2:P:18:UNK:CB	2.68	0.56
1:D:340:GLU:HG3	1:D:385:GLN:HG3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:TYR:HA	2:P:7:UNK:HA	1.87	0.56
1:E:636:GLU:OE1	1:D:647:VAL:HG21	2.05	0.56
1:E:638:MET:CB	1:D:685:ASP:CG	2.79	0.56
1:D:635:SER:HA	1:D:681:LYS:HE3	1.88	0.56
1:F:698:ARG:HG3	1:F:707:VAL:H	1.72	0.55
1:F:729:PHE:H	1:F:767:GLY:HA2	1.70	0.55
1:D:538:GLU:O	1:D:542:ARG:NH1	2.40	0.55
1:B:330:GLU:OE1	1:B:331:ARG:NH1	2.38	0.55
1:A:780:LYS:HA	1:A:783:TYR:HB2	1.88	0.55
1:C:332:ARG:NH1	3:D:901:AGS:O2G	2.35	0.55
1:E:819:ARG:NH2	1:D:755:ASN:O	2.40	0.55
1:D:601:PHE:HD1	1:D:759:GLU:HB2	1.70	0.55
1:A:741:VAL:HA	1:A:744:VAL:HG12	1.87	0.55
1:F:240:LEU:HD22	1:F:277:ILE:HG23	1.88	0.55
1:F:732:LEU:HB2	1:F:766:LEU:HA	1.88	0.55
1:B:775:ALA:HB2	1:B:817:LEU:HD21	1.88	0.55
1:A:789:ARG:NH1	1:A:833:ILE:O	2.40	0.55
1:C:525:ARG:NH1	1:C:527:LEU:O	2.40	0.55
1:D:692:GLN:HE21	1:D:699:LEU:HA	1.66	0.55
1:B:242:MET:HG2	1:B:245:LEU:HD12	1.88	0.55
1:E:314:THR:CB	1:E:319:TYR:HB2	2.35	0.55
1:C:543:TRP:HZ2	1:B:334:GLN:HE21	1.53	0.55
1:E:725:ILE:HG22	1:E:765:PRO:HD3	1.88	0.55
1:D:692:GLN:HE21	1:D:699:LEU:HD13	1.70	0.55
1:C:786:LEU:HD22	1:C:791:TYR:HB2	1.88	0.55
1:D:793:ILE:HG12	1:D:844:ILE:HB	1.88	0.55
1:B:603:PHE:O	1:B:611:LYS:NZ	2.40	0.55
1:C:744:VAL:O	1:C:749:PHE:N	2.35	0.55
1:F:250:LYS:O	1:E:252:ARG:NH1	2.40	0.55
1:E:563:GLU:OE1	1:E:574:ASN:OD1	2.24	0.55
1:A:193:VAL:HG12	1:A:196:ARG:HH21	1.71	0.55
1:C:331:ARG:HH12	1:D:385:GLN:H	1.54	0.55
1:F:802:LEU:CD2	1:F:803:LEU:HD11	2.34	0.55
1:E:325:LYS:HA	1:E:330:GLU:HB2	1.88	0.55
1:E:553:GLU:O	1:E:556:ARG:NH2	2.36	0.55
1:B:628:ALA:HB2	1:B:669:ARG:HH21	1.71	0.55
1:F:684:PRO:HA	1:F:687:PHE:HB2	1.89	0.54
1:E:641:HIS:C	1:E:643:VAL:H	2.15	0.54
1:F:751:PRO:O	1:F:755:ASN:ND2	2.40	0.54
1:E:246:VAL:O	1:E:246:VAL:CG1	2.54	0.54
1:E:361:HIS:HE1	1:D:196:ARG:HA	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:777:ILE:HD11	3:E:902:AGS:H2	1.88	0.54
1:D:167:ASP:HB3	1:D:170:GLU:HG2	1.90	0.54
1:C:207:GLU:O	1:C:210:VAL:CG2	2.49	0.54
1:C:725:ILE:HG23	1:C:734:TYR:HH	1.70	0.54
1:F:724:LEU:O	1:F:725:ILE:CB	2.55	0.54
1:A:563:GLU:O	1:A:567:HIS:ND1	2.41	0.54
1:C:601:PHE:HD1	1:C:759:GLU:HB2	1.72	0.54
1:E:196:ARG:NH2	1:E:199:LYS:O	2.40	0.54
1:D:551:MET:HG2	1:D:556:ARG:HG2	1.84	0.54
1:E:231:GLY:O	1:E:235:ARG:NH2	2.38	0.54
1:C:842:LYS:HE3	1:C:843:VAL:HG12	1.90	0.54
1:E:203:VAL:HG12	1:E:205:ILE:CG2	2.38	0.54
1:E:561:ARG:HD2	1:E:565:GLU:HG2	1.90	0.54
1:E:641:HIS:CB	1:D:653:TYR:OH	2.56	0.54
3:E:901:AGS:O2B	3:E:901:AGS:O1A	2.24	0.54
1:C:679:VAL:CG2	1:C:687:PHE:HE1	2.20	0.54
1:C:777:ILE:HD11	3:C:902:AGS:H2	1.88	0.54
1:F:162:LYS:NZ	1:F:163:LYS:HD2	2.23	0.54
1:F:797:ASP:HA	1:F:800:LEU:HB2	1.90	0.54
1:E:724:LEU:HD21	1:E:740:LEU:HD22	1.89	0.54
1:F:815:ARG:NE	1:E:758:ASP:O	2.41	0.54
1:E:633:ASP:CG	1:D:692:GLN:OE1	2.51	0.54
1:F:318:GLU:O	1:F:321:GLN:NE2	2.40	0.54
1:E:242:MET:HG2	1:D:301:PRO:HG3	1.90	0.54
1:D:637:PHE:N	1:D:637:PHE:CD2	2.76	0.54
1:B:546:ILE:HG22	1:B:547:PRO:N	2.22	0.54
1:C:596:ARG:NH2	1:C:756:ARG:O	2.40	0.53
1:C:679:VAL:HG22	1:C:687:PHE:HE1	1.72	0.53
1:E:315:THR:OG1	1:E:318:GLU:CG	2.56	0.53
1:E:623:PHE:HE2	1:E:673:VAL:HG23	1.73	0.53
1:E:834:LEU:CA	1:D:556:ARG:HH21	2.21	0.53
1:F:677:ASP:OD1	1:F:677:ASP:N	2.41	0.53
1:E:638:MET:CG	1:D:685:ASP:OD1	2.38	0.53
1:D:680:GLU:OE2	1:D:719:ASN:N	2.36	0.53
1:C:385:GLN:O	1:C:389:LYS:CE	2.42	0.53
1:D:634:MET:O	1:D:681:LYS:HE3	2.08	0.53
1:B:835:SER:O	1:A:556:ARG:NH2	2.40	0.53
1:E:365:ILE:HA	1:E:531:VAL:HG22	1.89	0.53
1:E:633:ASP:CB	1:D:692:GLN:OE1	2.56	0.53
1:D:744:VAL:CB	1:D:749:PHE:HB2	2.30	0.53
1:B:596:ARG:NH2	1:B:756:ARG:O	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ARG:O	1:A:389:LYS:NZ	2.39	0.53
1:E:641:HIS:C	1:E:643:VAL:N	2.65	0.53
1:D:405:ILE:HD11	1:D:529:ASN:HA	1.91	0.53
1:E:638:MET:SD	1:E:682:ALA:C	2.92	0.53
1:E:641:HIS:CG	1:D:653:TYR:CZ	2.96	0.53
1:B:602:LEU:HD21	1:B:749:PHE:CZ	2.43	0.53
1:C:643:VAL:HG23	1:C:686:VAL:HG13	1.90	0.53
1:D:551:MET:CE	1:D:556:ARG:NE	2.62	0.53
1:A:204:LEU:H	1:A:313:ALA:HA	1.74	0.53
1:B:611:LYS:HD3	1:B:717:THR:HB	1.89	0.53
1:E:809:ASP:N	1:E:809:ASP:OD1	2.41	0.53
1:B:203:VAL:HG21	1:B:333:PHE:HB3	1.91	0.53
1:C:316:LEU:CB	1:D:668:ARG:NH2	2.72	0.53
1:F:823:GLN:HG3	1:F:852:ARG:HA	1.91	0.53
1:E:381:ILE:HD11	1:E:540:LEU:HD11	1.91	0.53
1:E:834:LEU:HA	1:D:556:ARG:HH21	1.74	0.53
1:B:818:LYS:HG3	4:B:902:ADP:H4'	1.91	0.53
1:A:213:THR:HA	1:A:217:GLU:HG3	1.91	0.53
1:F:279:GLU:OE2	1:E:328:ALA:HB2	2.09	0.52
1:E:676:LEU:HD13	1:E:690:LEU:HD11	1.91	0.52
1:D:643:VAL:HG23	1:D:686:VAL:HG23	1.91	0.52
1:C:343:VAL:C	1:C:346:THR:HG22	2.34	0.52
1:F:597:PRO:HB3	1:F:694:LEU:HD22	1.89	0.52
1:F:604:LEU:HD13	1:F:721:GLY:HA2	1.91	0.52
1:F:765:PRO:O	1:F:766:LEU:O	2.28	0.52
1:E:310:CYS:SG	1:E:311:VAL:N	2.81	0.52
1:D:346:THR:HB	1:D:386:LEU:CD2	2.39	0.52
1:A:592:ALA:HB1	1:A:596:ARG:HH21	1.74	0.52
1:C:823:GLN:NE2	1:B:759:GLU:OE2	2.42	0.52
1:E:733:ASP:H	1:E:736:HIS:HB2	1.75	0.52
1:D:596:ARG:NH2	1:D:756:ARG:O	2.35	0.52
1:B:184:ASP:HA	1:B:187:ILE:HG22	1.90	0.52
1:C:263:LEU:HD11	1:C:299:LEU:HD22	1.91	0.52
1:E:631:ARG:NH1	1:D:696:ASP:OD2	2.43	0.52
1:D:680:GLU:CD	1:D:720:LEU:HD12	2.31	0.52
1:C:167:ASP:HB2	1:C:170:GLU:HB3	1.91	0.52
1:C:212:LYS:N	3:C:901:AGS:O1B	2.40	0.52
1:B:230:GLU:HA	1:B:233:LYS:HG3	1.92	0.52
1:B:322:TYR:C	1:B:322:TYR:CD2	2.86	0.52
1:D:386:LEU:N	1:D:387:PRO:CD	2.73	0.52
1:A:167:ASP:OD1	1:A:169:THR:OG1	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:663:THR:HG21	1:C:701:ASP:HB3	1.92	0.51
1:C:731:GLU:HG2	1:C:732:LEU:HG	1.91	0.51
1:F:237:VAL:HG22	1:F:274:ILE:HB	1.91	0.51
1:E:562:MET:HG2	1:E:585:ARG:NH2	2.25	0.51
1:E:793:ILE:HD13	1:E:844:ILE:HB	1.93	0.51
1:C:834:LEU:HB3	1:B:559:LEU:HD13	1.92	0.51
1:C:809:ASP:OD1	1:C:809:ASP:N	2.42	0.51
1:F:588:ARG:NH2	1:F:712:THR:O	2.42	0.51
1:E:202:PRO:HG2	1:E:311:VAL:HG22	1.92	0.51
1:F:366:THR:HB	1:F:530:LYS:HD2	1.93	0.51
1:A:646:LEU:HA	1:A:661:TYR:HB2	1.91	0.51
1:E:304:ALA:HA	1:E:332:ARG:HD2	1.93	0.51
1:D:750:ARG:HB3	1:D:750:ARG:HH11	1.74	0.51
1:B:842:LYS:HG3	1:B:857:GLN:HE22	1.76	0.51
3:B:901:AGS:O2A	3:B:901:AGS:O2B	2.29	0.51
1:A:554:SER:HB2	1:A:557:GLU:HG2	1.91	0.51
1:A:361:HIS:NE2	1:A:395:ASP:OD1	2.44	0.51
1:F:331:ARG:NH2	1:A:388:ASP:OD2	2.43	0.51
1:F:833:ILE:HG22	1:F:834:LEU:HD22	1.92	0.51
1:E:640:LYS:O	1:E:640:LYS:HG2	2.11	0.51
1:E:641:HIS:O	1:E:643:VAL:N	2.43	0.51
1:D:688:ASN:O	1:D:691:LEU:HB2	2.11	0.51
1:A:296:GLY:O	1:A:300:LYS:NZ	2.44	0.51
1:D:343:VAL:HA	1:D:346:THR:HG22	1.92	0.51
1:B:238:LEU:HD13	1:B:273:VAL:HG23	1.92	0.51
1:A:563:GLU:HA	1:A:566:LEU:HB2	1.92	0.51
1:C:815:ARG:NH2	3:C:902:AGS:O3G	2.36	0.51
1:F:386:LEU:O	1:F:390:ALA:N	2.44	0.51
1:F:768:GLU:O	1:F:769:GLN:NE2	2.44	0.51
1:D:732:LEU:HD12	1:D:734:TYR:H	1.76	0.51
1:D:203:VAL:HG12	1:D:203:VAL:O	2.11	0.51
1:B:323:ILE:HG22	1:B:326:ASP:H	1.76	0.51
1:B:600:SER:HB3	1:B:758:ASP:H	1.76	0.51
1:A:265:ASP:N	1:A:265:ASP:OD2	2.40	0.51
1:A:806:ASN:HD21	1:A:821:ILE:HD11	1.76	0.51
1:C:692:GLN:NE2	1:D:636:GLU:OE2	2.44	0.50
1:D:738:LYS:HA	1:D:741:VAL:HG12	1.92	0.50
1:E:189:ARG:NH1	1:E:334:GLN:OE1	2.37	0.50
1:D:744:VAL:HG11	1:D:749:PHE:CD2	2.41	0.50
1:A:363:VAL:HA	1:A:529:ASN:HB2	1.92	0.50
1:C:178:ASP:OD2	1:B:197:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:THR:OG1	3:E:901:AGS:S1G	2.69	0.50
1:B:377:SER:HB3	1:B:389:LYS:HG2	1.94	0.50
1:B:741:VAL:HA	1:B:745:VAL:HG12	1.94	0.50
1:A:405:ILE:HG12	1:A:527:LEU:HA	1.94	0.50
1:F:724:LEU:HD13	1:F:743:GLY:O	2.12	0.50
1:C:369:ALA:HB2	1:C:532:THR:HA	1.93	0.50
1:C:663:THR:HG23	1:C:707:VAL:HG21	1.93	0.50
1:F:241:ASP:OD1	1:F:241:ASP:N	2.36	0.50
1:C:199:LYS:HD2	1:C:332:ARG:HA	1.92	0.50
1:C:266:LEU:HD11	1:C:275:LEU:HD13	1.94	0.50
1:E:633:ASP:O	1:E:637:PHE:HE2	1.95	0.50
1:B:573:GLN:H	1:B:764:HIS:CE1	2.30	0.50
1:B:653:TYR:HB3	1:A:652:GLY:HA2	1.93	0.50
1:F:167:ASP:HB3	1:F:170:GLU:HB2	1.93	0.50
1:F:303:LEU:HD22	1:F:308:LEU:HD11	1.94	0.50
1:E:533:ASP:OD2	1:E:533:ASP:N	2.44	0.50
1:E:745:VAL:HA	1:E:749:PHE:HB2	1.92	0.50
1:B:241:ASP:OD1	1:B:241:ASP:N	2.38	0.50
1:F:175:GLY:HA2	1:F:221:GLN:HE22	1.77	0.50
1:E:171:ARG:HH21	1:E:176:LYS:HE2	1.76	0.50
1:C:340:GLU:OE2	1:C:386:LEU:HB2	2.12	0.49
1:D:374:ALA:HA	1:D:390:ALA:HB2	1.94	0.49
1:C:331:ARG:NH1	1:D:388:ASP:HB3	2.27	0.49
1:D:210:VAL:CG2	1:D:385:GLN:CG	2.84	0.49
1:C:196:ARG:HH21	1:D:396:GLU:HB2	1.76	0.49
1:D:169:THR:HG22	1:D:224:ILE:HD13	1.94	0.49
1:D:701:ASP:HB3	1:D:703:GLN:H	1.77	0.49
1:B:203:VAL:O	1:B:205:ILE:N	2.45	0.49
1:D:552:MET:HA	1:D:556:ARG:HD3	1.94	0.49
1:D:717:THR:O	1:D:717:THR:OG1	2.31	0.49
1:E:645:ARG:NH2	1:D:701:ASP:O	2.41	0.49
1:B:354:LYS:HD3	1:B:370:ILE:HD11	1.94	0.49
1:C:346:THR:CB	1:C:386:LEU:HD21	2.37	0.49
1:E:633:ASP:OD2	1:E:635:SER:HB3	2.12	0.49
1:D:555:GLU:OE1	1:D:588:ARG:NH2	2.34	0.49
1:B:798:GLU:OE2	1:B:848:VAL:N	2.44	0.49
1:C:386:LEU:H	1:C:387:PRO:HD2	1.78	0.49
1:C:602:LEU:HD23	1:C:760:VAL:HG13	1.95	0.49
1:E:187:ILE:HA	1:E:190:THR:HG22	1.94	0.49
1:B:654:VAL:CG1	1:A:656:TYR:CD2	2.96	0.49
1:C:199:LYS:NZ	1:D:388:ASP:OD1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:282:THR:CG2	1:E:327:ALA:HB1	2.41	0.49
1:F:396:GLU:OE2	1:E:189:ARG:NH1	2.46	0.49
1:E:183:ARG:HH22	1:E:341:PRO:HD3	1.77	0.49
1:E:632:ILE:CG2	1:E:637:PHE:CE2	2.96	0.49
1:E:832:GLN:HB3	1:E:838:LEU:HG	1.94	0.49
1:E:838:LEU:HD13	1:E:844:ILE:HD13	1.95	0.49
1:C:611:LYS:NZ	1:C:718:SER:O	2.41	0.49
1:C:744:VAL:HG23	1:C:748:ASN:HB3	1.94	0.49
1:C:815:ARG:NH1	1:B:695:ASP:OD1	2.46	0.49
1:E:641:HIS:HB2	1:D:653:TYR:OH	2.13	0.49
1:E:834:LEU:O	1:D:556:ARG:NH2	2.46	0.49
1:D:161:LEU:HD23	1:D:162:LYS:HG2	1.94	0.49
1:B:556:ARG:HA	1:B:559:LEU:HD12	1.95	0.49
1:B:679:VAL:HG22	1:B:687:PHE:HE1	1.77	0.49
1:E:354:LYS:NZ	1:E:358:GLU:OE2	2.44	0.48
1:D:266:LEU:HD11	1:D:275:LEU:HD22	1.95	0.48
1:D:386:LEU:N	1:D:387:PRO:HD2	2.21	0.48
1:E:171:ARG:HH21	1:E:176:LYS:HB3	1.79	0.48
1:E:562:MET:HG2	1:E:585:ARG:HH22	1.77	0.48
1:E:633:ASP:OD2	1:D:692:GLN:OE1	2.31	0.48
1:E:647:VAL:HG23	1:E:689:ILE:CD1	2.43	0.48
1:E:771:ILE:HD12	1:E:808:TYR:HD1	1.77	0.48
1:C:171:ARG:HH12	1:B:305:ARG:HH11	1.60	0.48
1:C:201:ASN:N	1:C:201:ASN:OD1	2.44	0.48
1:C:210:VAL:CG1	1:C:338:VAL:HG12	2.44	0.48
1:D:720:LEU:HD22	1:D:741:VAL:HG23	1.95	0.48
1:A:187:ILE:HA	1:A:190:THR:OG1	2.14	0.48
1:C:208:PRO:O	1:C:385:GLN:HG2	2.14	0.48
1:F:281:HIS:CD2	1:E:327:ALA:HA	2.48	0.48
1:F:672:SER:OG	1:F:673:VAL:N	2.46	0.48
1:E:253:GLY:HA2	1:E:256:GLU:HG2	1.94	0.48
1:D:776:GLN:HA	1:D:779:LEU:HB2	1.95	0.48
1:B:542:ARG:HH21	1:A:189:ARG:HH11	1.61	0.48
1:D:223:ILE:HD13	1:D:235:ARG:HB2	1.96	0.48
1:D:796:SER:OG	1:D:797:ASP:N	2.45	0.48
1:E:587:SER:O	1:E:587:SER:OG	2.32	0.48
1:D:798:GLU:HB2	1:D:848:VAL:HG21	1.96	0.48
1:A:719:ASN:ND2	1:A:723:ASP:OD1	2.47	0.48
1:E:695:ASP:HB3	1:E:756:ARG:HD2	1.95	0.48
1:C:803:LEU:HD11	1:C:825:ILE:HD11	1.96	0.48
1:F:602:LEU:HD13	1:F:604:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:611:LYS:NZ	3:D:902:AGS:O3B	2.46	0.48
1:B:550:ARG:HA	1:B:556:ARG:HH22	1.79	0.48
1:C:643:VAL:HG11	1:D:638:MET:HE3	1.96	0.48
1:E:629:MET:HE3	1:E:631:ARG:HB2	1.96	0.48
1:D:612:THR:HG21	1:D:677:ASP:OD1	2.14	0.48
1:B:632:ILE:HD11	1:B:662:LEU:HD13	1.96	0.48
1:D:213:THR:OG1	3:D:901:AGS:S1G	2.64	0.47
1:D:541:ALA:HB2	1:D:547:PRO:CB	2.35	0.47
1:A:679:VAL:HB	1:A:718:SER:HB2	1.96	0.47
1:E:323:ILE:HG22	1:E:323:ILE:O	2.14	0.47
1:B:185:GLU:O	1:B:189:ARG:CD	2.62	0.47
1:A:633:ASP:OD1	1:A:681:LYS:NZ	2.44	0.47
1:D:692:GLN:HG3	1:D:698:ARG:O	2.13	0.47
1:B:619:ALA:HA	1:B:673:VAL:HG21	1.97	0.47
1:C:679:VAL:HG12	1:C:718:SER:HB2	1.97	0.47
1:C:738:LYS:HE2	1:C:754:ILE:CG2	2.44	0.47
1:F:771:ILE:HG23	1:F:817:LEU:HD12	1.96	0.47
1:D:340:GLU:HB2	1:D:385:GLN:NE2	2.30	0.47
1:D:381:ILE:HB	1:D:389:LYS:HD2	1.95	0.47
1:A:280:LEU:HA	1:A:283:MET:HG2	1.96	0.47
1:A:652:GLY:O	2:P:22:UNK:N	2.47	0.47
1:C:645:ARG:HA	1:B:651:PRO:HD2	1.96	0.47
1:F:215:ILE:O	1:F:219:LEU:N	2.45	0.47
1:F:720:LEU:HB3	1:F:745:VAL:HG22	1.96	0.47
1:F:730:GLY:HA3	1:F:774:ILE:HD11	1.95	0.47
1:B:214:ALA:HA	1:B:217:GLU:HB2	1.96	0.47
1:A:190:THR:HG21	1:A:215:ILE:CG2	2.44	0.47
1:F:596:ARG:HD3	1:F:597:PRO:HD2	1.97	0.47
1:E:637:PHE:HA	1:E:642:SER:OG	2.14	0.47
1:D:210:VAL:HG22	1:D:385:GLN:CG	2.41	0.47
1:C:377:SER:HB2	1:C:389:LYS:HG3	1.96	0.47
1:C:606:PRO:HA	1:C:722:SER:HB3	1.97	0.47
1:E:367:ASP:HA	1:E:370:ILE:HG12	1.97	0.47
1:E:647:VAL:HG13	1:E:701:ASP:HA	1.96	0.47
1:D:562:MET:HE1	1:D:584:ILE:HB	1.96	0.47
1:D:637:PHE:CD1	1:D:645:ARG:CD	2.94	0.47
1:B:263:LEU:HD21	1:B:299:LEU:HD23	1.96	0.47
1:A:191:ILE:HG22	1:A:195:GLN:NE2	2.30	0.47
1:F:361:HIS:HB2	1:F:363:VAL:HG22	1.96	0.47
1:F:379:ARG:O	1:F:379:ARG:NH1	2.40	0.47
1:F:796:SER:HB3	1:F:846:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:280:LEU:HB3	1:E:314:THR:HG23	1.96	0.47
1:E:587:SER:HB2	1:E:590:GLY:HA2	1.96	0.47
1:E:596:ARG:NH1	1:E:758:ASP:OD1	2.47	0.47
1:A:741:VAL:HG12	1:A:745:VAL:HB	1.96	0.47
1:F:240:LEU:N	1:F:276:PHE:O	2.45	0.47
1:F:827:ASN:HA	1:F:830:ALA:HB3	1.97	0.47
1:E:393:LEU:HD11	1:E:540:LEU:HD13	1.97	0.47
1:D:210:VAL:HG23	1:D:385:GLN:CG	2.43	0.47
1:D:381:ILE:CG2	1:D:389:LYS:HD2	2.45	0.47
1:D:632:ILE:HD13	1:D:646:LEU:HD22	1.96	0.47
1:D:682:ALA:HB1	1:D:747:HIS:CD2	2.49	0.47
1:D:680:GLU:CD	1:D:720:LEU:CD1	2.87	0.47
1:C:815:ARG:HD3	1:B:756:ARG:HE	1.80	0.46
1:F:603:PHE:HA	1:F:762:VAL:HG23	1.96	0.46
1:D:199:LYS:HD2	1:D:332:ARG:HA	1.95	0.46
1:D:570:VAL:HG21	1:D:614:LEU:HA	1.97	0.46
1:B:607:THR:HG22	1:B:719:ASN:HD22	1.79	0.46
1:A:376:LEU:HD23	1:A:540:LEU:HD23	1.97	0.46
1:B:824:GLN:HG2	1:B:853:ILE:HD12	1.97	0.46
1:C:208:PRO:O	1:C:385:GLN:CG	2.64	0.46
1:C:551:MET:O	1:C:556:ARG:NH1	2.32	0.46
1:C:693:VAL:HG12	1:C:699:LEU:HB2	1.97	0.46
1:F:727:GLU:HG2	1:F:765:PRO:HA	1.98	0.46
1:E:602:LEU:HB3	1:E:760:VAL:HG13	1.97	0.46
1:D:771:ILE:HD12	1:D:808:TYR:HD1	1.80	0.46
1:A:724:LEU:HB2	1:A:737:MET:HE1	1.98	0.46
1:C:643:VAL:HG11	1:D:638:MET:CE	2.45	0.46
1:E:350:LEU:HD11	1:E:390:ALA:HB1	1.96	0.46
1:D:177:LEU:HD13	1:D:217:GLU:HB3	1.97	0.46
1:B:749:PHE:HB3	1:B:754:ILE:HG13	1.97	0.46
1:A:205:ILE:HB	1:A:337:PHE:HA	1.97	0.46
1:C:678:GLU:HB3	1:C:681:LYS:HD2	1.96	0.46
1:F:625:SER:HB2	1:F:673:VAL:HG22	1.96	0.46
1:D:350:LEU:HD21	1:D:391:ILE:HA	1.98	0.46
1:A:263:LEU:HD23	1:A:266:LEU:HD12	1.97	0.46
1:A:616:LYS:HG3	1:A:629:MET:HE3	1.97	0.46
1:C:785:ARG:NH1	1:B:592:ALA:O	2.49	0.46
1:F:601:PHE:HZ	1:F:741:VAL:HA	1.80	0.46
1:D:819:ARG:HA	1:D:822:GLN:HG2	1.98	0.46
1:F:809:ASP:OD1	1:F:809:ASP:N	2.47	0.46
1:D:300:LYS:HG2	1:D:332:ARG:HE	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:ARG:HD2	1:D:388:ASP:OD2	2.15	0.46
1:F:579:ALA:HA	1:F:582:ASN:HB2	1.98	0.46
1:E:341:PRO:HB3	1:E:345:ASP:HB2	1.97	0.46
1:D:350:LEU:HD11	1:D:390:ALA:HB1	1.98	0.46
1:D:401:ILE:HD12	1:D:528:ARG:HB2	1.97	0.46
1:D:633:ASP:O	1:D:637:PHE:HE2	1.99	0.46
1:F:583:ALA:HA	1:F:586:ARG:HB2	1.98	0.46
1:F:815:ARG:HG3	1:F:816:PRO:HD3	1.96	0.46
1:E:240:LEU:HD12	1:E:240:LEU:HA	1.81	0.46
1:E:771:ILE:HA	1:E:774:ILE:HG12	1.96	0.46
1:B:404:GLN:HB2	1:B:528:ARG:HH12	1.80	0.46
1:A:674:ILE:HD11	1:A:714:VAL:HG12	1.98	0.46
1:C:247:ALA:O	1:C:249:ALA:N	2.42	0.46
1:E:634:MET:C	1:E:637:PHE:HD2	2.24	0.46
1:A:663:THR:HG21	1:A:701:ASP:HB3	1.98	0.46
1:A:688:ASN:HA	1:A:691:LEU:HD13	1.97	0.46
1:E:315:THR:OG1	1:E:318:GLU:HG3	2.16	0.45
3:E:902:AGS:O1A	3:E:902:AGS:O2B	2.28	0.45
1:B:640:LYS:HE3	1:B:640:LYS:HB3	1.75	0.45
1:A:280:LEU:HD22	1:A:313:ALA:H	1.80	0.45
1:A:305:ARG:HG3	1:A:307:GLU:H	1.80	0.45
1:F:181:ILE:HB	1:F:349:ILE:HG12	1.96	0.45
1:F:588:ARG:NH1	1:F:710:ARG:O	2.49	0.45
1:F:694:LEU:HA	1:F:716:MET:HE1	1.96	0.45
1:B:605:GLY:HA2	1:B:725:ILE:HD11	1.98	0.45
1:C:183:ARG:NH2	1:C:341:PRO:HD3	2.30	0.45
1:B:298:MET:HE2	1:B:298:MET:HB3	1.81	0.45
1:B:345:ASP:O	1:B:349:ILE:N	2.46	0.45
1:A:559:LEU:HA	1:A:562:MET:HB2	1.99	0.45
1:B:738:LYS:HA	1:B:741:VAL:HG22	1.99	0.45
1:F:343:VAL:HG11	1:F:375:THR:HG22	1.99	0.45
1:E:389:LYS:HA	1:E:389:LYS:HD2	1.73	0.45
1:E:595:ASN:HA	1:E:710:ARG:HE	1.82	0.45
1:D:686:VAL:HG22	1:D:686:VAL:O	2.15	0.45
1:A:370:ILE:HA	1:A:394:ILE:HD11	1.97	0.45
1:A:663:THR:O	1:A:667:ARG:N	2.40	0.45
1:C:771:ILE:HD12	1:C:808:TYR:HD1	1.82	0.45
1:E:401:ILE:HG13	1:E:531:VAL:HG12	1.98	0.45
1:B:347:ILE:HG12	1:B:371:VAL:HA	1.99	0.45
1:C:755:ASN:O	1:D:819:ARG:NH1	2.49	0.45
1:E:193:VAL:HA	1:E:196:ARG:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:681:LYS:HA	1:D:681:LYS:HD3	1.42	0.45
1:D:793:ILE:HD11	1:D:829:LEU:HD11	1.98	0.45
1:A:213:THR:N	4:A:901:ADP:O2A	2.50	0.45
1:C:215:ILE:O	1:C:219:LEU:N	2.50	0.45
1:C:343:VAL:HA	1:C:346:THR:CG2	2.45	0.45
1:C:376:LEU:HB3	1:C:540:LEU:HD13	1.98	0.45
1:B:347:ILE:HG23	1:B:370:ILE:HG22	1.97	0.45
1:B:562:MET:HE3	1:B:562:MET:HB2	1.82	0.45
1:B:652:GLY:O	2:P:20:UNK:N	2.50	0.45
1:B:848:VAL:HG13	1:B:853:ILE:HA	1.98	0.45
1:A:383:ASP:OD1	1:A:383:ASP:N	2.50	0.45
1:C:802:LEU:HD21	1:C:853:ILE:HD11	1.98	0.45
1:F:740:LEU:HD22	1:F:743:GLY:HA3	1.97	0.45
1:E:637:PHE:HE1	1:E:646:LEU:HD22	1.81	0.45
1:F:282:THR:OG1	1:F:283:MET:N	2.51	0.44
1:E:632:ILE:CG2	1:E:637:PHE:CZ	3.00	0.44
1:D:280:LEU:HD22	1:D:312:GLY:HA3	1.98	0.44
1:C:210:VAL:HG12	1:C:338:VAL:HG12	1.99	0.44
1:C:679:VAL:CG1	1:C:718:SER:HB2	2.46	0.44
1:F:204:LEU:HD13	1:F:215:ILE:HB	1.98	0.44
1:E:695:ASP:OD1	1:E:696:ASP:N	2.48	0.44
1:B:800:LEU:O	1:B:804:SER:OG	2.33	0.44
1:C:279:GLU:O	1:C:282:THR:OG1	2.32	0.44
1:C:343:VAL:CA	1:C:346:THR:HG22	2.47	0.44
1:C:384:ARG:CZ	1:B:331:ARG:HA	2.48	0.44
1:C:550:ARG:HG2	1:C:553:GLU:HB2	1.99	0.44
1:C:564:GLN:O	1:C:568:HIS:ND1	2.49	0.44
1:C:721:GLY:O	1:C:725:ILE:HG13	2.17	0.44
3:D:902:AGS:O2B	3:D:902:AGS:O1A	2.35	0.44
1:B:380:TYR:CD2	1:B:546:ILE:HG21	2.53	0.44
1:A:787:GLU:H	1:A:787:GLU:HG2	1.63	0.44
1:D:275:LEU:N	1:D:309:HIS:O	2.51	0.44
1:D:569:ARG:HE	1:D:569:ARG:HB3	1.61	0.44
1:B:363:VAL:HA	1:B:529:ASN:HB2	1.99	0.44
1:A:785:ARG:HD2	1:A:789:ARG:HH21	1.83	0.44
1:F:751:PRO:HA	1:F:754:ILE:HG12	1.98	0.44
1:E:365:ILE:HD13	1:E:394:ILE:HG23	1.99	0.44
1:E:651:PRO:HA	1:E:656:TYR:CD1	2.52	0.44
1:B:255:PHE:HE2	1:B:295:ALA:HB2	1.83	0.44
1:C:386:LEU:N	1:C:387:PRO:HD2	2.32	0.44
1:E:750:ARG:HE	1:E:752:GLU:H	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:559:LEU:HD21	1:C:588:ARG:HG3	2.00	0.44
1:E:203:VAL:HG12	1:E:205:ILE:HG22	1.99	0.44
1:E:645:ARG:HA	1:D:651:PRO:HD2	1.99	0.44
1:B:802:LEU:HD13	1:B:848:VAL:HG21	2.00	0.44
1:B:826:GLU:HG2	1:A:586:ARG:HD2	2.00	0.44
1:E:183:ARG:HD2	1:E:215:ILE:HD11	2.00	0.44
1:E:735:ALA:HA	1:E:738:LYS:HG2	2.00	0.44
1:A:205:ILE:O	1:A:338:VAL:N	2.50	0.44
1:A:386:LEU:HD13	1:A:389:LYS:HE2	1.99	0.44
1:A:741:VAL:O	1:A:745:VAL:N	2.42	0.44
1:E:540:LEU:O	1:E:544:THR:OG1	2.35	0.44
1:E:658:GLU:OE2	1:D:656:TYR:OH	2.35	0.44
1:E:812:TYR:HE2	1:D:738:LYS:HZ1	1.66	0.44
1:D:388:ASP:O	1:D:392:ASP:OD2	2.35	0.44
1:A:238:LEU:N	1:A:274:ILE:O	2.47	0.44
1:F:676:LEU:HD21	1:F:679:VAL:HG21	2.00	0.43
1:E:641:HIS:CG	1:D:653:TYR:OH	2.70	0.43
1:B:199:LYS:HG2	1:B:304:ALA:HA	2.00	0.43
1:B:604:LEU:O	1:B:763:PHE:N	2.50	0.43
1:C:541:ALA:CB	1:C:547:PRO:CA	2.94	0.43
1:C:550:ARG:O	1:C:555:GLU:CD	2.61	0.43
1:C:692:GLN:HE22	1:D:636:GLU:CG	2.31	0.43
1:C:700:THR:OG1	1:D:636:GLU:OE1	2.29	0.43
1:E:360:HIS:CD2	1:D:197:ARG:HB3	2.53	0.43
1:D:187:ILE:HG12	1:D:215:ILE:HG23	1.99	0.43
1:D:663:THR:OG1	1:D:701:ASP:OD2	2.23	0.43
1:B:588:ARG:HD2	1:B:588:ARG:HA	1.73	0.43
1:A:302:ALA:O	1:A:305:ARG:NH1	2.51	0.43
1:A:405:ILE:HD13	1:A:527:LEU:HG	2.00	0.43
1:A:767:GLY:HA3	1:A:770:HIS:HD2	1.83	0.43
1:F:171:ARG:HH21	1:F:176:LYS:HB3	1.83	0.43
1:D:177:LEU:HB2	1:D:221:GLN:HE21	1.83	0.43
1:D:207:GLU:HB3	1:D:385:GLN:OE1	2.17	0.43
1:D:343:VAL:C	1:D:346:THR:HG22	2.41	0.43
1:D:637:PHE:CE1	1:D:645:ARG:CD	3.01	0.43
1:D:638:MET:HE3	1:D:638:MET:HB2	1.77	0.43
1:B:380:TYR:CE2	1:B:546:ILE:CG2	3.01	0.43
1:A:795:ILE:HB	1:A:798:GLU:HG3	2.00	0.43
1:E:634:MET:SD	1:E:637:PHE:CE2	3.12	0.43
1:D:378:HIS:O	1:D:378:HIS:CG	2.70	0.43
1:D:638:MET:O	1:D:683:HIS:CD2	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:674:ILE:HD12	1:B:712:THR:HG21	2.00	0.43
1:A:197:ARG:HG3	1:A:198:THR:HG23	2.00	0.43
1:A:265:ASP:O	1:A:269:GLN:NE2	2.44	0.43
1:A:758:ASP:OD2	1:A:759:GLU:N	2.51	0.43
1:E:241:ASP:HB3	1:E:244:ALA:HB3	1.99	0.43
1:D:401:ILE:HD13	1:D:401:ILE:HA	1.87	0.43
1:A:564:GLN:O	1:A:568:HIS:ND1	2.42	0.43
1:A:644:SER:HB2	1:A:649:ALA:HA	2.01	0.43
1:D:744:VAL:HB	1:D:749:PHE:CB	2.32	0.43
1:B:322:TYR:OH	1:B:329:LEU:C	2.61	0.43
1:B:634:MET:HE3	1:B:676:LEU:HD23	2.01	0.43
1:A:779:LEU:HD11	1:A:803:LEU:HD11	2.00	0.43
1:E:351:ARG:HG2	1:E:370:ILE:HD12	1.99	0.43
1:D:205:ILE:HG22	1:D:337:PHE:HA	2.01	0.43
1:A:171:ARG:HA	1:A:174:GLN:HE21	1.83	0.43
1:C:203:VAL:HG12	1:C:205:ILE:HG23	2.00	0.43
1:C:243:GLY:H	1:C:246:VAL:HG12	1.84	0.43
1:F:765:PRO:C	1:F:766:LEU:O	2.60	0.43
1:D:633:ASP:O	1:D:637:PHE:CE2	2.71	0.43
1:B:809:ASP:OD1	1:B:809:ASP:N	2.49	0.43
1:C:812:TYR:HE1	1:B:751:PRO:HB3	1.84	0.43
1:F:598:ILE:HB	1:F:716:MET:HG2	2.01	0.43
1:E:183:ARG:NH2	1:E:341:PRO:HD3	2.34	0.43
1:E:664:GLU:OE2	1:E:705:ARG:NH1	2.52	0.43
1:B:345:ASP:OD1	1:B:345:ASP:N	2.50	0.43
1:A:541:ALA:HA	1:A:551:MET:HE1	2.01	0.43
1:C:653:TYR:O	1:C:656:TYR:HB3	2.18	0.42
1:C:683:HIS:HB3	1:C:686:VAL:HG23	2.01	0.42
1:C:737:MET:HE3	1:C:760:VAL:HG11	1.84	0.42
1:D:191:ILE:HG23	1:D:232:LEU:HD22	1.99	0.42
1:D:543:TRP:CD1	1:D:543:TRP:O	2.71	0.42
1:D:667:ARG:HD2	1:D:705:ARG:HD3	2.01	0.42
1:B:537:ALA:O	1:B:541:ALA:N	2.44	0.42
1:C:692:GLN:HE22	1:D:636:GLU:HG3	1.84	0.42
1:C:745:VAL:HA	1:C:749:PHE:HB2	2.01	0.42
1:D:194:LEU:HD22	1:D:309:HIS:HB3	2.01	0.42
1:B:381:ILE:HB	1:B:389:LYS:HD2	2.00	0.42
1:A:180:VAL:HG11	1:A:218:GLY:HA3	2.00	0.42
1:A:646:LEU:HG	1:A:647:VAL:HG23	2.01	0.42
1:C:192:GLN:O	1:D:399:SER:OG	2.31	0.42
1:C:213:THR:OG1	3:C:901:AGS:S1G	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:PRO:HG2	1:C:386:LEU:HD22	2.01	0.42
1:C:362:HIS:O	1:C:402:ARG:NH2	2.52	0.42
1:E:633:ASP:O	1:E:637:PHE:CE2	2.72	0.42
1:B:561:ARG:NH2	1:B:565:GLU:OE2	2.52	0.42
1:B:766:LEU:HD22	1:B:774:ILE:HD11	2.02	0.42
1:A:223:ILE:HD13	1:A:228:VAL:HG11	2.01	0.42
1:A:807:GLY:H	1:A:817:LEU:HD23	1.84	0.42
1:C:842:LYS:HD2	1:C:842:LYS:HA	1.81	0.42
1:D:277:ILE:HD13	1:D:283:MET:HG3	2.01	0.42
1:D:563:GLU:O	1:D:567:HIS:ND1	2.51	0.42
1:D:683:HIS:HB2	1:D:686:VAL:HG12	2.01	0.42
1:B:280:LEU:HD22	1:B:312:GLY:HA3	2.01	0.42
1:B:605:GLY:HA3	1:B:763:PHE:HB2	2.01	0.42
1:A:190:THR:O	1:A:194:LEU:HB2	2.20	0.42
1:C:168:LEU:HD11	1:C:276:PHE:CD2	2.55	0.42
1:C:331:ARG:HD2	1:D:388:ASP:CG	2.44	0.42
1:C:637:PHE:CE2	1:C:646:LEU:HD22	2.55	0.42
1:C:752:GLU:O	1:C:756:ARG:HD3	2.19	0.42
1:C:832:GLN:N	1:C:832:GLN:OE1	2.52	0.42
1:D:606:PRO:HG2	1:D:765:PRO:HG3	2.01	0.42
1:A:611:LYS:HB3	1:A:631:ARG:HH22	1.84	0.42
1:C:819:ARG:HA	1:C:822:GLN:HG2	2.02	0.42
1:F:183:ARG:NH2	1:F:339:ALA:O	2.45	0.42
1:C:561:ARG:HB2	1:C:564:GLN:HB2	2.01	0.42
3:C:902:AGS:O2B	3:C:902:AGS:O2A	2.37	0.42
1:F:210:VAL:HA	1:F:387:PRO:HB2	2.01	0.42
1:F:281:HIS:CD2	1:E:327:ALA:HB1	2.53	0.42
1:E:698:ARG:NH2	1:E:708:ASP:OD1	2.52	0.42
1:D:377:SER:O	1:D:389:LYS:CE	2.54	0.42
1:D:377:SER:HA	1:D:381:ILE:HG13	2.02	0.42
1:B:546:ILE:HG23	1:B:547:PRO:HD2	2.02	0.42
1:C:721:GLY:O	1:C:725:ILE:N	2.51	0.42
1:E:323:ILE:HG23	1:E:326:ASP:CG	2.44	0.42
1:E:744:VAL:O	1:E:749:PHE:N	2.39	0.42
1:D:346:THR:HB	1:D:386:LEU:HD21	2.02	0.42
1:B:629:MET:HE2	1:B:629:MET:HB3	1.83	0.42
1:C:800:LEU:HD12	1:C:800:LEU:HA	1.88	0.42
1:C:802:LEU:HA	1:C:805:GLU:HB3	2.02	0.42
1:E:361:HIS:CE1	1:D:196:ARG:HA	2.54	0.42
1:A:526:LEU:O	1:A:526:LEU:HG	2.20	0.42
1:C:171:ARG:HH12	1:B:305:ARG:NH1	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:THR:CB	1:C:386:LEU:CD2	2.94	0.42
1:F:179:PRO:HD2	1:F:353:LEU:HD11	2.01	0.42
1:F:335:LYS:HE2	1:F:335:LYS:HB2	1.95	0.42
1:F:579:ALA:HB3	1:F:761:VAL:HG11	2.02	0.42
1:D:634:MET:HE3	1:D:676:LEU:HD22	2.02	0.42
1:F:709:PHE:HA	1:F:712:THR:HB	2.01	0.41
1:D:741:VAL:HG23	1:D:749:PHE:CZ	2.54	0.41
1:B:195:GLN:NE2	1:B:232:LEU:HD13	2.34	0.41
1:A:689:ILE:HG13	1:A:690:LEU:HD13	2.02	0.41
1:F:168:LEU:HD23	1:F:168:LEU:HA	1.84	0.41
1:F:260:LYS:HE3	1:F:260:LYS:HB3	1.94	0.41
1:F:746:SER:HB3	1:F:754:ILE:HG21	2.02	0.41
1:E:600:SER:HB2	1:E:758:ASP:H	1.85	0.41
1:E:826:GLU:HB2	1:D:586:ARG:HD3	2.02	0.41
1:D:216:VAL:HG11	1:D:276:PHE:CG	2.56	0.41
1:A:539:VAL:HA	1:A:542:ARG:HD3	2.01	0.41
1:A:610:GLY:HA2	1:A:613:GLU:HB3	2.01	0.41
1:A:644:SER:OG	1:A:645:ARG:NH1	2.53	0.41
1:C:578:ASP:HA	1:C:581:SER:HB2	2.01	0.41
1:C:606:PRO:HG2	1:C:609:VAL:HG11	2.02	0.41
1:F:601:PHE:CZ	1:F:741:VAL:HA	2.56	0.41
1:E:275:LEU:HD23	1:E:275:LEU:HA	1.92	0.41
1:D:221:GLN:O	1:D:225:ASN:ND2	2.54	0.41
1:A:380:TYR:HB3	1:A:544:THR:HG21	2.02	0.41
1:C:721:GLY:CA	1:C:725:ILE:CD1	2.91	0.41
1:D:353:LEU:CD1	1:D:391:ILE:HD11	2.50	0.41
1:B:205:ILE:HD12	1:B:335:LYS:HB3	2.01	0.41
1:B:602:LEU:CD1	1:B:749:PHE:HZ	2.33	0.41
1:A:664:GLU:HA	1:A:667:ARG:HB2	2.03	0.41
1:C:358:GLU:HG2	1:C:364:GLN:HA	2.02	0.41
1:F:283:MET:O	1:F:322:TYR:OH	2.38	0.41
1:F:731:GLU:HG2	1:F:770:HIS:HB2	2.02	0.41
1:E:668:ARG:HA	1:E:668:ARG:HD3	1.61	0.41
1:D:744:VAL:HG21	1:D:749:PHE:CD2	2.56	0.41
1:B:207:GLU:HB3	1:B:385:GLN:HG3	2.03	0.41
1:A:232:LEU:HD12	1:A:235:ARG:HD2	2.02	0.41
1:A:681:LYS:HE3	1:A:681:LYS:HB2	1.90	0.41
1:C:605:GLY:HA3	1:C:763:PHE:HB2	2.02	0.41
1:C:742:LEU:HA	1:C:746:SER:HB2	2.02	0.41
1:F:724:LEU:CD1	1:F:743:GLY:O	2.68	0.41
1:E:317:ASP:OD1	1:E:318:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:555:GLU:H	1:E:555:GLU:HG3	1.64	0.41
1:E:744:VAL:HG23	1:E:748:ASN:HB3	2.03	0.41
1:D:786:LEU:HD22	1:D:791:TYR:HB2	2.02	0.41
1:B:749:PHE:CE1	1:B:753:PHE:CE2	3.08	0.41
1:A:171:ARG:HA	1:A:174:GLN:HG2	2.03	0.41
1:A:588:ARG:HA	1:A:588:ARG:HD3	1.94	0.41
1:C:560:LEU:HD21	1:D:834:LEU:HB3	2.01	0.41
1:F:205:ILE:HD12	1:F:335:LYS:HB3	2.03	0.41
1:F:787:GLU:HG2	1:F:788:GLU:HG2	2.03	0.41
1:E:562:MET:HB3	1:E:577:VAL:HB	2.01	0.41
1:D:637:PHE:HE1	1:D:645:ARG:HG3	1.86	0.41
1:B:380:TYR:HD2	1:B:546:ILE:HD13	1.82	0.41
1:C:717:THR:O	1:C:717:THR:OG1	2.38	0.41
1:F:204:LEU:HD22	1:F:215:ILE:HD12	2.02	0.41
1:F:789:ARG:NE	1:E:533:ASP:OD1	2.54	0.41
1:E:540:LEU:HD12	1:E:540:LEU:HA	1.79	0.41
1:E:680:GLU:HG3	1:E:720:LEU:HD21	2.02	0.41
1:D:547:PRO:HG3	1:D:550:ARG:HB2	2.03	0.41
1:B:532:THR:HG22	1:B:533:ASP:H	1.86	0.41
1:A:546:ILE:HD11	1:A:550:ARG:HB2	2.03	0.41
1:C:612:THR:HG23	1:C:675:LEU:HD21	2.03	0.41
1:F:770:HIS:CD2	1:F:773:SER:HB3	2.56	0.41
1:E:548:VAL:HG13	1:E:589:ALA:HB1	2.03	0.41
1:E:732:LEU:HD11	1:E:737:MET:HB2	2.02	0.41
1:E:754:ILE:HG23	1:E:757:ILE:HD11	2.02	0.41
1:D:569:ARG:NH2	1:D:626:ASP:OD2	2.43	0.41
1:B:796:SER:OG	1:B:846:LEU:O	2.28	0.41
1:A:256:GLU:HG3	1:A:297:ASN:H	1.85	0.41
1:A:280:LEU:HD13	1:A:312:GLY:HA3	2.03	0.41
1:A:802:LEU:HD22	1:A:824:GLN:HE22	1.86	0.41
1:E:526:LEU:HG	1:E:527:LEU:HG	2.03	0.41
1:B:274:ILE:HD13	1:B:274:ILE:HG21	1.87	0.41
1:A:283:MET:HE2	1:A:299:LEU:HD21	2.03	0.41
1:C:401:ILE:HD13	1:C:401:ILE:HA	1.86	0.40
1:F:341:PRO:HD2	1:F:387:PRO:HD3	2.01	0.40
1:D:553:GLU:OE1	1:D:553:GLU:N	2.50	0.40
1:D:573:GLN:HB3	1:D:576:ALA:HB3	2.02	0.40
1:B:544:THR:HG23	1:B:546:ILE:HG13	2.03	0.40
1:C:365:ILE:HD13	1:C:394:ILE:HG23	2.02	0.40
1:C:550:ARG:O	1:C:555:GLU:OE1	2.39	0.40
1:C:724:LEU:CG	1:C:740:LEU:HD23	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:839:VAL:O	1:C:857:GLN:NE2	2.54	0.40
1:F:397:ALA:HB1	1:F:536:ILE:HG12	2.03	0.40
1:F:728:ARG:HB3	1:F:768:GLU:N	2.32	0.40
1:E:319:TYR:O	1:E:319:TYR:CG	2.74	0.40
1:E:394:ILE:HD13	1:E:394:ILE:HA	1.88	0.40
1:E:662:LEU:HD11	1:E:674:ILE:HD13	2.03	0.40
1:D:676:LEU:HD13	1:D:690:LEU:HD21	2.03	0.40
1:D:779:LEU:HA	1:D:779:LEU:HD23	1.90	0.40
1:B:725:ILE:HB	1:B:737:MET:HE2	2.03	0.40
3:E:901:AGS:O2B	3:E:901:AGS:O2G	2.36	0.40
1:D:612:THR:OG1	3:D:902:AGS:O2A	2.40	0.40
1:D:680:GLU:CG	1:D:720:LEU:CD1	2.96	0.40
1:C:741:VAL:O	1:C:745:VAL:HG12	2.21	0.40
1:F:298:MET:HA	1:A:244:ALA:HA	2.03	0.40
1:E:200:ASN:OD1	1:E:200:ASN:N	2.54	0.40
1:E:401:ILE:HD11	1:E:535:GLU:HG2	2.04	0.40
1:D:675:LEU:HG	1:D:677:ASP:HB2	2.04	0.40
1:D:692:GLN:HE22	1:D:699:LEU:HD12	1.75	0.40
1:D:716:MET:HE3	1:D:716:MET:HB2	1.98	0.40
1:B:655:GLY:HA3	1:A:651:PRO:HB3	2.04	0.40
1:B:740:LEU:HA	1:B:744:VAL:HB	2.04	0.40
1:A:678:GLU:HB3	1:A:681:LYS:HE2	2.03	0.40
1:C:603:PHE:HB2	1:C:717:THR:HA	2.04	0.40
1:F:802:LEU:HD23	1:F:802:LEU:C	2.47	0.40
1:E:611:LYS:NZ	3:E:902:AGS:O3B	2.54	0.40
1:D:384:ARG:HB2	1:D:389:LYS:CD	2.51	0.40
3:B:901:AGS:H4'	1:A:331:ARG:HH22	1.87	0.40
1:A:195:GLN:HE22	1:A:229:PRO:HG2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	542/867 (62%)	486 (90%)	56 (10%)	0	100	100
1	B	564/867 (65%)	505 (90%)	52 (9%)	7 (1%)	10	37
1	C	564/867 (65%)	505 (90%)	55 (10%)	4 (1%)	18	49
1	D	564/867 (65%)	523 (93%)	40 (7%)	1 (0%)	43	71
1	E	564/867 (65%)	511 (91%)	50 (9%)	3 (0%)	24	55
1	F	550/867 (63%)	470 (86%)	78 (14%)	2 (0%)	30	60
All	All	3348/5202 (64%)	3000 (90%)	331 (10%)	17 (0%)	26	55

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	725	ILE
1	F	766	LEU
1	E	639	GLU
1	B	747	HIS
1	C	247	ALA
1	C	386	LEU
1	D	386	LEU
1	B	748	ASN
1	E	248	GLY
1	E	642	SER
1	B	386	LEU
1	C	315	THR
1	B	749	PHE
1	B	751	PRO
1	C	248	GLY
1	B	323	ILE
1	B	750	ARG

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	463/726 (64%)	460 (99%)	3 (1%)	78	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	482/726 (66%)	476 (99%)	6 (1%)	63	75
1	C	482/726 (66%)	467 (97%)	15 (3%)	35	60
1	D	482/726 (66%)	474 (98%)	8 (2%)	53	71
1	E	482/726 (66%)	476 (99%)	6 (1%)	63	75
1	F	475/726 (65%)	474 (100%)	1 (0%)	87	88
All	All	2866/4356 (66%)	2827 (99%)	39 (1%)	57	73

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	216	VAL
1	C	232	LEU
1	C	383	ASP
1	C	389	LYS
1	C	391	ILE
1	C	539	VAL
1	C	546	ILE
1	C	571	ILE
1	C	626	ASP
1	C	693	VAL
1	C	713	VAL
1	C	734	TYR
1	C	738	LYS
1	C	741	VAL
1	C	744	VAL
1	F	238	LEU
1	E	331	ARG
1	E	531	VAL
1	E	693	VAL
1	E	741	VAL
1	E	754	ILE
1	E	856	VAL
1	D	180	VAL
1	D	381	ILE
1	D	391	ILE
1	D	637	PHE
1	D	638	MET
1	D	681	LYS
1	D	691	LEU
1	D	762	VAL

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Mol	Chain	Res	Type
1	B	246	VAL
1	B	322	TYR
1	B	368	PRO
1	B	548	VAL
1	B	748	ASN
1	B	749	PHE
1	A	714	VAL
1	A	777	ILE
1	A	802	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	195	GLN
1	C	269	GLN
1	C	385	GLN
1	C	404	GLN
1	C	595	ASN
1	C	620	ASN
1	C	688	ASN
1	C	703	GLN
1	C	736	HIS
1	C	824	GLN
1	C	849	ASN
1	C	857	GLN
1	F	221	GLN
1	F	264	ASN
1	F	272	ASN
1	F	281	HIS
1	F	385	GLN
1	F	711	ASN
1	F	748	ASN
1	F	755	ASN
1	F	770	HIS
1	F	824	GLN
1	E	264	ASN
1	E	321	GLN
1	E	360	HIS
1	E	404	GLN
1	E	683	HIS
1	E	688	ASN
1	E	832	GLN

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Mol	Chain	Res	Type
1	D	192	GLN
1	D	201	ASN
1	D	264	ASN
1	D	309	HIS
1	D	378	HIS
1	D	385	GLN
1	D	574	ASN
1	D	595	ASN
1	D	641	HIS
1	D	703	GLN
1	D	747	HIS
1	B	221	GLN
1	B	264	ASN
1	B	334	GLN
1	B	360	HIS
1	B	692	GLN
1	B	726	GLN
1	B	764	HIS
1	B	778	GLN
1	B	794	HIS
1	B	822	GLN
1	B	831	GLN
1	B	857	GLN
1	A	272	ASN
1	A	309	HIS
1	A	404	GLN
1	A	573	GLN
1	A	620	ASN
1	A	726	GLN
1	A	755	ASN
1	A	770	HIS
1	A	794	HIS
1	A	806	ASN
1	A	824	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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
3	AGS	D	901	-	32,33,33	1.44	5 (15%)	45,52,52	0.64	1 (2%)
4	ADP	F	901	-	28,29,29	1.39	4 (14%)	43,45,45	1.83	9 (20%)
3	AGS	B	901	-	32,33,33	0.81	2 (6%)	45,52,52	0.91	2 (4%)
3	AGS	E	902	-	32,33,33	1.40	5 (15%)	45,52,52	0.75	2 (4%)
4	ADP	A	901	-	28,29,29	1.39	5 (17%)	43,45,45	1.80	9 (20%)
3	AGS	D	902	-	32,33,33	1.57	5 (15%)	45,52,52	0.79	2 (4%)
4	ADP	B	902	-	28,29,29	1.37	4 (14%)	43,45,45	1.90	9 (20%)
3	AGS	E	901	-	32,33,33	1.39	4 (12%)	45,52,52	0.95	1 (2%)
3	AGS	C	902	-	32,33,33	1.24	3 (9%)	45,52,52	1.05	2 (4%)
3	AGS	C	901	-	32,33,33	1.64	5 (15%)	45,52,52	0.97	3 (6%)
4	ADP	A	902	-	28,29,29	1.41	4 (14%)	43,45,45	1.82	8 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AGS	D	901	-	-	2/21/38/38	0/3/3/3
4	ADP	F	901	-	-	4/16/32/32	0/3/3/3
3	AGS	B	901	-	-	6/21/38/38	0/3/3/3
3	AGS	E	902	-	-	2/21/38/38	0/3/3/3
4	ADP	A	901	-	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AGS	D	902	-	-	2/21/38/38	0/3/3/3
4	ADP	B	902	-	-	4/16/32/32	0/3/3/3
3	AGS	E	901	-	-	3/21/38/38	0/3/3/3
3	AGS	C	902	-	-	5/21/38/38	0/3/3/3
3	AGS	C	901	-	-	2/21/38/38	0/3/3/3
4	ADP	A	902	-	-	1/16/32/32	0/3/3/3

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	901	AGS	PB-O3B	-6.21	1.52	1.59
3	D	902	AGS	PA-O3A	-5.05	1.54	1.59
3	D	902	AGS	PB-O3A	-5.01	1.54	1.59
3	E	901	AGS	PB-O3A	-4.97	1.54	1.59
4	F	901	ADP	C5-C4	4.63	1.47	1.39
3	E	902	AGS	PB-O3A	-4.62	1.54	1.59
3	D	901	AGS	PB-O3A	-4.62	1.54	1.59
4	A	902	ADP	C5-C4	4.62	1.47	1.39
4	A	901	ADP	C5-C4	4.51	1.47	1.39
4	B	902	ADP	C5-C4	4.43	1.47	1.39
3	D	901	AGS	PA-O3A	-4.15	1.55	1.59
3	E	902	AGS	PA-O3A	-4.03	1.55	1.59
3	C	901	AGS	PA-O3A	-4.00	1.55	1.59
3	C	902	AGS	PA-O3A	-3.98	1.55	1.59
3	C	901	AGS	PB-O3A	-3.98	1.55	1.59
3	E	901	AGS	PA-O3A	-3.89	1.55	1.59
3	C	902	AGS	PB-O3A	-3.73	1.55	1.59
3	D	901	AGS	PB-O3B	-3.42	1.55	1.59
3	C	902	AGS	PB-O3B	-3.17	1.56	1.59
3	E	902	AGS	PB-O3B	-2.80	1.56	1.59
3	D	902	AGS	PA-O1A	-2.76	1.41	1.50
3	B	901	AGS	PB-O3B	-2.74	1.56	1.59
4	A	901	ADP	C5-C6	2.64	1.48	1.41
4	F	901	ADP	C5-C6	2.61	1.48	1.41
4	B	902	ADP	C5-N7	-2.60	1.34	1.39
4	B	902	ADP	C5-C6	2.58	1.48	1.41
4	A	902	ADP	C5-N7	-2.57	1.34	1.39
3	E	901	AGS	PB-O3B	-2.48	1.56	1.59
4	A	902	ADP	C5-C6	2.48	1.47	1.41
3	E	902	AGS	PA-O1A	-2.45	1.42	1.50
4	F	901	ADP	C5-N7	-2.39	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	ADP	C5-N7	-2.38	1.34	1.39
3	D	901	AGS	PA-O1A	-2.38	1.42	1.50
3	E	901	AGS	PA-O1A	-2.37	1.42	1.50
3	D	902	AGS	PB-O3B	-2.33	1.57	1.59
4	F	901	ADP	C8-N7	2.24	1.36	1.31
3	E	902	AGS	PG-S1G	2.14	1.95	1.90
4	A	902	ADP	C8-N7	2.12	1.35	1.31
3	C	901	AGS	PA-O1A	-2.11	1.43	1.50
3	D	902	AGS	PG-S1G	2.09	1.95	1.90
4	A	901	ADP	C4-N9	-2.08	1.33	1.37
3	C	901	AGS	PG-S1G	2.08	1.95	1.90
3	D	901	AGS	PG-S1G	2.08	1.95	1.90
3	B	901	AGS	PG-S1G	2.08	1.95	1.90
4	B	902	ADP	C8-N9	-2.04	1.34	1.37
4	A	901	ADP	C8-N7	2.01	1.35	1.31

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	902	ADP	C5-C4-N3	-6.29	118.06	126.72
4	A	902	ADP	C5-C4-N3	-5.95	118.52	126.72
4	A	901	ADP	C5-C4-N3	-5.82	118.70	126.72
4	F	901	ADP	C5-C4-N3	-5.74	118.81	126.72
4	B	902	ADP	N3-C4-N9	5.10	135.84	127.17
3	E	901	AGS	PB-O3B-PG	-5.06	114.66	133.17
4	A	902	ADP	N3-C4-N9	4.94	135.57	127.17
3	B	901	AGS	PB-O3B-PG	-4.92	115.15	133.17
3	C	902	AGS	PB-O3B-PG	-4.73	115.87	133.17
4	A	901	ADP	N3-C4-N9	4.67	135.11	127.17
4	F	901	ADP	N3-C4-N9	4.57	134.94	127.17
3	C	901	AGS	PB-O3B-PG	-4.48	116.76	133.17
4	A	902	ADP	C2-N3-C4	3.73	120.95	111.83
4	F	901	ADP	C2-N3-C4	3.69	120.84	111.83
4	B	902	ADP	C2-N3-C4	3.67	120.79	111.83
4	A	901	ADP	C2-N3-C4	3.64	120.73	111.83
4	A	901	ADP	C4-C5-N7	-3.48	106.60	110.58
4	B	902	ADP	C4-C5-N7	-3.47	106.62	110.58
4	F	901	ADP	N3-C2-N1	-3.38	123.46	128.58
4	A	902	ADP	N3-C2-N1	-3.28	123.62	128.58
4	F	901	ADP	C4-C5-N7	-3.24	106.88	110.58
3	D	902	AGS	PB-O3B-PG	-3.19	121.50	133.17
4	A	901	ADP	N3-C2-N1	-3.16	123.79	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	902	ADP	C4-C5-N7	-2.94	107.22	110.58
3	D	901	AGS	PB-O3B-PG	-2.76	123.08	133.17
4	B	902	ADP	N3-C2-N1	-2.75	124.42	128.58
4	A	901	ADP	C4-N9-C8	2.72	108.59	105.74
4	B	902	ADP	C4-N9-C8	2.57	108.44	105.74
4	B	902	ADP	C5-N7-C8	2.57	107.48	103.45
4	F	901	ADP	C3'-C2'-C1'	2.55	106.29	101.46
3	C	902	AGS	O2A-PA-O3A	-2.53	100.42	107.27
4	B	902	ADP	C3'-C2'-C1'	2.53	106.25	101.46
4	A	902	ADP	C4-N9-C8	2.52	108.38	105.74
4	A	901	ADP	C5-N7-C8	2.44	107.29	103.45
3	C	901	AGS	O2B-PB-O3B	-2.43	100.71	107.27
4	F	901	ADP	C4-N9-C8	2.43	108.29	105.74
3	C	901	AGS	O2G-PG-O3B	2.40	112.66	104.64
3	E	902	AGS	O2B-PB-O3A	-2.39	100.81	107.27
3	E	902	AGS	PB-O3B-PG	-2.39	124.42	133.17
4	F	901	ADP	C5-N7-C8	2.36	107.16	103.45
4	A	902	ADP	C3'-C2'-C1'	2.24	105.71	101.46
4	A	902	ADP	C5-N7-C8	2.21	106.93	103.45
4	B	902	ADP	O3B-PB-O2B	2.19	116.02	107.80
4	F	901	ADP	C2-N1-C6	2.05	122.09	118.73
4	A	901	ADP	C6-C5-N7	2.02	135.99	132.09
3	B	901	AGS	O2G-PG-O3B	2.02	111.39	104.64
3	D	902	AGS	PA-O5'-C5'	-2.01	109.81	121.35
4	A	901	ADP	C2-N1-C6	2.01	122.03	118.73

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	902	AGS	C5'-O5'-PA-O1A
3	C	902	AGS	C5'-O5'-PA-O3A
3	C	902	AGS	O4'-C4'-C5'-O5'
3	D	901	AGS	PB-O3B-PG-O2G
3	D	901	AGS	PB-O3B-PG-O3G
3	B	901	AGS	C5'-O5'-PA-O1A
3	B	901	AGS	C5'-O5'-PA-O3A
4	F	901	ADP	C5'-O5'-PA-O3A
4	B	902	ADP	C5'-O5'-PA-O2A
4	B	902	ADP	C5'-O5'-PA-O3A
4	A	901	ADP	C5'-O5'-PA-O1A
4	A	901	ADP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
4	A	901	ADP	C5'-O5'-PA-O3A
4	A	902	ADP	C5'-O5'-PA-O1A
3	C	902	AGS	C3'-C4'-C5'-O5'
4	F	901	ADP	C3'-C4'-C5'-O5'
3	D	902	AGS	C3'-C4'-C5'-O5'
4	F	901	ADP	O4'-C4'-C5'-O5'
3	D	902	AGS	O4'-C4'-C5'-O5'
3	B	901	AGS	PA-O3A-PB-O2B
3	C	902	AGS	C5'-O5'-PA-O2A
4	F	901	ADP	C5'-O5'-PA-O1A
4	B	902	ADP	C5'-O5'-PA-O1A
3	C	901	AGS	PG-O3B-PB-O2B
3	E	901	AGS	O4'-C4'-C5'-O5'
3	E	901	AGS	PB-O3A-PA-O1A
3	B	901	AGS	PB-O3B-PG-O2G
3	E	902	AGS	PB-O3A-PA-O1A
3	E	902	AGS	PB-O3A-PA-O2A
3	B	901	AGS	PA-O3A-PB-O1B
4	B	902	ADP	PB-O3A-PA-O2A
3	B	901	AGS	O4'-C4'-C5'-O5'
3	C	901	AGS	O4'-C4'-C5'-O5'
3	E	901	AGS	PB-O3A-PA-O2A

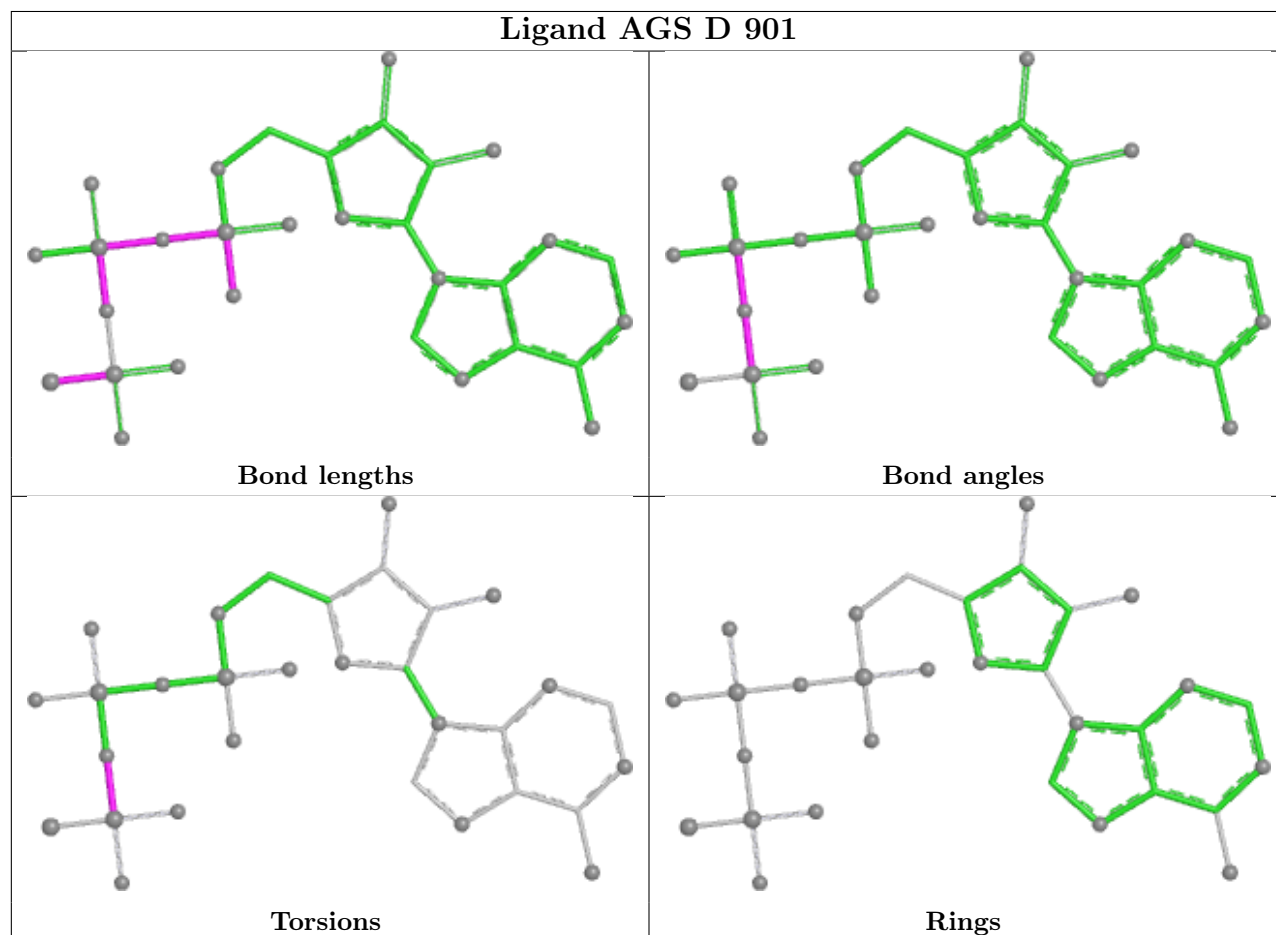
There are no ring outliers.

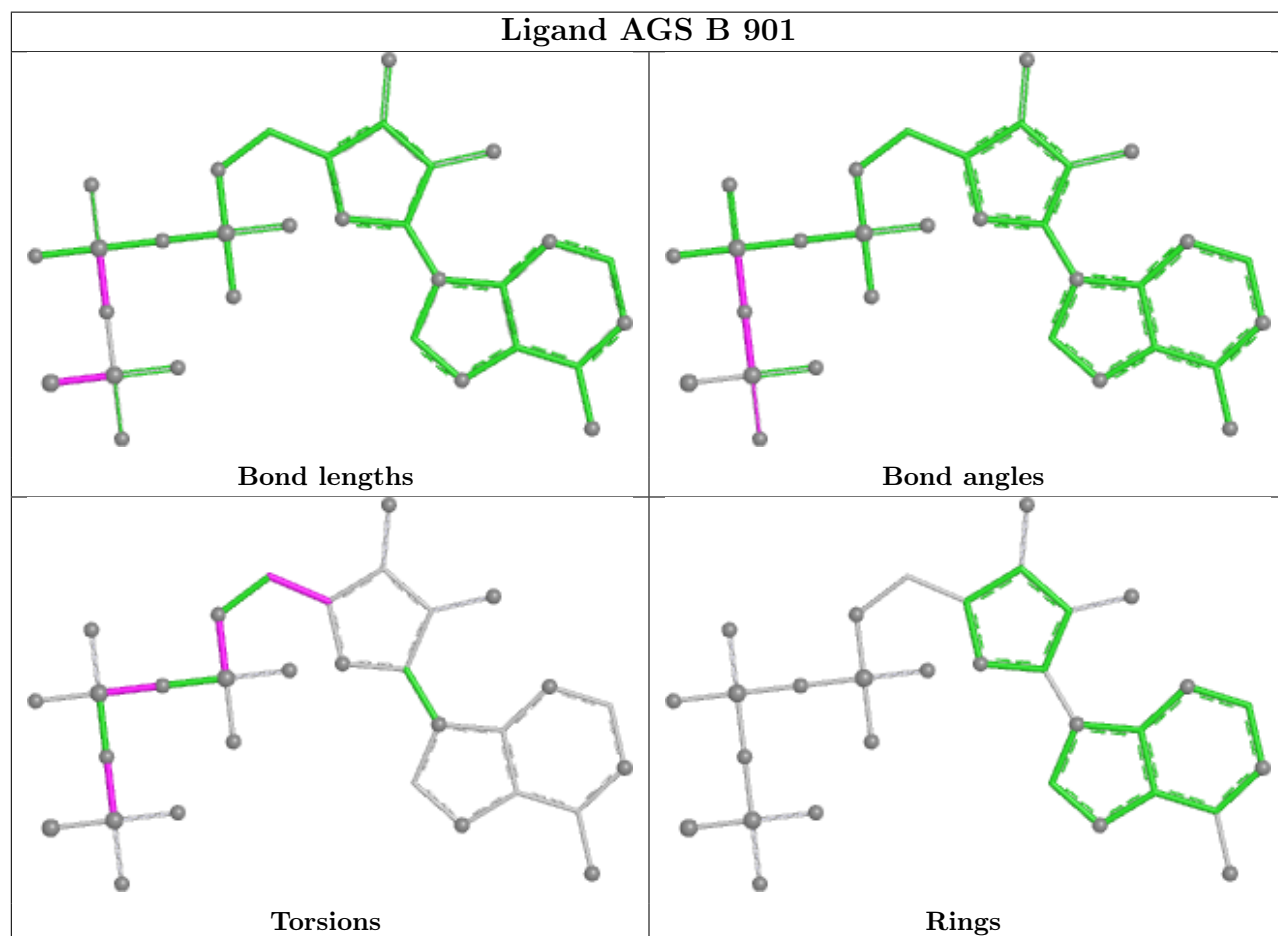
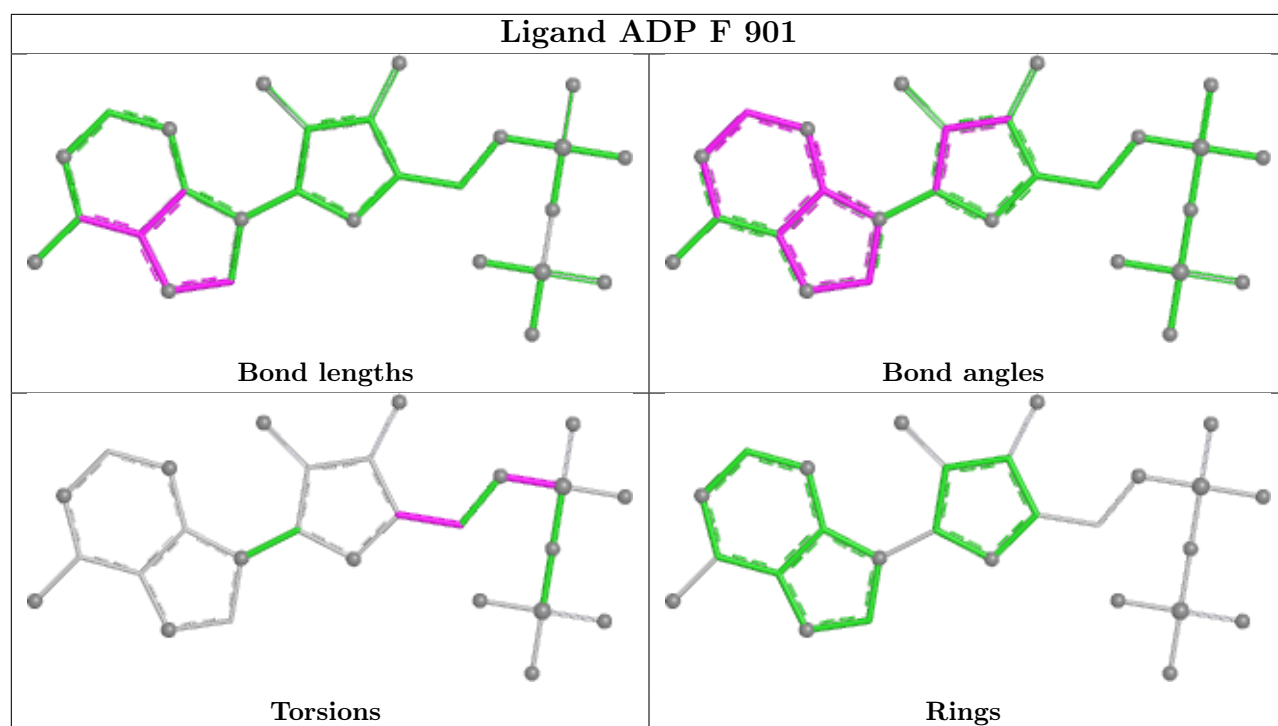
9 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	901	AGS	3	0
3	B	901	AGS	2	0
3	E	902	AGS	4	0
4	A	901	ADP	1	0
3	D	902	AGS	4	0
4	B	902	ADP	1	0
3	E	901	AGS	5	0
3	C	902	AGS	5	0
3	C	901	AGS	3	0

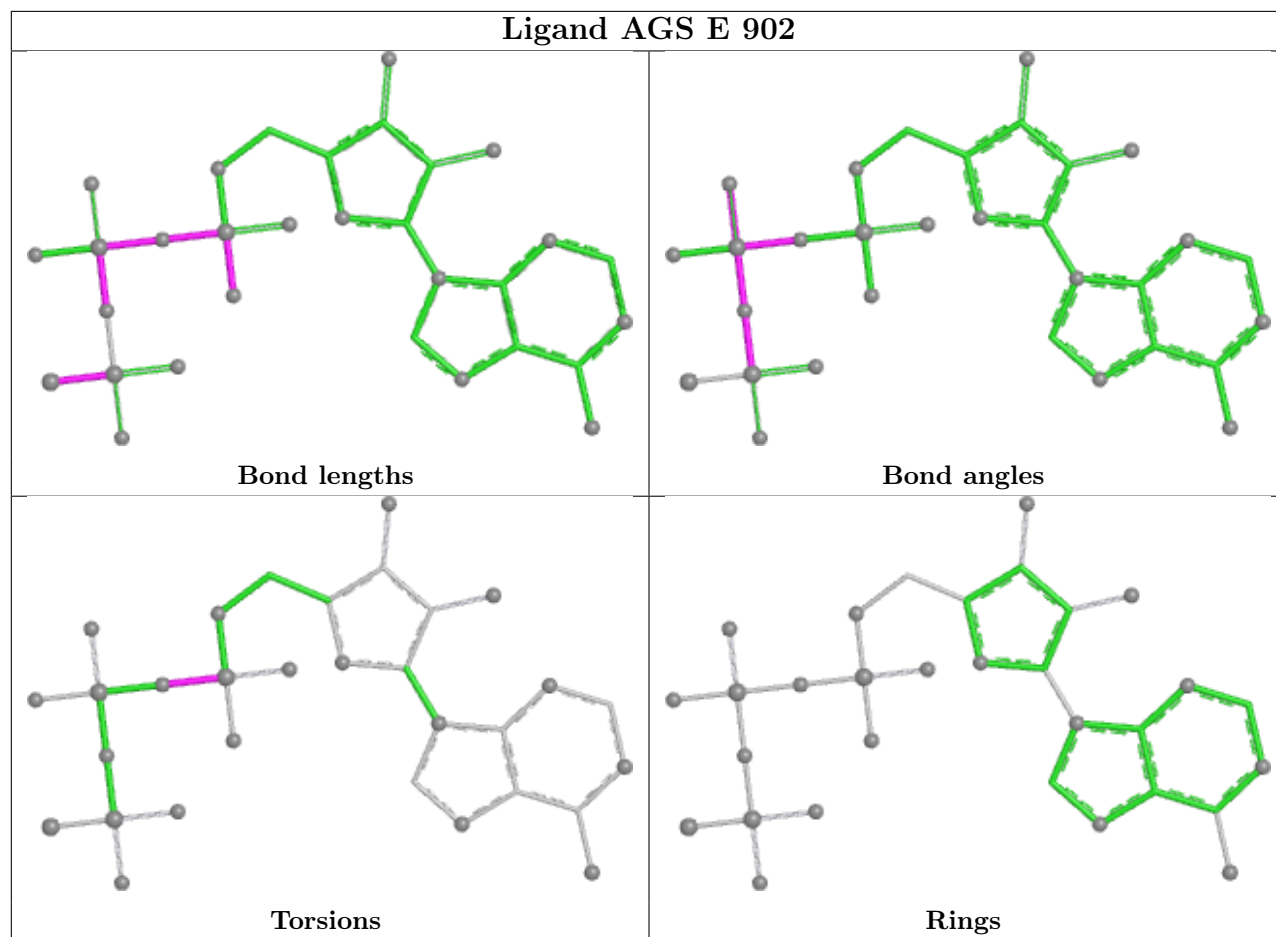
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

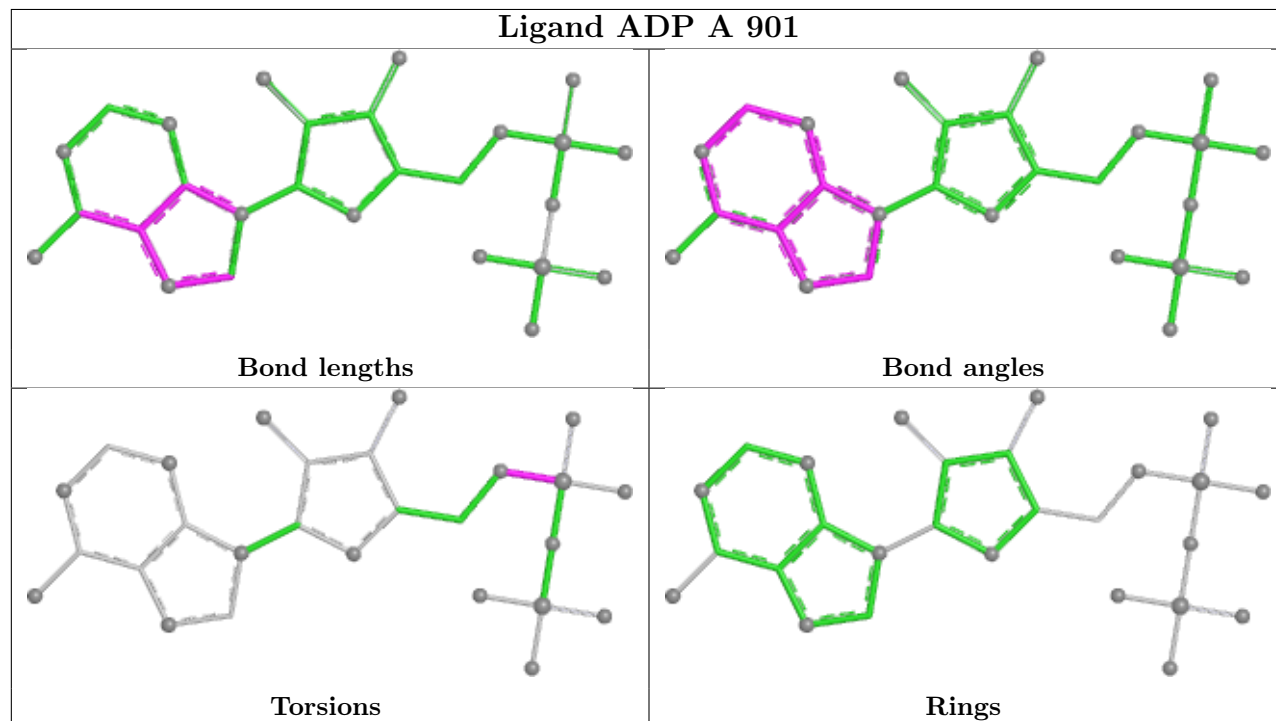




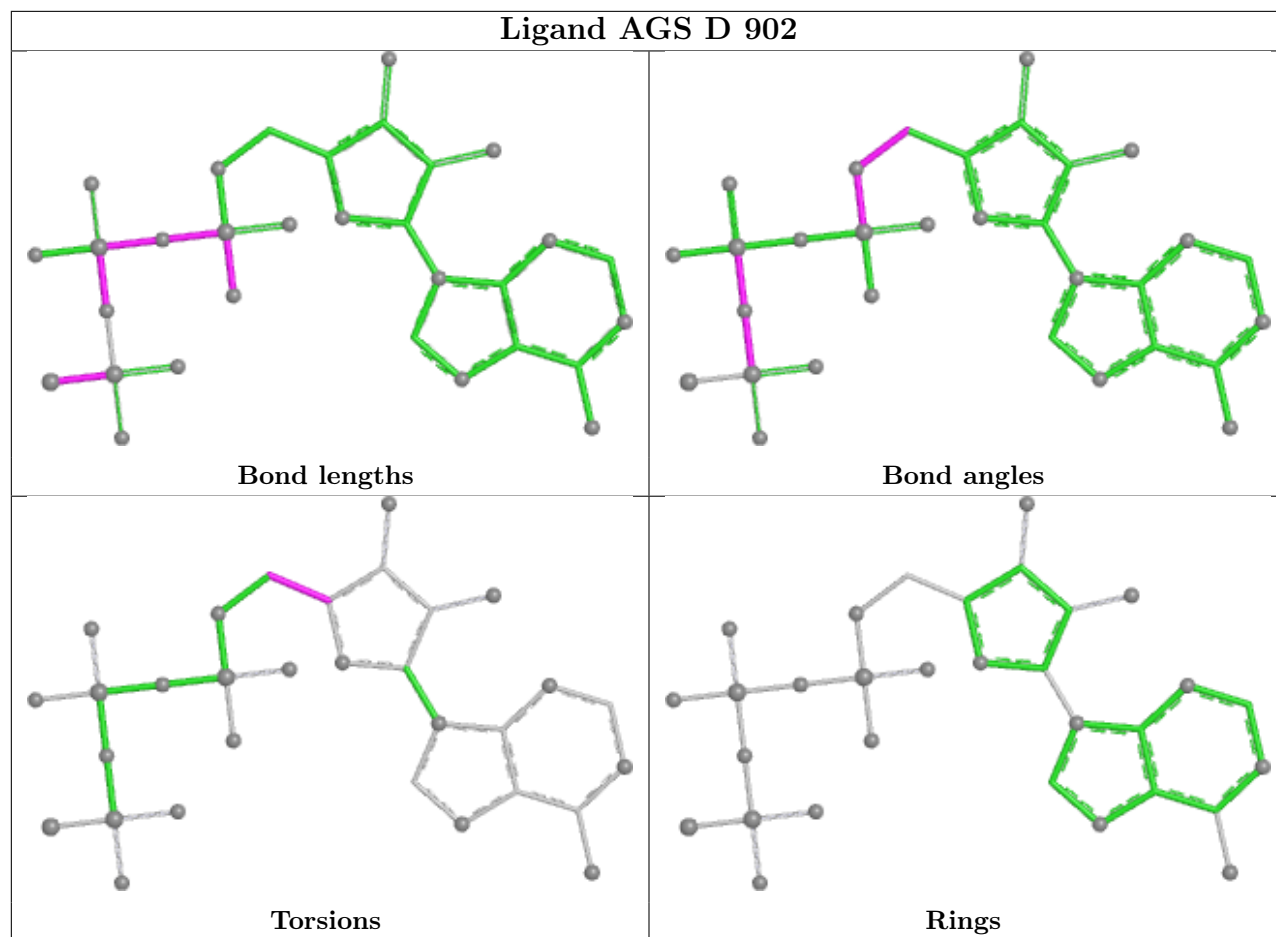
Ligand AGS E 902



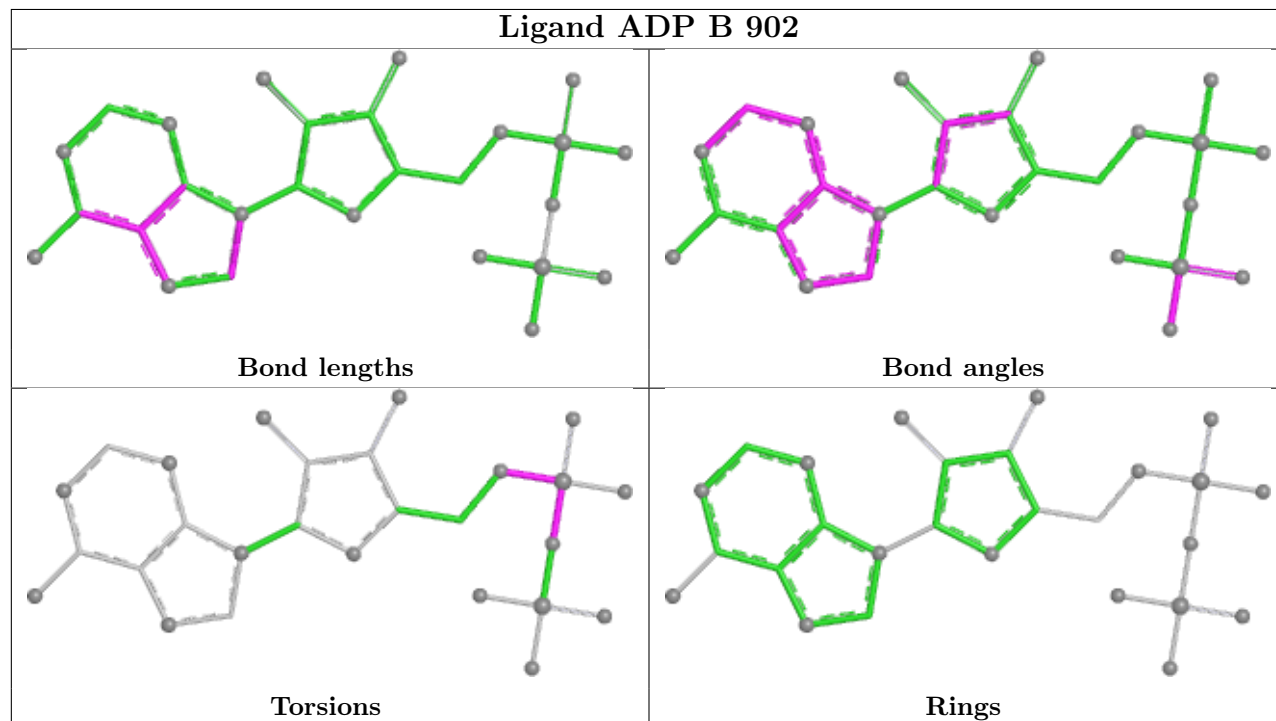
Ligand ADP A 901

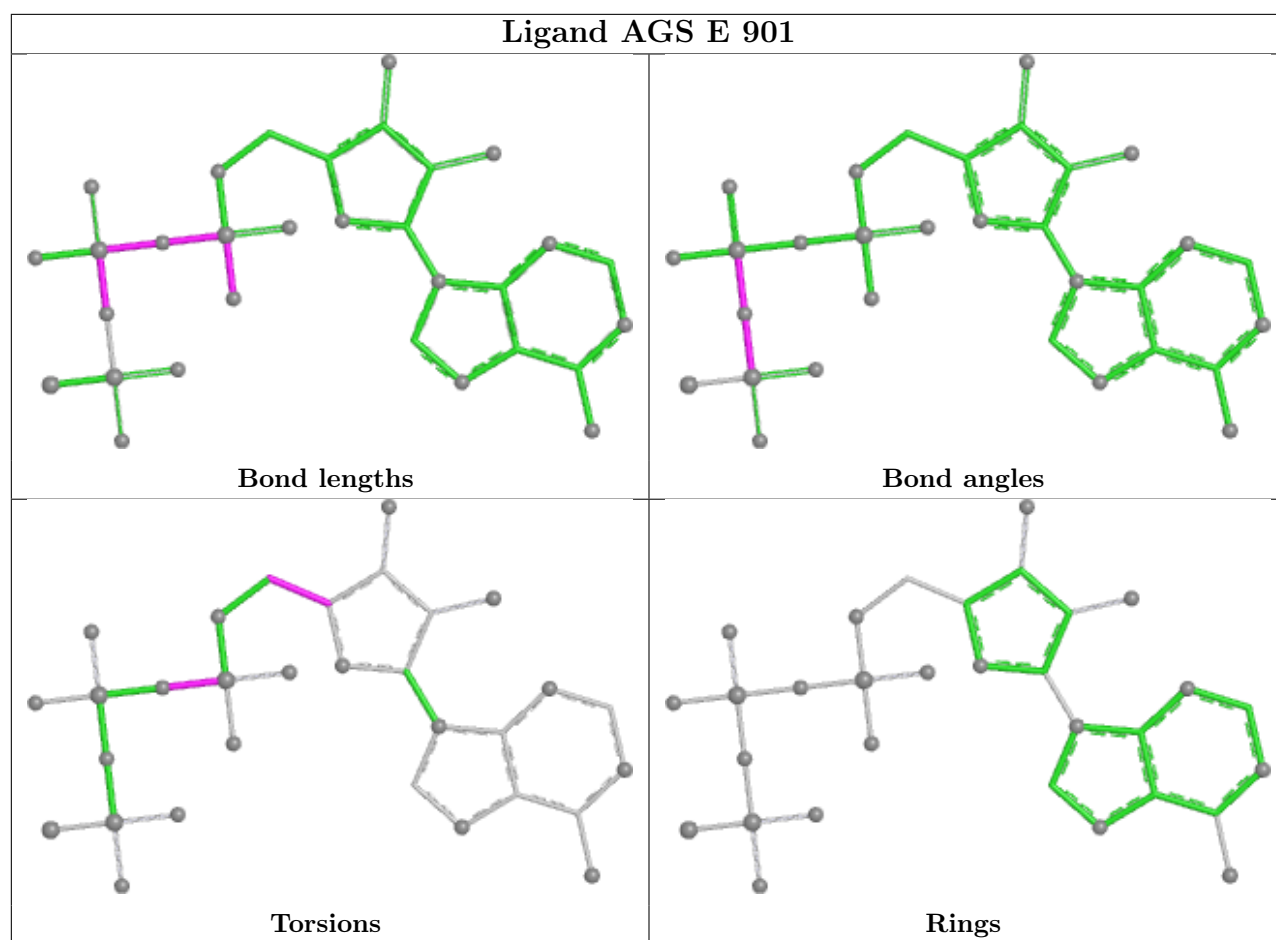


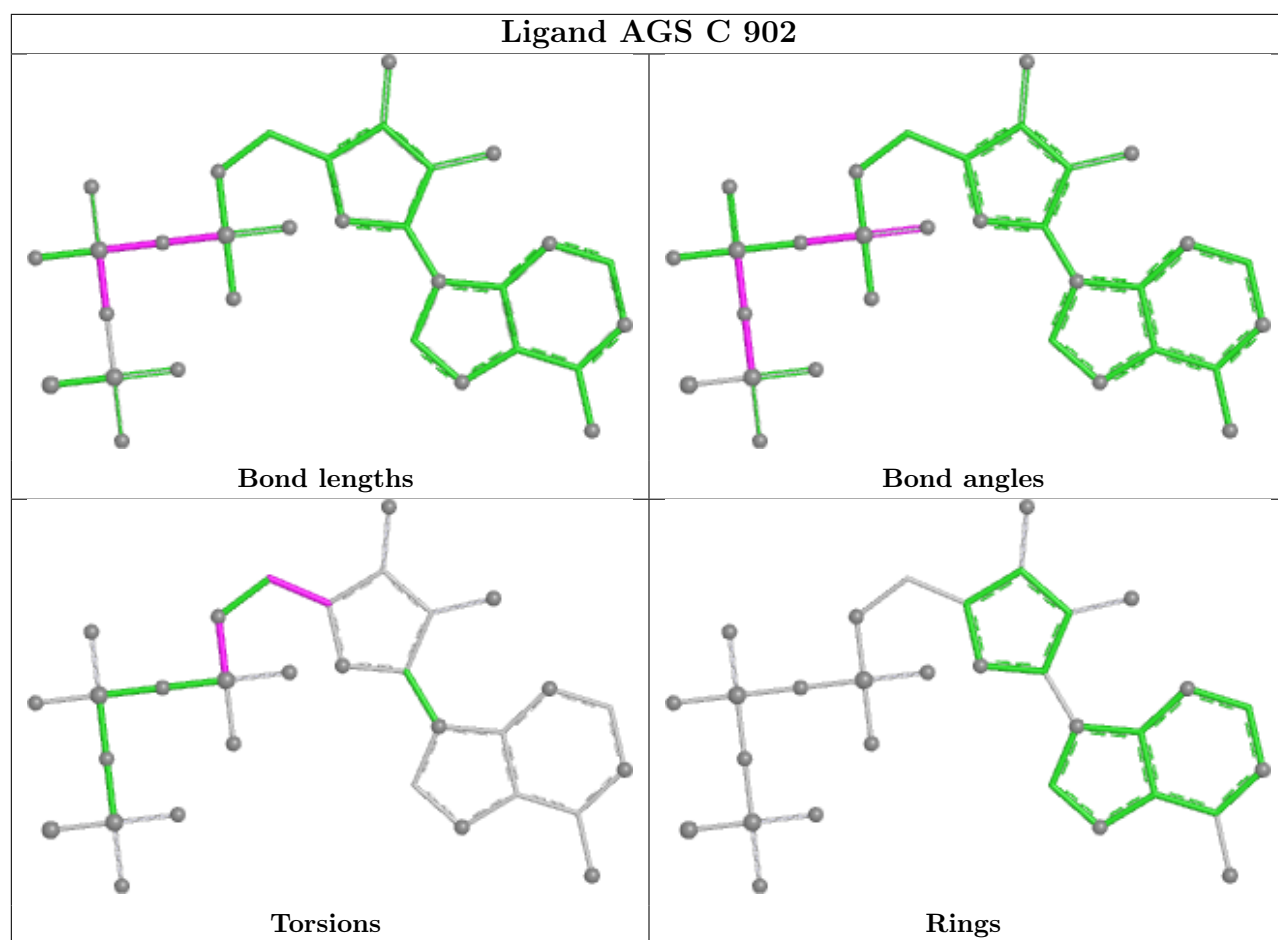
Ligand AGS D 902



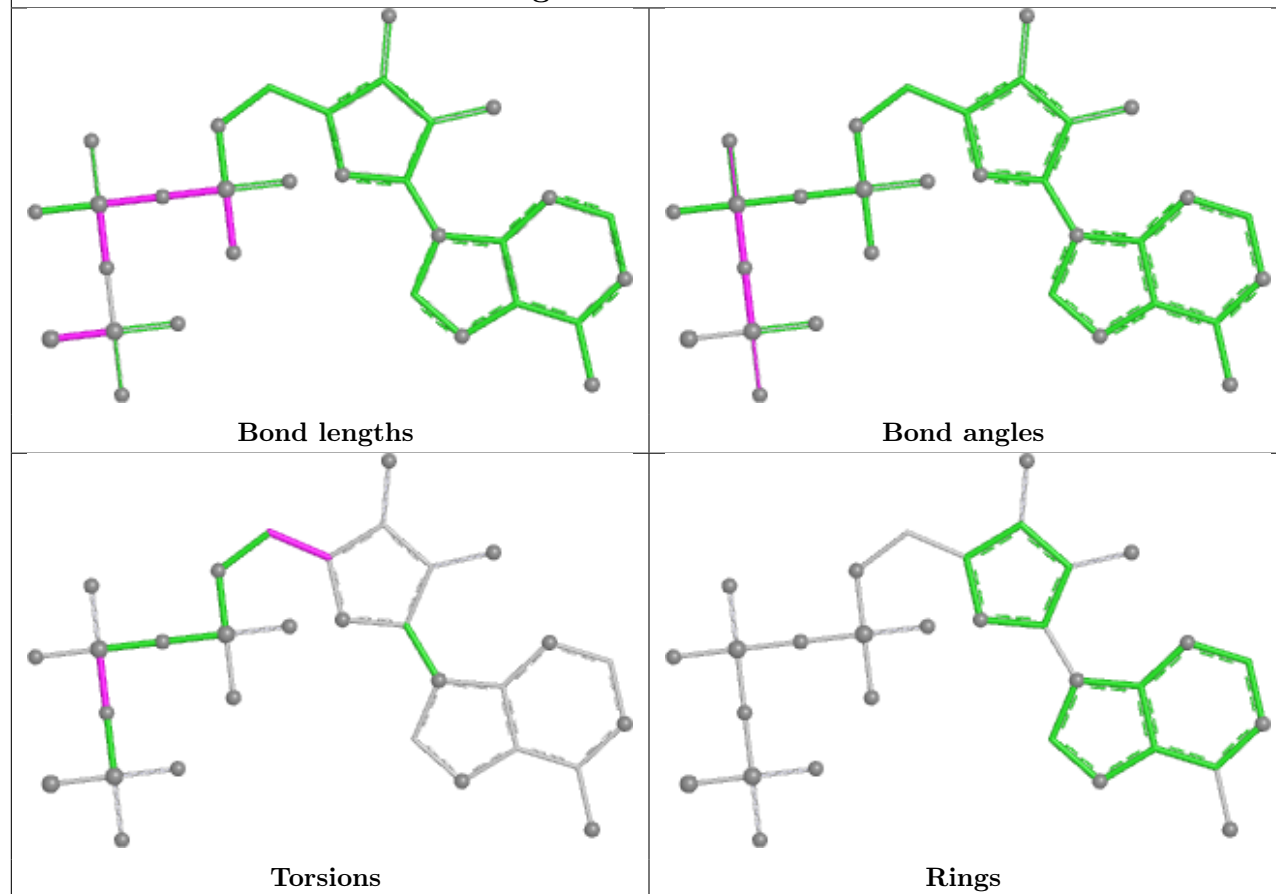
Ligand ADP B 902



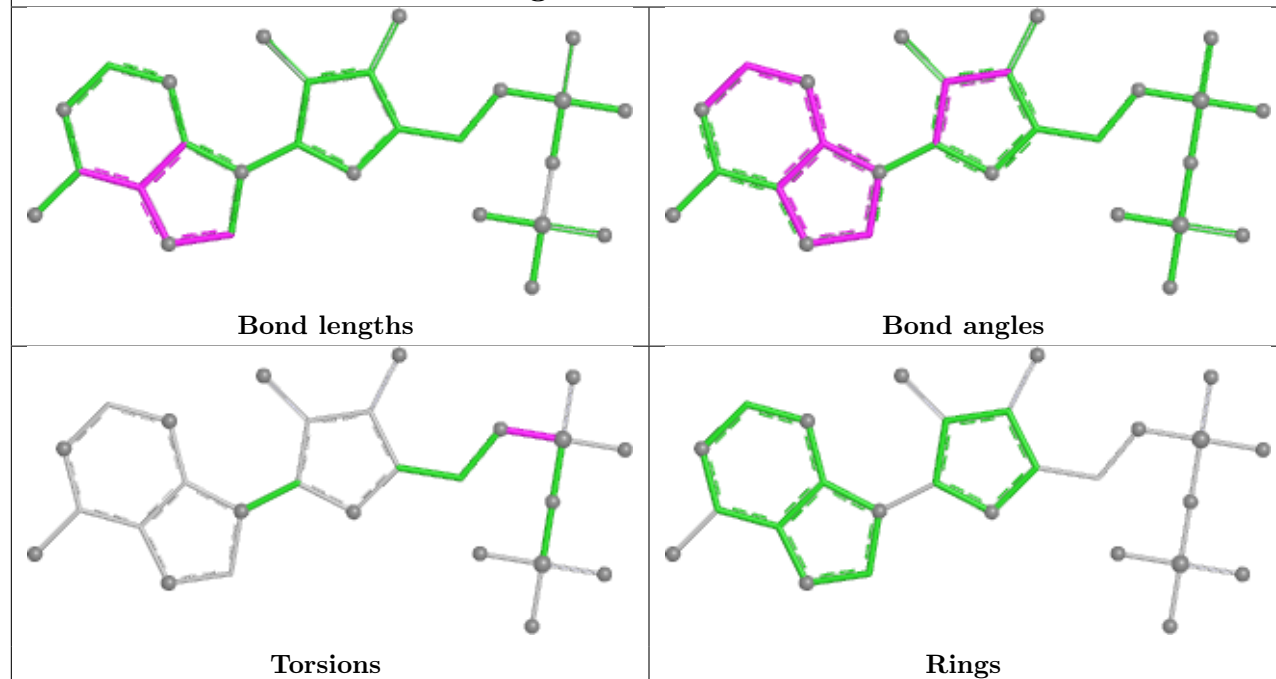




Ligand AGS C 901



Ligand ADP A 902



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

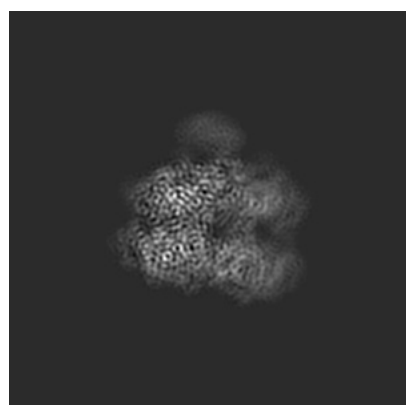
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20005. These allow visual inspection of the internal detail of the map and identification of artifacts.

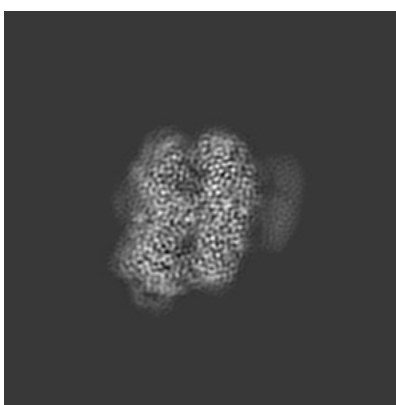
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

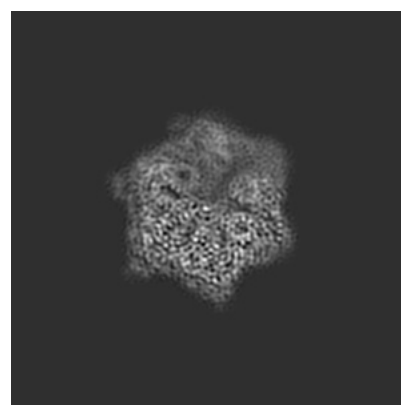
6.1.1 Primary map



X



Y

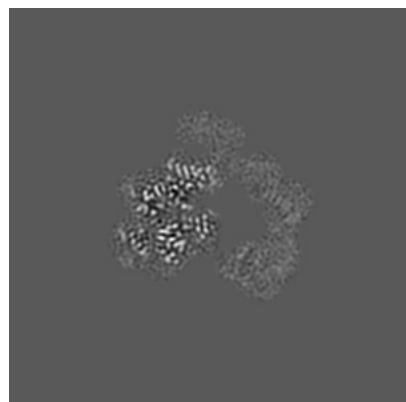


Z

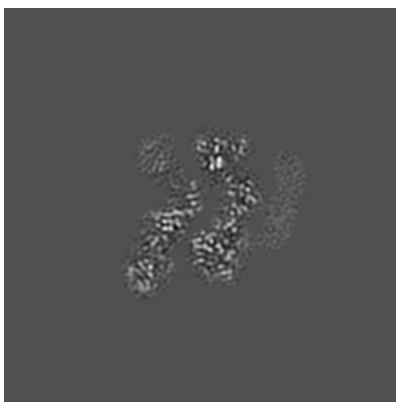
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

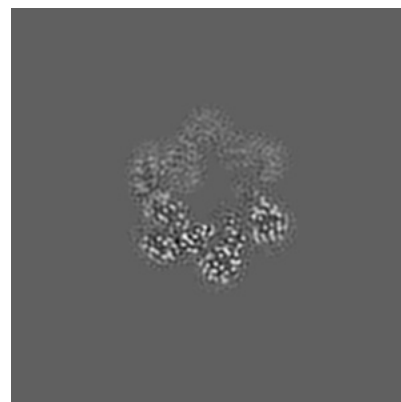
6.2.1 Primary map



X Index: 128



Y Index: 128

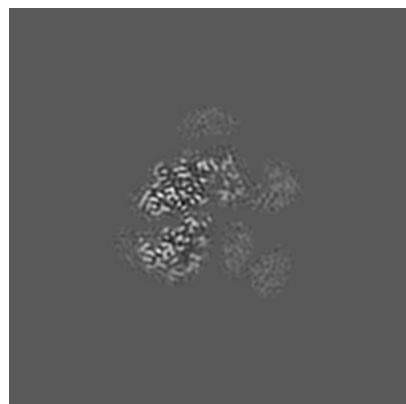


Z Index: 128

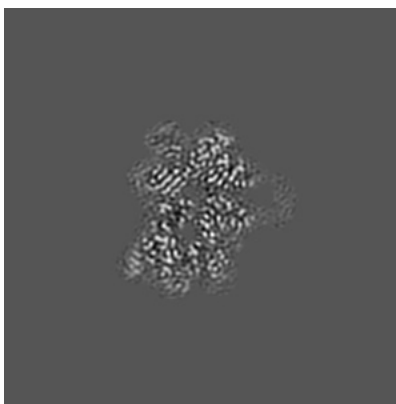
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

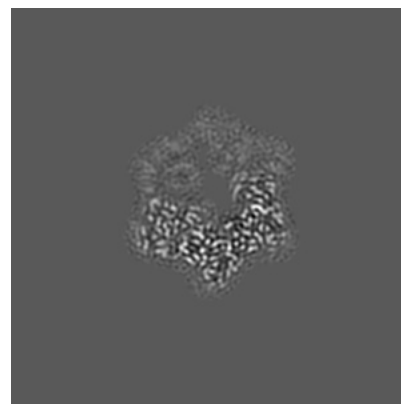
6.3.1 Primary map



X Index: 143



Y Index: 110

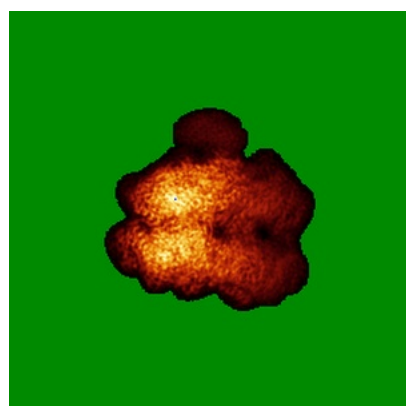


Z Index: 137

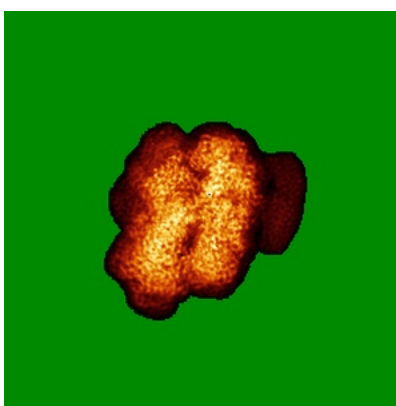
The images above show the largest variance slices of the map in three orthogonal directions.

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

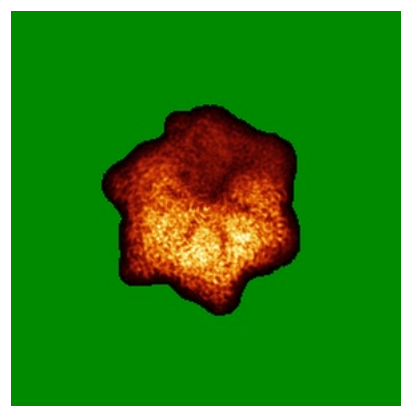
6.4.1 Primary map



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

This section was not generated.

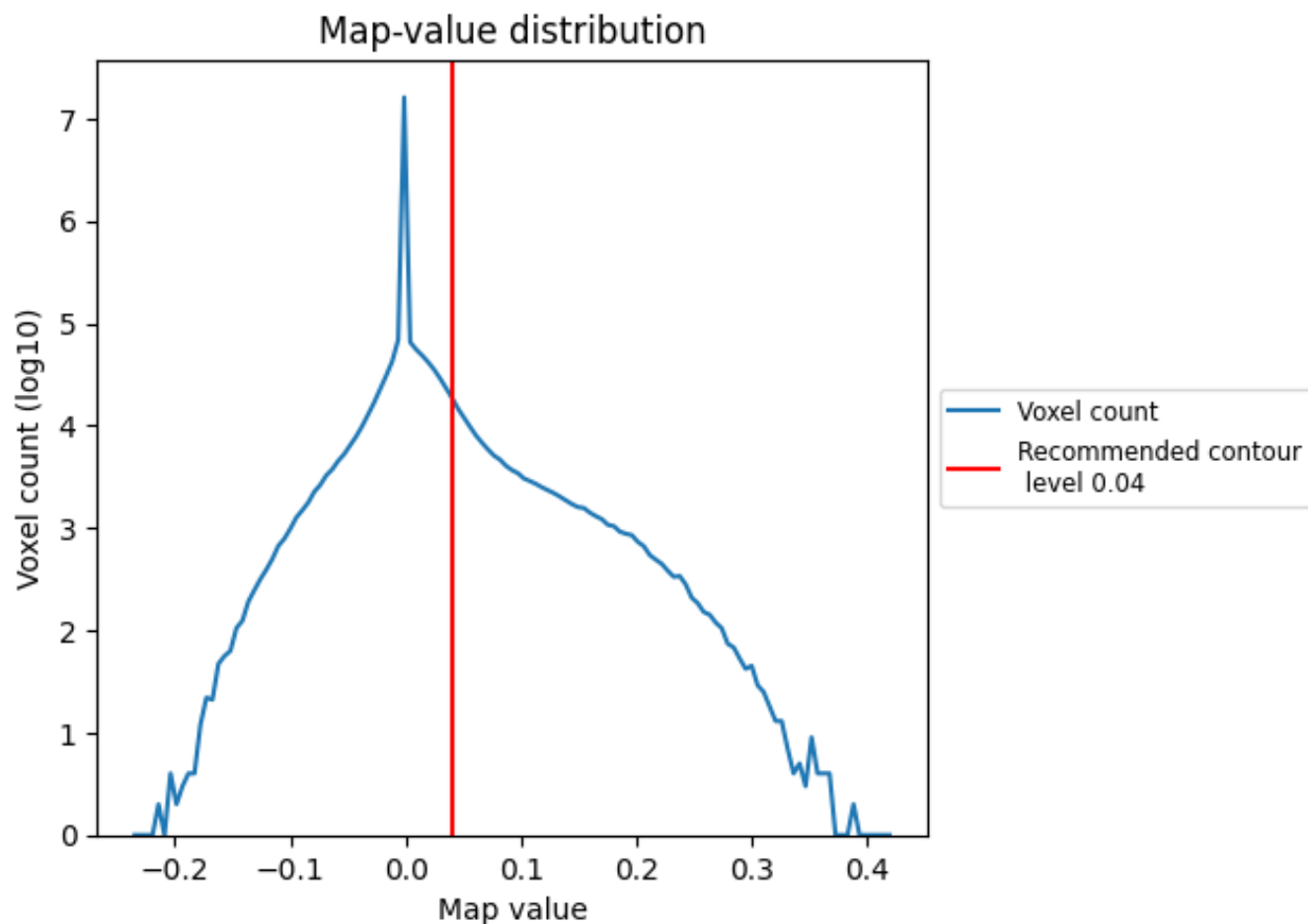
6.6 Mask visualisation

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

7 Map analysis [i](#)

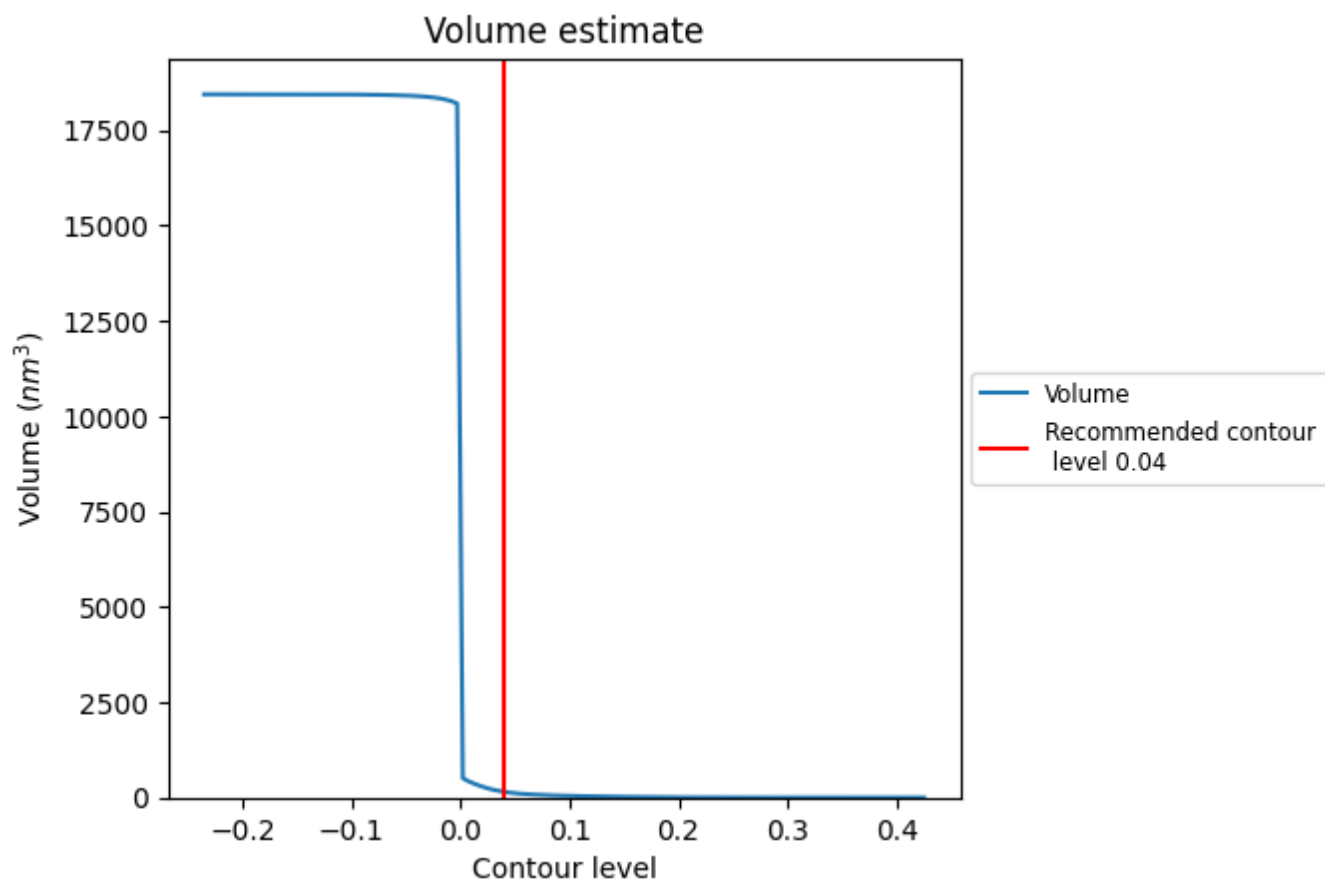
This section contains the results of statistical analysis of the map.

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.

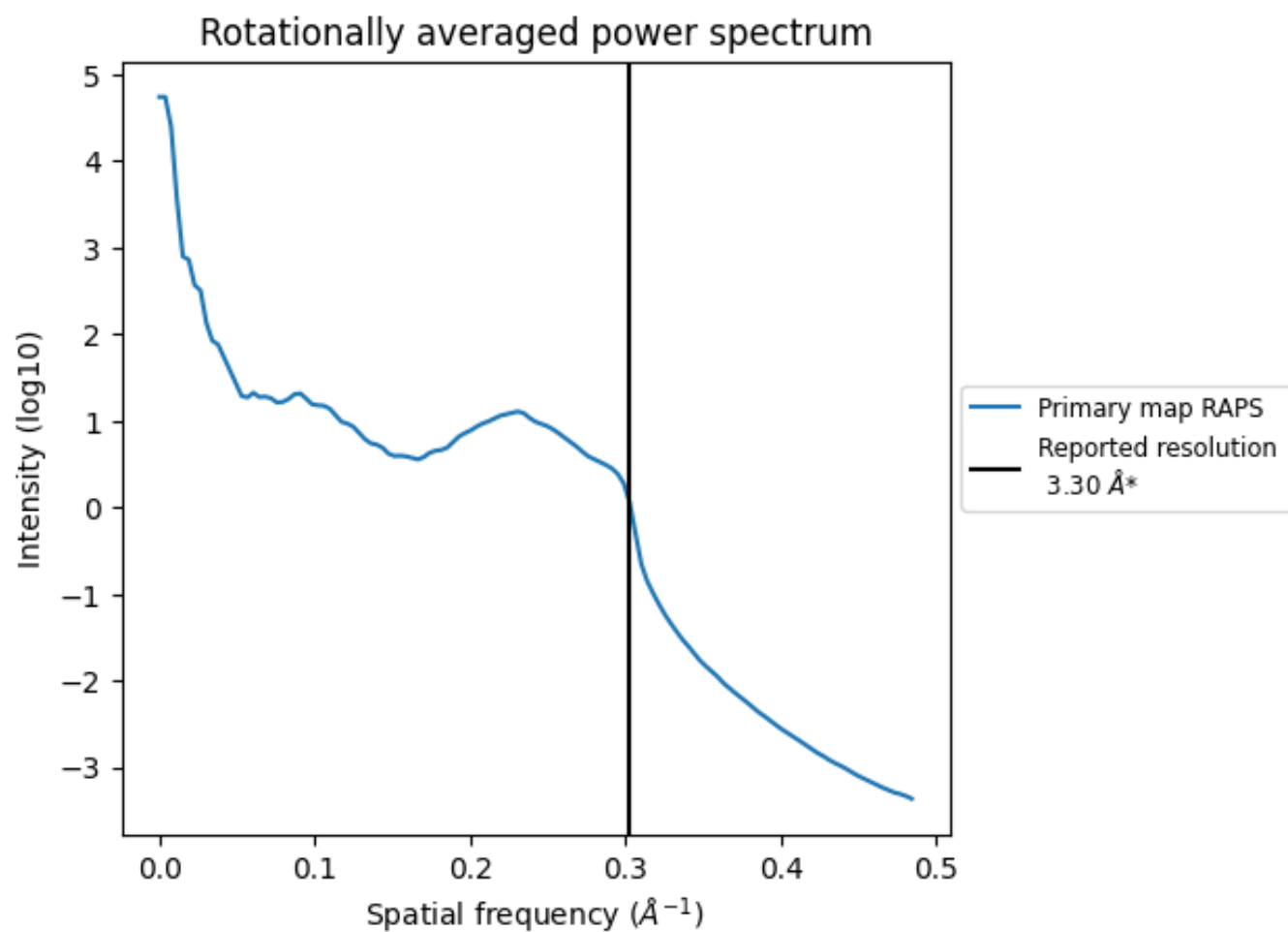
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 151 nm³; this corresponds to an approximate mass of 136 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 0.303 Å⁻¹

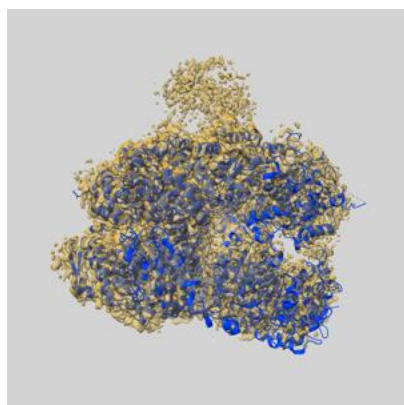
8 Fourier-Shell correlation ⓘ

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

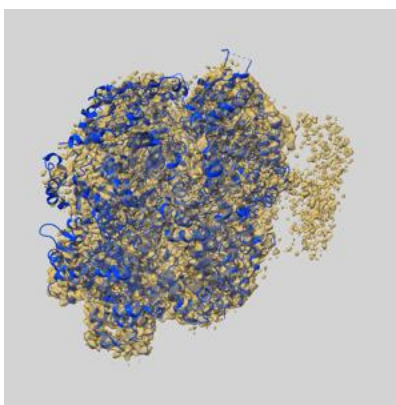
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20005 and PDB model 6OAY. Per-residue inclusion information can be found in section [3](#) on page [7](#).

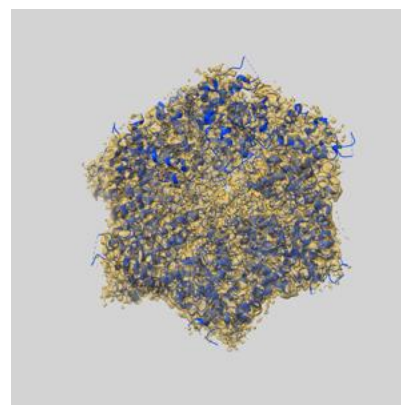
9.1 Map-model overlay [i](#)



X



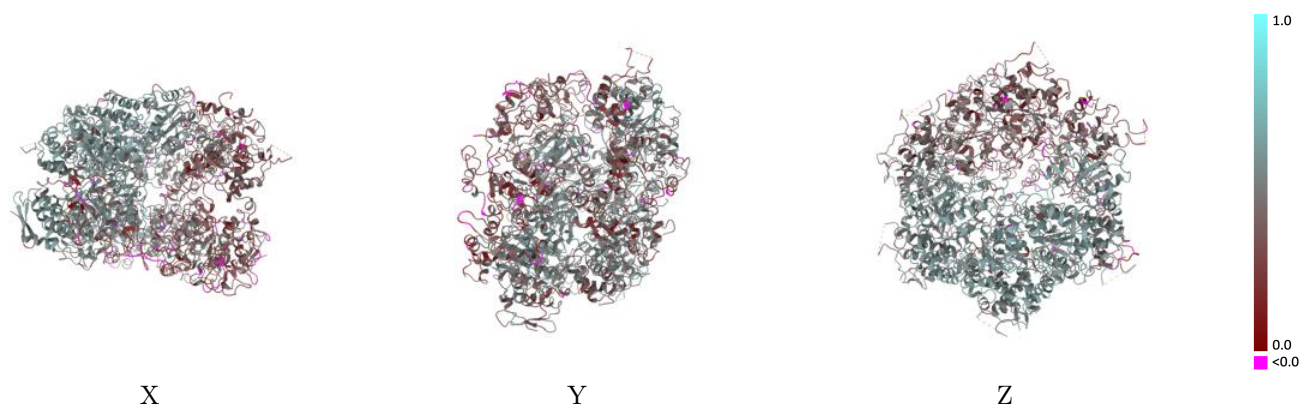
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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](#)

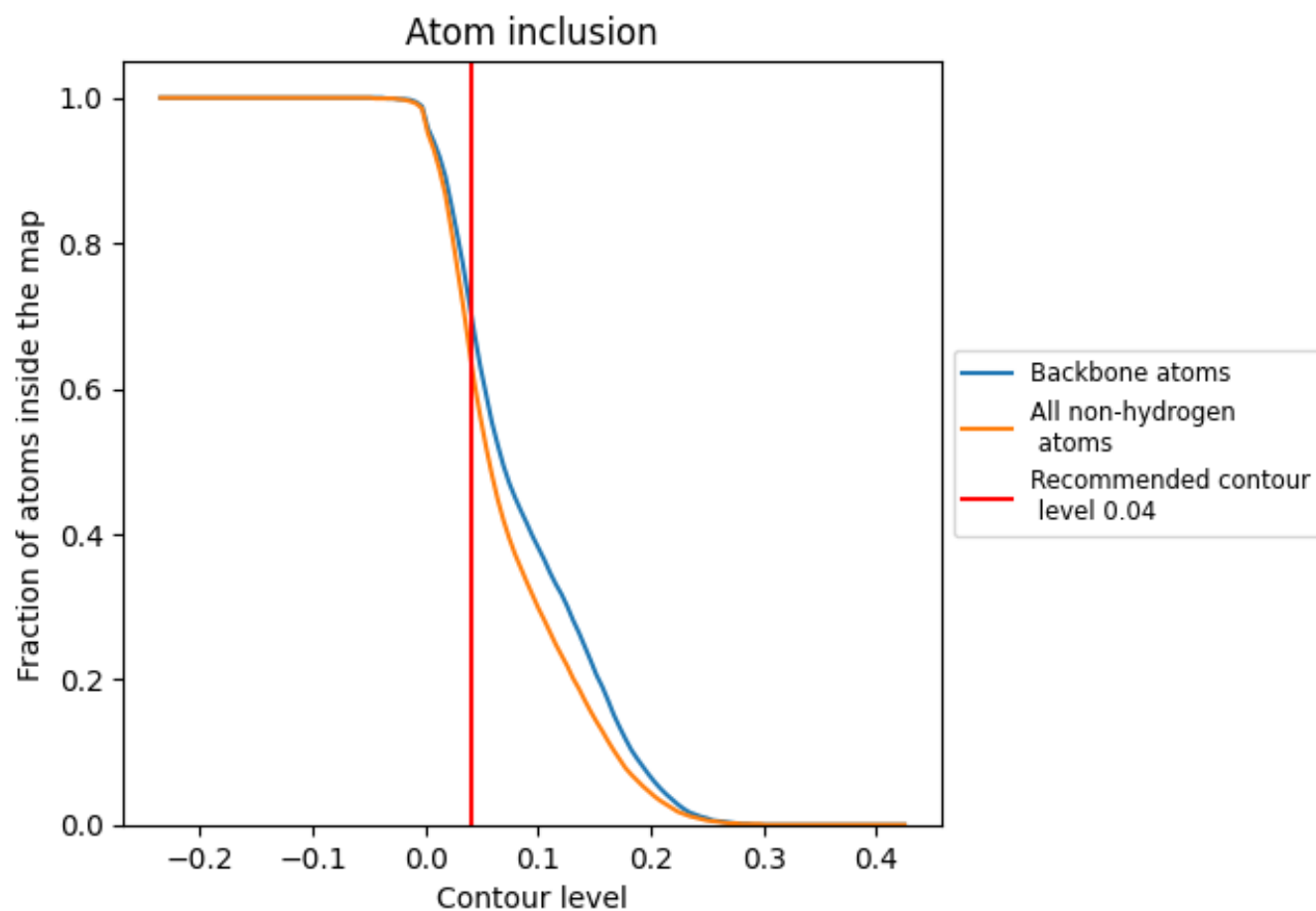


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6430	0.4370
A	0.3840	0.3320
B	0.6760	0.4420
C	0.8120	0.5050
D	0.8430	0.5280
E	0.8110	0.5090
F	0.3150	0.2990
P	0.7080	0.4500

1.0

0.0

<0.0