



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 04:31 AM UTC

PDB ID : 5VYA / pdb_00005vya
EMDB ID : EMD-8746
Title : S. cerevisiae Hsp104:casein complex, Extended Conformation
Authors : Gates, S.N.; Yokom, A.L.; Lin, J.-B.; Jackrel, M.E.; Rizo, A.N.; Kendsersky, N.M.; Buell, C.E.; Sweeny, E.A.; Chuang, E.; Torrente, M.P.; Mack, K.L.; Su, M.; Shorter, J.; Southworth, D.R.
Deposited on : 2017-05-24
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

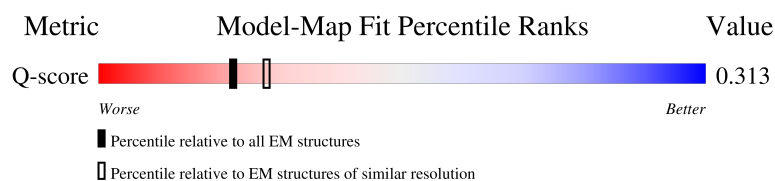
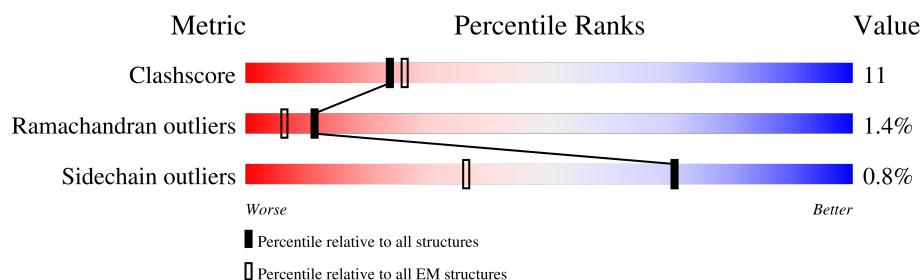
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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	7587 (3.50 - 4.50)

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	908	
1	B	908	
1	C	908	
1	D	908	

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Mol	Chain	Length	Quality of chain
1	E	908	
1	F	908	
2	P	28	

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	B	1002	-	-	X	-
3	AGS	C	1003	-	-	X	-
3	AGS	D	1002	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27691 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.

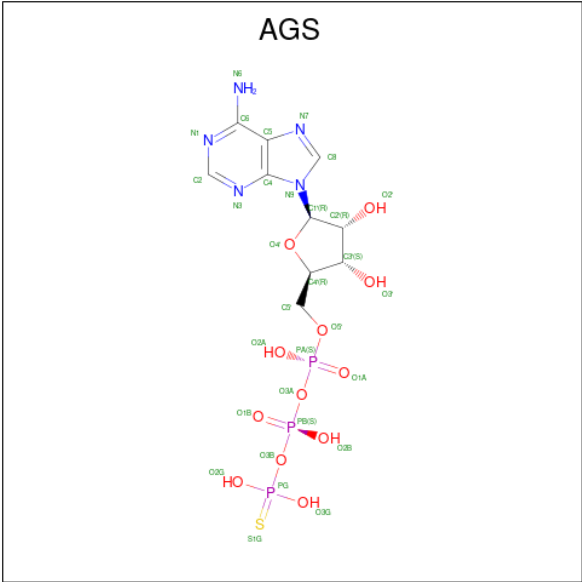
- Molecule 1 is a protein called Heat shock protein 104.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	579	Total	C	N	O	S	0	0
			4530	2850	794	868	18		
1	B	579	Total	C	N	O	S	0	0
			4530	2850	794	868	18		
1	C	579	Total	C	N	O	S	0	0
			4530	2850	794	868	18		
1	D	579	Total	C	N	O	S	0	0
			4530	2850	794	868	18		
1	E	579	Total	C	N	O	S	0	0
			4530	2850	794	868	18		
1	F	579	Total	C	N	O	S	0	0
			4530	2850	794	868	18		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	P	28	Total	C	N	O	0	0
			139	83	28	28		

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

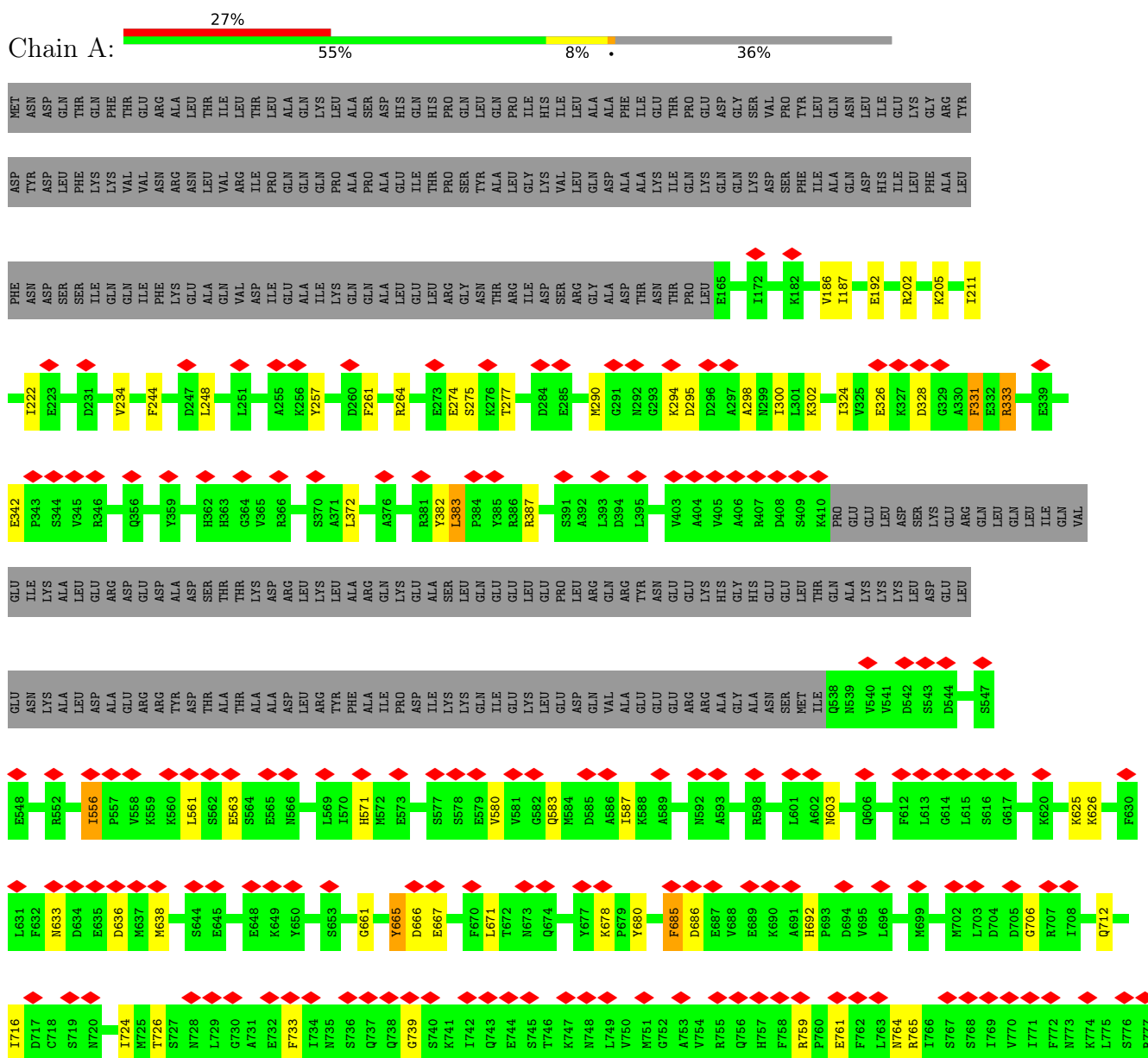


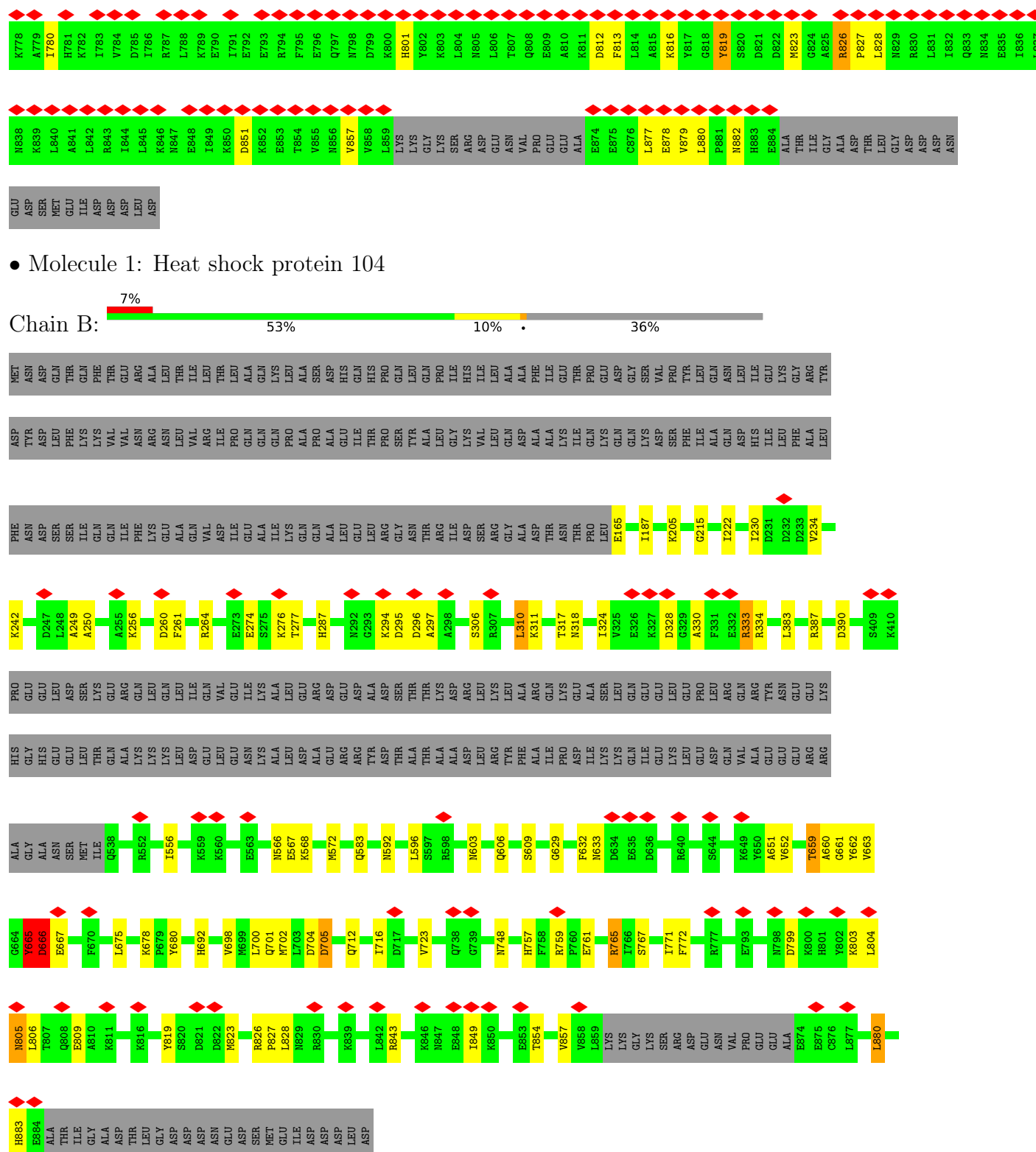
Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	C	1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

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.

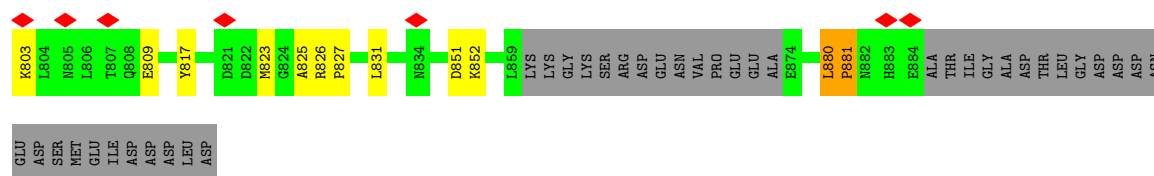
• Molecule 1: Heat shock protein 104



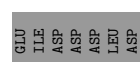
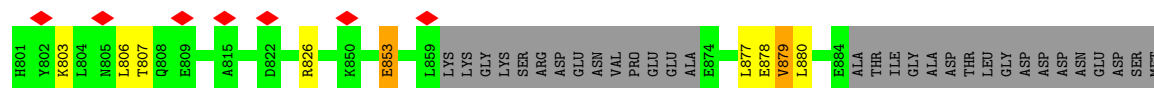
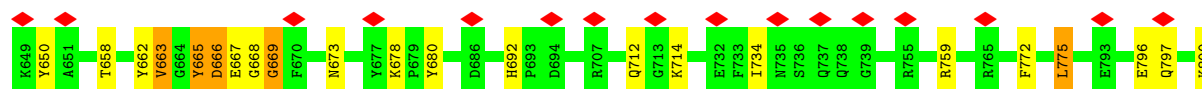
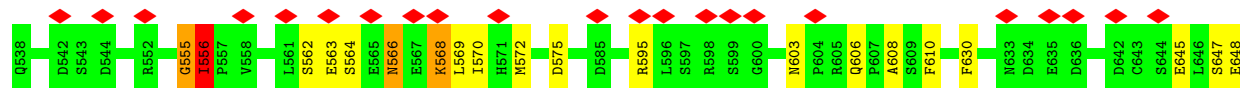
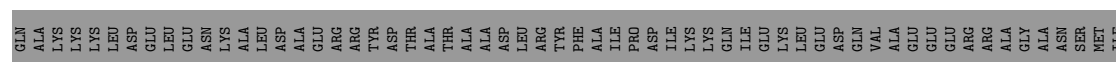
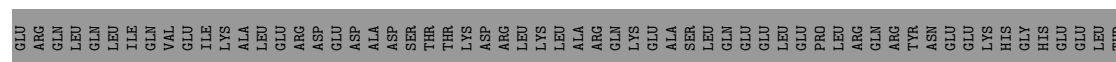
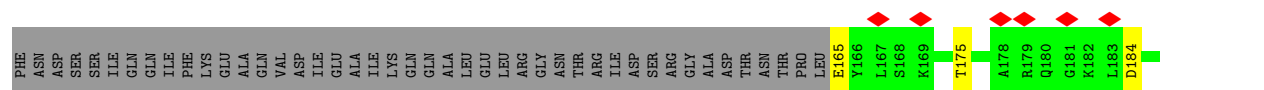
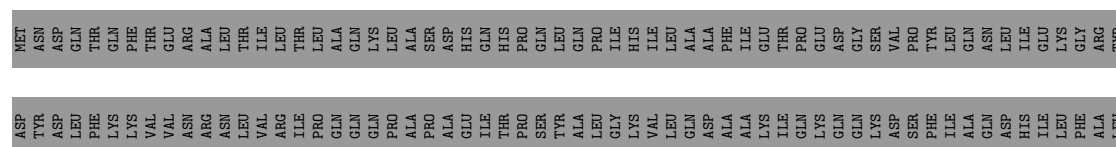


• Molecule 1: Heat shock protein 104

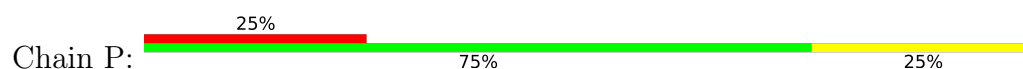
Chain C: 52% 10% 36%

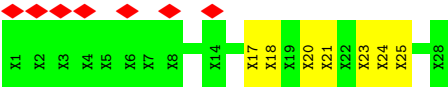


• Molecule 1: Heat shock protein 104



• Molecule 2: Alpha-S1-casein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	146463	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 ($e^-/\text{\AA}^2$)	0.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	50000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.175	Depositor
Minimum map value	-0.061	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0248	Depositor
Map size (Å)	256.0, 256.0, 256.0	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	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

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	1.16	7/4586 (0.2%)	1.32	44/6171 (0.7%)
1	B	1.27	5/4586 (0.1%)	1.29	35/6171 (0.6%)
1	C	1.34	10/4586 (0.2%)	1.27	36/6171 (0.6%)
1	D	1.32	9/4586 (0.2%)	1.29	32/6171 (0.5%)
1	E	1.30	10/4586 (0.2%)	1.28	25/6171 (0.4%)
1	F	1.21	5/4586 (0.1%)	1.29	38/6171 (0.6%)
All	All	1.27	46/27516 (0.2%)	1.29	210/37026 (0.6%)

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	287	HIS	CB-CG	-8.74	1.38	1.50
1	F	673	ASN	CB-CG	-8.27	1.31	1.52
1	B	287	HIS	CB-CG	-6.72	1.40	1.50
1	D	281	LEU	CB-CG	-6.42	1.40	1.53
1	C	595	ARG	CD-NE	-6.26	1.37	1.46
1	D	230	ILE	CB-CG1	-6.26	1.41	1.53
1	A	324	ILE	CB-CG1	-6.13	1.41	1.53
1	C	287	HIS	CB-CG	-6.09	1.41	1.50
1	D	801	HIS	CB-CG	-6.08	1.41	1.50
1	D	610	PHE	CB-CG	-6.07	1.36	1.50
1	D	222	ILE	CB-CG1	-6.02	1.41	1.53
1	E	207	ASN	CB-CG	-5.99	1.37	1.52
1	A	692	HIS	CB-CG	-5.98	1.41	1.50
1	B	230	ILE	CB-CG1	-5.93	1.41	1.53
1	F	282	PHE	CB-CG	-5.93	1.37	1.50
1	C	310	LEU	CB-CG	-5.92	1.41	1.53
1	D	207	ASN	CB-CG	-5.89	1.37	1.52
1	A	571	HIS	CB-CG	5.75	1.58	1.50
1	A	780	ILE	CB-CG1	-5.72	1.42	1.53
1	F	734	ILE	CB-CG1	-5.70	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	571	HIS	CB-CG	-5.68	1.42	1.50
1	D	708	ILE	CB-CG1	-5.68	1.42	1.53
1	C	281	LEU	CB-CG	-5.63	1.42	1.53
1	B	596	LEU	CB-CG	-5.62	1.42	1.53
1	E	248	LEU	CB-CG	-5.56	1.42	1.53
1	C	883	HIS	CB-CG	5.47	1.57	1.50
1	A	264	ARG	CD-NE	-5.45	1.38	1.46
1	E	305	LEU	CG-CD2	-5.39	1.34	1.52
1	E	378	LEU	CB-CG	-5.37	1.42	1.53
1	C	207	ASN	CB-CG	-5.36	1.38	1.52
1	C	244	PHE	CB-CG	-5.33	1.38	1.50
1	B	716	ILE	CA-CB	-5.32	1.49	1.55
1	E	758	PHE	CB-CG	-5.29	1.38	1.50
1	F	692	HIS	CB-CG	-5.28	1.42	1.50
1	E	826	ARG	CG-CD	-5.27	1.36	1.52
1	A	587	ILE	CB-CG1	-5.23	1.43	1.53
1	B	757	HIS	CB-CG	-5.23	1.42	1.50
1	F	216	ILE	CB-CG1	-5.16	1.43	1.53
1	E	234	VAL	N-CA	-5.15	1.41	1.47
1	C	283	ILE	CA-C	-5.14	1.47	1.52
1	C	806	LEU	CB-CG	-5.14	1.43	1.53
1	E	632	PHE	CB-CG	-5.10	1.39	1.50
1	A	716	ILE	CB-CG1	-5.06	1.43	1.53
1	E	299	ASN	CA-C	-5.04	1.46	1.52
1	C	695	VAL	CA-C	-5.03	1.46	1.52
1	D	244	PHE	CB-CG	-5.02	1.39	1.50

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	266	LYS	N-CA-C	15.14	130.85	112.38
1	E	803	LYS	N-CA-C	-11.41	99.49	113.41
1	B	883	HIS	N-CA-C	-10.29	101.04	114.31
1	A	342	GLU	CA-C-N	9.66	129.59	120.03
1	A	342	GLU	C-N-CA	9.66	129.59	120.03
1	B	799	ASP	N-CA-C	-9.30	102.51	114.04
1	A	880	LEU	CA-C-N	8.81	128.67	120.21
1	A	880	LEU	C-N-CA	8.81	128.67	120.21
1	A	733	PHE	CA-CB-CG	-8.71	105.09	113.80
1	F	880	LEU	CA-C-N	8.67	128.53	120.21
1	F	880	LEU	C-N-CA	8.67	128.53	120.21
1	C	261	PHE	CA-CB-CG	8.45	122.25	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	ILE	CB-CA-C	-8.29	101.16	112.02
1	B	880	LEU	CA-C-N	7.97	129.81	119.84
1	B	880	LEU	C-N-CA	7.97	129.81	119.84
1	A	685	PHE	CA-CB-CG	-7.90	105.90	113.80
1	C	803	LYS	N-CA-C	-7.84	104.23	113.88
1	B	256	LYS	N-CA-C	-7.80	99.50	110.50
1	A	234	VAL	CA-C-N	7.73	128.19	119.92
1	A	234	VAL	C-N-CA	7.73	128.19	119.92
1	D	555	GLY	CA-C-N	-7.57	117.45	122.60
1	D	555	GLY	C-N-CA	-7.57	117.45	122.60
1	F	267	GLY	N-CA-C	-7.47	95.47	113.18
1	E	555	GLY	CA-C-N	-7.40	117.57	122.60
1	E	555	GLY	C-N-CA	-7.40	117.57	122.60
1	C	256	LYS	N-CA-C	-7.34	99.29	110.30
1	F	556	ILE	CA-C-N	7.33	127.98	119.47
1	F	556	ILE	C-N-CA	7.33	127.98	119.47
1	A	739	GLY	N-CA-C	-7.19	103.78	112.48
1	F	673	ASN	CA-CB-CG	-7.10	105.50	112.60
1	F	800	LYS	N-CA-C	-7.02	99.11	110.20
1	D	256	LYS	N-CA-C	-6.98	100.11	110.23
1	D	388	LEU	N-CA-C	6.96	122.29	113.25
1	F	603	ASN	CA-C-N	6.92	128.49	119.84
1	F	603	ASN	C-N-CA	6.92	128.49	119.84
1	A	823	MET	N-CA-C	-6.84	105.49	114.31
1	D	733	PHE	CA-CB-CG	-6.83	106.97	113.80
1	B	310	LEU	CB-CA-C	-6.79	102.20	112.11
1	C	310	LEU	CB-CA-C	-6.77	102.22	112.11
1	A	686	ASP	CA-CB-CG	6.73	119.33	112.60
1	B	698	VAL	CB-CA-C	-6.71	103.08	112.14
1	B	324	ILE	CB-CA-C	-6.67	100.36	111.29
1	C	642	ASP	CA-CB-CG	-6.67	105.93	112.60
1	B	748	ASN	CA-CB-CG	-6.60	106.00	112.60
1	D	544	ASP	CA-CB-CG	-6.46	106.14	112.60
1	C	849	ILE	N-CA-C	6.42	117.06	108.27
1	E	556	ILE	CA-C-N	6.40	126.03	119.56
1	E	556	ILE	C-N-CA	6.40	126.03	119.56
1	A	828	LEU	N-CA-C	-6.33	104.46	111.36
1	E	234	VAL	CA-C-N	6.33	126.30	119.78
1	E	234	VAL	C-N-CA	6.33	126.30	119.78
1	C	740	SER	N-CA-C	-6.32	101.25	111.04
1	B	666	ASP	N-CA-C	-6.31	97.36	110.80
1	C	556	ILE	CA-C-N	6.30	127.71	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	556	ILE	C-N-CA	6.30	127.71	119.84
1	E	545	THR	N-CA-C	-6.28	104.52	111.36
1	D	759	ARG	CA-C-N	6.27	125.96	119.56
1	D	759	ARG	C-N-CA	6.27	125.96	119.56
1	D	234	VAL	CA-C-N	6.22	126.57	119.92
1	D	234	VAL	C-N-CA	6.22	126.57	119.92
1	D	383	LEU	CA-C-N	6.21	125.90	119.56
1	D	383	LEU	C-N-CA	6.21	125.90	119.56
1	C	651	ALA	N-CA-C	6.21	118.04	111.28
1	F	803	LYS	N-CA-C	-6.19	104.79	112.90
1	A	211	ILE	N-CA-C	6.18	117.39	108.48
1	D	556	ILE	CA-C-N	6.18	125.87	119.56
1	D	556	ILE	C-N-CA	6.18	125.87	119.56
1	B	556	ILE	CA-C-N	6.17	125.80	119.56
1	B	556	ILE	C-N-CA	6.17	125.80	119.56
1	E	383	LEU	CA-C-N	6.16	125.79	119.56
1	E	383	LEU	C-N-CA	6.16	125.79	119.56
1	F	555	GLY	N-CA-C	-6.16	101.11	112.62
1	B	803	LYS	N-CA-C	-6.15	106.10	113.97
1	D	603	ASN	CA-C-N	6.14	125.82	119.56
1	D	603	ASN	C-N-CA	6.14	125.82	119.56
1	B	234	VAL	CA-C-N	6.08	126.43	119.92
1	B	234	VAL	C-N-CA	6.08	126.43	119.92
1	B	603	ASN	CA-C-N	6.06	125.74	119.56
1	B	603	ASN	C-N-CA	6.06	125.74	119.56
1	D	667	GLU	N-CA-C	-6.06	101.87	110.35
1	F	678	LYS	CA-C-N	5.98	126.41	119.47
1	F	678	LYS	C-N-CA	5.98	126.41	119.47
1	E	216	ILE	N-CA-C	5.97	116.75	110.72
1	D	219	THR	N-CA-C	-5.96	104.86	111.36
1	C	324	ILE	CB-CA-C	-5.95	101.54	111.29
1	B	592	ASN	CA-CB-CG	-5.93	106.67	112.60
1	A	724	ILE	N-CA-C	5.93	116.41	108.11
1	C	695	VAL	CB-CA-C	-5.91	104.28	112.02
1	C	648	GLU	N-CA-C	5.91	118.48	111.33
1	E	799	ASP	N-CA-C	-5.88	104.98	114.09
1	C	390	ASP	CA-CB-CG	5.87	118.47	112.60
1	A	244	PHE	N-CA-C	5.86	118.45	108.90
1	F	397	ASP	CA-CB-CG	5.86	118.46	112.60
1	A	331	PHE	CA-CB-CG	-5.86	107.94	113.80
1	F	175	THR	N-CA-C	-5.85	105.97	113.23
1	E	603	ASN	CA-C-N	5.84	127.15	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	603	ASN	C-N-CA	5.84	127.15	119.84
1	A	383	LEU	CA-C-N	5.81	125.92	119.87
1	A	383	LEU	C-N-CA	5.81	125.92	119.87
1	D	299	ASN	N-CA-C	-5.80	103.00	111.30
1	C	592	ASN	CA-CB-CG	-5.80	106.80	112.60
1	A	671	LEU	N-CA-C	5.78	120.05	112.13
1	A	302	LYS	CA-C-N	5.76	127.04	119.84
1	A	302	LYS	C-N-CA	5.76	127.04	119.84
1	C	295	ASP	CA-C-N	5.75	128.56	120.28
1	C	295	ASP	C-N-CA	5.75	128.56	120.28
1	B	692	HIS	CA-C-N	5.74	127.01	119.84
1	B	692	HIS	C-N-CA	5.74	127.01	119.84
1	F	362	HIS	CA-CB-CG	5.73	119.53	113.80
1	F	564	SER	N-CA-C	5.72	117.97	108.13
1	A	187	ILE	N-CA-C	5.71	116.08	107.75
1	A	328	ASP	CA-CB-CG	-5.69	106.91	112.60
1	E	881	PRO	N-CA-C	-5.69	101.25	110.40
1	D	728	ASN	CA-CB-CG	-5.68	106.92	112.60
1	E	334	ARG	N-CA-C	5.66	117.44	111.28
1	E	632	PHE	CA-CB-CG	-5.66	108.14	113.80
1	A	556	ILE	CA-C-N	5.62	125.99	119.47
1	A	556	ILE	C-N-CA	5.62	125.99	119.47
1	F	324	ILE	CB-CA-C	-5.61	104.80	111.97
1	A	248	LEU	CB-CA-C	-5.59	110.11	116.54
1	F	606	GLN	CA-C-N	5.59	125.53	119.78
1	F	606	GLN	C-N-CA	5.59	125.53	119.78
1	A	274	GLU	N-CA-C	5.56	118.70	109.46
1	D	853	GLU	N-CA-C	5.56	118.30	109.96
1	F	566	ASN	N-CA-C	-5.55	104.04	112.04
1	F	383	LEU	CA-C-N	5.55	125.64	119.87
1	F	383	LEU	C-N-CA	5.55	125.64	119.87
1	D	545	THR	N-CA-C	-5.52	105.16	111.07
1	C	741	LYS	N-CA-C	-5.51	102.12	110.28
1	E	764	ASN	CA-CB-CG	-5.51	107.09	112.60
1	A	234	VAL	N-CA-CB	-5.51	106.99	111.67
1	C	259	GLY	N-CA-C	-5.51	108.14	114.69
1	C	390	ASP	CB-CA-C	-5.50	102.01	110.81
1	D	696	LEU	N-CA-C	-5.48	105.32	112.23
1	A	264	ARG	NE-CZ-NH2	5.46	124.11	119.20
1	F	268	VAL	CB-CA-C	-5.46	104.98	111.97
1	A	275	SER	N-CA-C	5.46	122.43	110.80
1	B	678	LYS	CA-C-N	5.46	125.80	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	678	LYS	C-N-CA	5.46	125.80	119.47
1	C	806	LEU	CB-CA-C	-5.44	103.86	111.80
1	A	759	ARG	CA-C-N	5.44	125.10	119.56
1	A	759	ARG	C-N-CA	5.44	125.10	119.56
1	F	247	ASP	CA-CB-CG	5.44	118.04	112.60
1	B	805	ASN	N-CA-C	-5.43	99.23	110.80
1	C	342	GLU	CA-C-N	5.43	125.42	120.21
1	C	342	GLU	C-N-CA	5.43	125.42	120.21
1	E	299	ASN	CB-CA-C	-5.42	102.65	111.06
1	A	726	THR	N-CA-C	5.42	118.40	109.72
1	B	854	THR	CA-C-N	5.42	130.09	123.10
1	B	854	THR	C-N-CA	5.42	130.09	123.10
1	C	223	GLU	CA-C-N	5.38	125.91	119.94
1	C	223	GLU	C-N-CA	5.38	125.91	119.94
1	D	274	GLU	N-CA-C	5.38	118.12	108.17
1	F	759	ARG	CA-C-N	5.38	125.70	119.47
1	F	759	ARG	C-N-CA	5.38	125.70	119.47
1	E	672	THR	N-CA-C	-5.37	105.51	111.36
1	C	826	ARG	CA-C-N	5.35	125.67	119.47
1	C	826	ARG	C-N-CA	5.35	125.67	119.47
1	A	638	MET	N-CA-C	5.34	117.42	110.43
1	C	681	SER	N-CA-C	5.34	117.41	110.53
1	D	819	TYR	N-CA-C	5.32	117.85	109.39
1	F	282	PHE	CA-CB-CG	-5.30	108.50	113.80
1	D	776	SER	N-CA-C	5.30	116.93	110.41
1	A	603	ASN	CA-C-N	5.29	126.46	119.84
1	A	603	ASN	C-N-CA	5.29	126.46	119.84
1	B	823	MET	N-CA-C	-5.27	106.62	114.64
1	A	678	LYS	CA-C-N	5.27	126.43	119.84
1	A	678	LYS	C-N-CA	5.27	126.43	119.84
1	A	633	ASN	N-CA-C	-5.26	104.64	111.74
1	B	857	VAL	N-CA-C	5.25	115.67	108.12
1	B	828	LEU	N-CA-C	-5.24	105.65	111.36
1	F	575	ASP	CA-CB-CG	-5.23	107.37	112.60
1	C	383	LEU	CA-C-N	5.21	125.29	119.87
1	C	383	LEU	C-N-CA	5.21	125.29	119.87
1	A	826	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	E	298	ALA	CB-CA-C	-5.19	110.57	116.54
1	B	297	ALA	N-CA-C	-5.18	105.63	111.28
1	B	383	LEU	CA-C-N	5.18	125.26	119.87
1	B	383	LEU	C-N-CA	5.18	125.26	119.87
1	F	608	ALA	N-CA-C	-5.18	102.72	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	324	ILE	CB-CA-C	-5.17	105.15	112.14
1	C	744	GLU	N-CA-C	-5.17	103.66	110.43
1	C	261	PHE	CB-CA-C	-5.16	103.02	110.96
1	C	796	GLU	N-CA-C	-5.15	105.57	111.14
1	F	313	ILE	CA-C-N	-5.15	115.44	122.03
1	F	313	ILE	C-N-CA	-5.15	115.44	122.03
1	A	851	ASP	N-CA-C	5.15	116.89	108.55
1	E	207	ASN	CA-CB-CG	-5.15	107.45	112.60
1	F	775	LEU	N-CA-C	5.15	117.48	108.52
1	F	244	PHE	N-CA-C	5.14	117.83	109.24
1	B	632	PHE	CA-CB-CG	-5.14	108.66	113.80
1	E	648	GLU	N-CA-C	5.12	119.81	111.37
1	A	857	VAL	CB-CA-C	-5.11	103.25	110.82
1	B	723	VAL	N-CA-C	5.11	115.21	107.75
1	C	546	ILE	CB-CA-C	-5.10	105.25	112.14
1	D	397	ASP	CA-CB-CG	5.10	117.70	112.60
1	C	234	VAL	CA-C-N	5.08	125.06	120.03
1	C	234	VAL	C-N-CA	5.08	125.06	120.03
1	B	759	ARG	CA-C-N	5.07	125.36	119.47
1	B	759	ARG	C-N-CA	5.07	125.36	119.47
1	E	678	LYS	CA-C-N	5.07	124.68	119.56
1	E	678	LYS	C-N-CA	5.07	124.68	119.56
1	A	372	LEU	N-CA-C	-5.07	105.84	111.36
1	F	256	LYS	N-CA-C	-5.05	103.38	110.50
1	F	261	PHE	CA-CB-CG	-5.05	108.75	113.80
1	D	856	ASN	N-CA-C	5.04	116.62	108.41
1	F	295	ASP	CA-CB-CG	5.04	117.64	112.60
1	D	275	SER	N-CA-C	5.03	121.52	110.80
1	D	678	LYS	CA-C-N	5.00	124.66	119.56
1	D	678	LYS	C-N-CA	5.00	124.66	119.56

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	4530	0	4648	75	0
1	B	4530	0	4645	148	0
1	C	4530	0	4645	132	0
1	D	4530	0	4644	142	0
1	E	4530	0	4645	132	0
1	F	4530	0	4643	83	0
2	P	139	0	39	19	0
3	A	62	0	24	7	0
3	B	62	0	24	13	0
3	C	93	0	36	19	0
3	D	62	0	24	21	0
3	E	93	0	36	13	0
All	All	27691	0	28053	608	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (608) 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:B:662:TYR:HD2	1:C:650:TYR:CE1	1.13	1.60
1:B:662:TYR:CD2	1:C:650:TYR:CE1	1.86	1.56
1:D:665:TYR:CE1	1:D:712:GLN:CG	1.87	1.52
1:E:662:TYR:CD2	1:F:650:TYR:HE1	1.21	1.52
1:D:665:TYR:CE1	1:D:712:GLN:HG2	0.98	1.50
1:E:662:TYR:CD2	1:F:650:TYR:CE1	1.97	1.49
1:D:333:ARG:HE	1:E:215:GLY:CA	1.28	1.43
1:D:333:ARG:NE	1:E:215:GLY:HA2	1.30	1.42
1:D:334:ARG:NH1	3:D:1002:AGS:S1G	1.96	1.38
1:B:663:VAL:CG2	2:P:24:UNK:O	1.71	1.34
1:E:662:TYR:CE2	1:F:650:TYR:CD1	2.15	1.34
1:A:326:GLU:OE2	1:B:712:GLN:CD	1.72	1.31
1:E:333:ARG:NH1	1:F:215:GLY:CA	1.93	1.31
1:E:662:TYR:HD2	1:F:650:TYR:CE1	1.39	1.31
1:E:662:TYR:CE2	1:F:650:TYR:CE1	2.20	1.29
1:D:662:TYR:CD2	1:E:650:TYR:CE1	2.22	1.27
1:D:662:TYR:CD2	1:E:650:TYR:HE1	1.51	1.26
1:D:333:ARG:NH2	3:D:1002:AGS:O5'	1.65	1.26
1:D:665:TYR:CG	1:D:712:GLN:NE2	2.04	1.25
1:B:205:LYS:CE	1:B:333:ARG:NH2	1.99	1.25
1:E:333:ARG:NH1	1:F:215:GLY:HA3	1.47	1.25
1:D:213:GLU:CG	1:D:214:PRO:HD2	1.67	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:662:TYR:HD2	1:E:650:TYR:CE1	1.56	1.23
1:B:665:TYR:O	1:B:666:ASP:C	1.82	1.23
3:C:1003:AGS:S1G	1:D:826:ARG:NH2	2.13	1.21
1:E:666:ASP:O	1:E:667:GLU:O	1.58	1.20
1:B:662:TYR:CD2	1:C:650:TYR:HE1	1.33	1.19
1:D:665:TYR:CZ	1:D:712:GLN:HG2	1.79	1.17
1:B:662:TYR:CD2	1:C:650:TYR:CD1	2.31	1.17
1:A:765:ARG:NH2	3:B:1002:AGS:S1G	2.16	1.16
1:A:665:TYR:CD2	1:A:712:GLN:NE2	2.16	1.14
1:E:333:ARG:CZ	1:F:215:GLY:HA2	1.78	1.13
3:C:1003:AGS:O3A	1:D:826:ARG:NH2	1.83	1.12
1:E:662:TYR:HE2	1:F:650:TYR:CD1	1.59	1.11
1:D:665:TYR:CD1	1:D:712:GLN:NE2	2.14	1.11
1:B:205:LYS:HE2	1:B:333:ARG:NH2	1.63	1.10
1:A:665:TYR:CE2	1:A:712:GLN:NE2	2.21	1.09
1:B:663:VAL:CG2	2:P:24:UNK:C	2.31	1.09
1:A:667:GLU:OE1	1:A:712:GLN:OE1	1.70	1.08
1:B:663:VAL:HG23	2:P:24:UNK:O	1.29	1.08
1:C:667:GLU:OE1	1:C:712:GLN:OE1	1.71	1.08
1:B:663:VAL:HG22	2:P:24:UNK:O	1.51	1.07
1:A:205:LYS:HD3	1:A:333:ARG:HH11	1.17	1.06
1:D:662:TYR:CE2	1:E:650:TYR:CD1	2.44	1.05
1:D:662:TYR:OH	1:E:649:LYS:O	1.75	1.04
1:D:213:GLU:HG2	1:D:214:PRO:CD	1.88	1.03
1:D:665:TYR:CD2	1:D:712:GLN:NE2	2.27	1.02
1:A:765:ARG:HH22	3:B:1002:AGS:PG	1.82	1.02
1:B:333:ARG:HE	1:C:390:ASP:CG	1.66	1.02
1:E:333:ARG:HH11	1:F:215:GLY:HA3	1.07	1.02
1:B:662:TYR:CE2	1:C:650:TYR:CD1	2.48	1.01
1:D:665:TYR:CZ	1:D:712:GLN:CG	2.40	1.01
1:D:662:TYR:CE2	1:E:650:TYR:CE1	2.48	1.00
1:B:306:SER:HB3	1:B:334:ARG:NH2	1.76	1.00
3:C:1003:AGS:S1G	3:C:1003:AGS:O2B	2.21	0.98
1:D:326:GLU:OE2	1:E:667:GLU:OE2	1.82	0.98
1:D:334:ARG:CZ	3:D:1002:AGS:S1G	2.51	0.97
3:E:1001:AGS:S1G	3:E:1001:AGS:O2B	2.21	0.97
1:D:333:ARG:HD2	1:E:215:GLY:N	1.80	0.96
1:B:662:TYR:CE2	1:C:650:TYR:CE1	2.53	0.96
1:E:712:GLN:HG2	1:E:714:LYS:HZ3	1.29	0.95
3:A:1001:AGS:O1A	3:A:1001:AGS:O1B	1.66	0.95
1:E:712:GLN:HG2	1:E:714:LYS:NZ	1.81	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:ARG:NH2	3:D:1002:AGS:S1G	2.40	0.94
3:E:1003:AGS:S1G	3:E:1003:AGS:O1B	2.25	0.93
1:B:205:LYS:NZ	1:B:333:ARG:HH21	1.66	0.93
3:C:1001:AGS:O2G	3:C:1001:AGS:O1B	1.85	0.93
1:E:333:ARG:HD3	1:E:334:ARG:NH2	1.83	0.92
1:A:765:ARG:HH11	1:B:826:ARG:NH2	1.67	0.92
1:B:663:VAL:HG22	2:P:24:UNK:C	1.96	0.92
1:D:665:TYR:CE1	1:D:712:GLN:CD	2.48	0.91
3:C:1003:AGS:S1G	3:C:1003:AGS:O3A	2.29	0.91
3:E:1001:AGS:S1G	3:E:1001:AGS:O3A	2.29	0.90
1:E:662:TYR:CD2	1:F:650:TYR:CD1	2.48	0.90
1:D:213:GLU:HG2	1:D:214:PRO:HD2	0.93	0.90
1:E:662:TYR:CE2	1:F:650:TYR:HD1	1.85	0.90
1:B:205:LYS:NZ	1:C:390:ASP:OD1	2.04	0.89
1:F:645:GLU:O	1:F:645:GLU:CD	2.15	0.89
1:A:665:TYR:CG	1:A:712:GLN:NE2	2.40	0.89
1:A:333:ARG:NE	1:B:390:ASP:OD2	2.04	0.89
1:B:205:LYS:CE	1:B:333:ARG:HH21	1.71	0.89
1:D:333:ARG:NE	1:E:215:GLY:CA	2.05	0.88
1:E:809:GLU:N	1:E:809:GLU:OE1	2.05	0.88
1:B:205:LYS:HZ1	1:B:333:ARG:HH21	1.20	0.88
1:D:662:TYR:CD2	1:E:650:TYR:CD1	2.61	0.87
1:A:205:LYS:HD3	1:A:333:ARG:NH1	1.89	0.87
1:D:662:TYR:CE1	1:F:650:TYR:OH	2.25	0.87
1:B:659:THR:HG23	1:C:650:TYR:HB3	1.54	0.87
1:C:665:TYR:CE1	1:C:712:GLN:HG2	2.10	0.87
1:A:326:GLU:OE2	1:B:712:GLN:OE1	1.91	0.87
1:D:322:ARG:HH22	1:E:666:ASP:HA	1.38	0.87
1:F:665:TYR:O	1:F:667:GLU:N	2.08	0.87
1:B:663:VAL:CG2	2:P:25:UNK:CB	2.53	0.86
3:C:1003:AGS:O1A	3:C:1003:AGS:O1B	1.89	0.86
1:C:192:GLU:OE1	1:C:192:GLU:N	2.08	0.86
1:A:765:ARG:HD3	1:B:826:ARG:CZ	2.04	0.86
1:A:333:ARG:NE	1:A:333:ARG:O	2.08	0.85
1:D:322:ARG:NH2	1:E:666:ASP:HA	1.91	0.85
1:D:662:TYR:HE2	1:E:650:TYR:CD1	1.94	0.85
1:F:216:ILE:HG22	1:F:216:ILE:O	1.74	0.85
3:D:1002:AGS:O2G	3:D:1002:AGS:O1B	1.90	0.85
1:C:333:ARG:HB2	1:C:333:ARG:CZ	2.05	0.85
1:B:663:VAL:HG23	2:P:24:UNK:C	2.01	0.85
1:B:665:TYR:O	1:B:667:GLU:N	2.09	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:ARG:HD3	3:D:1002:AGS:S1G	2.17	0.84
3:E:1002:AGS:O3G	3:E:1002:AGS:O2B	1.84	0.84
1:D:216:ILE:HD11	1:D:340:VAL:HG12	1.58	0.84
1:D:333:ARG:CD	1:E:215:GLY:N	2.40	0.84
1:D:662:TYR:HE1	1:F:650:TYR:OH	1.60	0.84
1:E:765:ARG:HH12	1:F:826:ARG:NH2	1.76	0.84
1:A:765:ARG:NH2	3:B:1002:AGS:PG	2.51	0.83
1:B:659:THR:HG1	1:C:653:SER:HG	1.19	0.83
1:E:712:GLN:CG	1:E:714:LYS:HZ3	1.91	0.83
1:A:205:LYS:CD	1:A:333:ARG:HH11	1.90	0.83
1:D:665:TYR:CE1	1:D:712:GLN:NE2	2.46	0.83
1:D:665:TYR:O	1:D:712:GLN:NE2	2.12	0.83
1:B:330:ALA:O	1:B:334:ARG:HG2	1.78	0.82
1:E:666:ASP:O	1:E:667:GLU:C	2.22	0.82
1:D:665:TYR:CZ	1:D:712:GLN:CD	2.57	0.82
1:A:765:ARG:HH11	1:B:826:ARG:CZ	1.93	0.81
1:C:556:ILE:O	1:C:556:ILE:HG13	1.78	0.81
1:A:192:GLU:N	1:A:192:GLU:OE1	2.12	0.81
1:A:326:GLU:CD	1:B:712:GLN:CD	2.48	0.81
1:A:665:TYR:CZ	1:A:712:GLN:NE2	2.48	0.81
1:B:663:VAL:HG21	2:P:25:UNK:CB	2.10	0.80
1:B:660:ALA:O	1:C:658:THR:HG22	1.82	0.80
1:E:666:ASP:C	1:E:667:GLU:O	2.21	0.80
1:D:333:ARG:NE	1:E:215:GLY:N	2.30	0.79
1:F:665:TYR:O	1:F:666:ASP:C	2.26	0.79
3:B:1002:AGS:O1B	3:B:1002:AGS:O3G	1.98	0.79
1:E:665:TYR:C	1:E:667:GLU:H	1.90	0.79
1:C:665:TYR:CZ	1:C:712:GLN:HG2	2.18	0.78
1:B:205:LYS:HE2	1:B:333:ARG:CZ	2.12	0.78
1:F:645:GLU:O	1:F:645:GLU:OE1	2.02	0.78
1:B:205:LYS:HE3	1:B:333:ARG:NH2	1.96	0.78
1:E:645:GLU:O	1:E:645:GLU:HG3	1.85	0.77
1:B:205:LYS:NZ	1:B:333:ARG:NH2	2.30	0.77
1:B:663:VAL:HG23	2:P:25:UNK:CB	2.15	0.77
1:F:563:GLU:OE1	1:F:563:GLU:N	2.17	0.77
1:B:261:PHE:CD1	1:B:261:PHE:C	2.64	0.76
3:E:1001:AGS:O1A	3:E:1001:AGS:O1B	1.89	0.76
3:C:1002:AGS:O3G	3:C:1002:AGS:O1B	1.98	0.76
1:E:386:ARG:HD3	1:E:390:ASP:OD2	1.85	0.76
1:C:659:THR:CG2	1:D:650:TYR:HB3	2.16	0.76
1:E:324:ILE:HG13	1:E:325:VAL:H	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:765:ARG:NH1	1:F:826:ARG:NH2	2.33	0.75
3:C:1002:AGS:S1G	3:C:1002:AGS:O2B	2.45	0.75
1:D:333:ARG:CZ	3:D:1002:AGS:O3A	2.34	0.74
1:C:583:GLN:HA	1:C:583:GLN:OE1	1.86	0.74
1:A:765:ARG:NH1	1:B:826:ARG:NH2	2.35	0.74
1:A:333:ARG:CD	1:B:390:ASP:OD2	2.35	0.74
1:A:764:ASN:OD1	1:A:765:ARG:HG2	1.87	0.74
1:B:306:SER:HB3	1:B:334:ARG:HH22	1.47	0.74
1:E:305:LEU:HB2	1:E:334:ARG:HG2	1.70	0.74
3:B:1002:AGS:S1G	3:B:1002:AGS:O2B	2.45	0.74
1:C:659:THR:HG21	1:D:650:TYR:HB3	1.69	0.74
1:A:819:TYR:O	1:A:819:TYR:CD2	2.41	0.73
1:B:665:TYR:O	1:B:666:ASP:O	2.06	0.73
1:E:761:GLU:N	1:E:761:GLU:OE1	2.21	0.73
1:B:330:ALA:O	1:B:334:ARG:CD	2.36	0.73
1:E:333:ARG:NH1	1:F:215:GLY:HA2	1.76	0.73
1:D:665:TYR:CD1	1:D:712:GLN:CG	2.69	0.73
1:D:333:ARG:NH2	3:D:1002:AGS:PA	2.61	0.73
1:D:662:TYR:CZ	1:E:649:LYS:O	2.42	0.73
1:B:660:ALA:HB3	1:C:658:THR:HG23	1.70	0.72
1:E:765:ARG:HH12	1:F:826:ARG:HH22	1.34	0.72
1:A:765:ARG:HH12	3:B:1002:AGS:PB	2.12	0.72
1:D:216:ILE:HD12	1:D:341:ALA:C	2.15	0.72
1:D:333:ARG:CD	1:E:215:GLY:CA	2.68	0.71
3:E:1002:AGS:H8	3:E:1002:AGS:H5'2	1.72	0.71
1:F:797:GLN:OE1	1:F:797:GLN:O	2.06	0.71
1:A:765:ARG:NH1	1:B:826:ARG:HH21	1.89	0.71
1:C:645:GLU:CD	1:C:645:GLU:O	2.34	0.70
1:A:326:GLU:CD	1:B:712:GLN:OE1	2.34	0.70
1:D:665:TYR:CE2	1:D:712:GLN:NE2	2.58	0.70
1:D:583:GLN:OE1	1:D:583:GLN:HA	1.91	0.70
1:D:662:TYR:CE2	1:E:649:LYS:O	2.45	0.70
1:C:387:ARG:HA	1:C:387:ARG:NE	2.06	0.70
3:D:1001:AGS:O1B	3:D:1001:AGS:O1A	2.05	0.70
1:A:326:GLU:OE2	1:B:712:GLN:CG	2.39	0.69
1:A:667:GLU:CD	1:A:712:GLN:OE1	2.35	0.69
3:A:1002:AGS:O2A	3:A:1002:AGS:O1B	2.10	0.69
1:B:330:ALA:O	1:B:334:ARG:CG	2.41	0.69
1:B:661:GLY:O	2:P:23:UNK:O	2.09	0.69
1:C:645:GLU:O	1:C:645:GLU:OE1	2.11	0.69
1:B:306:SER:HB3	1:B:334:ARG:HH21	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:616:SER:HB2	3:C:1002:AGS:S1G	2.32	0.69
1:D:661:GLY:HA2	1:E:662:TYR:HB3	1.75	0.68
1:B:333:ARG:NE	1:C:390:ASP:CG	2.46	0.68
1:B:334:ARG:HD2	1:B:334:ARG:N	2.08	0.68
1:D:662:TYR:HE1	1:F:650:TYR:HH	0.77	0.68
1:B:660:ALA:O	1:C:658:THR:CG2	2.41	0.68
1:D:333:ARG:HE	1:E:215:GLY:HA2	0.54	0.68
1:A:333:ARG:HD2	1:B:390:ASP:OD2	1.93	0.68
1:C:386:ARG:HD3	1:C:390:ASP:OD2	1.94	0.68
3:E:1003:AGS:H8	3:E:1003:AGS:C5'	2.23	0.68
1:B:659:THR:CG2	1:C:650:TYR:HB3	2.23	0.67
1:E:387:ARG:HA	1:E:387:ARG:NE	2.08	0.67
1:C:336:GLN:C	1:C:336:GLN:CD	2.62	0.67
3:C:1003:AGS:H2'	1:D:622:GLU:HG3	1.77	0.67
3:D:1002:AGS:H8	3:D:1002:AGS:H5'2	1.77	0.66
1:C:659:THR:HG22	1:D:650:TYR:CD1	2.30	0.66
3:A:1001:AGS:S1G	3:A:1001:AGS:O2B	2.53	0.66
3:C:1003:AGS:O3A	1:D:826:ARG:CZ	2.44	0.66
1:C:660:ALA:O	1:D:658:THR:OG1	2.09	0.66
1:D:216:ILE:CD1	1:D:340:VAL:HG12	2.25	0.66
1:E:333:ARG:NE	1:F:215:GLY:HA2	2.10	0.66
1:A:583:GLN:HG3	1:A:583:GLN:O	1.96	0.66
1:B:583:GLN:OE1	1:B:583:GLN:HA	1.96	0.65
1:D:662:TYR:CE2	1:E:650:TYR:HD1	2.13	0.65
1:A:333:ARG:HD2	1:B:215:GLY:HA3	1.77	0.65
1:D:333:ARG:NH2	3:D:1002:AGS:O3A	2.29	0.65
1:D:333:ARG:HD2	1:E:214:PRO:C	2.21	0.65
3:E:1002:AGS:H5'2	3:E:1002:AGS:C8	2.27	0.65
1:F:645:GLU:CD	1:F:645:GLU:C	2.65	0.65
1:C:256:LYS:HD2	1:C:256:LYS:N	2.12	0.65
1:E:205:LYS:NZ	1:F:390:ASP:OD1	2.30	0.64
1:C:205:LYS:NZ	1:C:333:ARG:HE	1.96	0.64
1:B:333:ARG:NE	1:C:390:ASP:OD2	2.31	0.64
1:D:665:TYR:CZ	1:D:712:GLN:NE2	2.66	0.64
1:C:237:ILE:N	1:C:237:ILE:HD12	2.13	0.64
1:B:662:TYR:CE2	1:C:649:LYS:C	2.65	0.63
1:C:642:ASP:OD1	1:C:642:ASP:C	2.38	0.63
1:B:663:VAL:HG23	2:P:25:UNK:CA	2.28	0.63
1:C:237:ILE:H	1:C:237:ILE:CD1	2.12	0.63
1:F:853:GLU:OE1	1:F:853:GLU:O	2.17	0.63
1:C:237:ILE:N	1:C:237:ILE:CD1	2.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ARG:CD	1:B:215:GLY:CA	2.77	0.62
1:D:665:TYR:HE1	1:D:712:GLN:HG2	0.80	0.62
1:D:216:ILE:HG13	1:D:216:ILE:O	1.99	0.62
1:D:216:ILE:CD1	1:D:341:ALA:C	2.73	0.62
1:C:663:VAL:HG23	2:P:23:UNK:HA	1.80	0.62
1:D:310:LEU:HG	1:D:310:LEU:O	2.00	0.62
1:E:712:GLN:CD	1:E:714:LYS:HZ3	2.08	0.62
1:B:333:ARG:CG	1:B:333:ARG:HH11	2.13	0.62
1:C:661:GLY:HA3	1:D:658:THR:HG21	1.80	0.62
1:E:333:ARG:NH2	3:E:1002:AGS:O5'	2.34	0.61
1:F:680:TYR:O	1:F:680:TYR:CD2	2.54	0.61
1:F:797:GLN:CD	1:F:797:GLN:C	2.69	0.60
1:B:663:VAL:N	2:P:24:UNK:O	2.34	0.60
1:E:662:TYR:HA	2:P:18:UNK:O	2.01	0.60
1:E:765:ARG:HH11	1:E:765:ARG:CG	2.14	0.60
1:B:205:LYS:O	1:B:205:LYS:HG2	2.01	0.59
1:B:662:TYR:HE2	1:C:649:LYS:C	2.07	0.59
3:B:1001:AGS:H3'	3:B:1001:AGS:PA	2.42	0.59
1:D:666:ASP:O	1:D:667:GLU:C	2.45	0.59
1:A:205:LYS:CD	1:A:333:ARG:NH1	2.57	0.59
1:E:662:TYR:HE2	1:F:650:TYR:CE1	1.88	0.59
1:F:556:ILE:O	1:F:556:ILE:HG22	2.03	0.59
1:D:390:ASP:OD1	1:D:394:ASP:OD1	2.20	0.59
1:C:542:ASP:C	1:C:542:ASP:OD1	2.42	0.59
1:C:333:ARG:HB2	1:C:333:ARG:NH2	2.17	0.58
1:F:266:LYS:O	1:F:270:LYS:HG3	2.03	0.58
1:B:680:TYR:CD2	1:B:680:TYR:N	2.71	0.58
1:E:333:ARG:HD2	1:F:215:GLY:CA	2.33	0.58
1:B:662:TYR:CE2	1:C:649:LYS:HB3	2.38	0.58
1:C:704:ASP:CB	1:C:765:ARG:HG2	2.33	0.58
1:A:333:ARG:HD2	1:B:215:GLY:CA	2.33	0.58
1:D:665:TYR:OH	1:D:712:GLN:HB3	2.04	0.58
1:E:189:ARG:HG2	1:E:189:ARG:HH11	1.69	0.58
1:E:286:ILE:C	1:E:286:ILE:HD12	2.29	0.58
1:B:660:ALA:CB	1:C:658:THR:CG2	2.81	0.58
1:A:387:ARG:HA	1:A:387:ARG:NE	2.20	0.57
1:B:333:ARG:HD3	1:C:215:GLY:HA2	1.86	0.57
1:A:333:ARG:HD3	1:B:215:GLY:CA	2.34	0.57
1:E:542:ASP:OD1	1:E:542:ASP:C	2.45	0.57
1:B:805:ASN:O	1:B:806:LEU:C	2.47	0.57
3:D:1001:AGS:O1B	3:D:1001:AGS:O2G	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:ASN:C	1:D:299:ASN:OD1	2.48	0.57
1:D:333:ARG:HH22	3:D:1002:AGS:PA	2.20	0.57
1:D:680:TYR:CD1	1:D:680:TYR:C	2.82	0.57
1:E:583:GLN:HA	1:E:583:GLN:OE1	2.04	0.57
1:B:665:TYR:O	1:B:667:GLU:CA	2.53	0.56
1:C:617:GLY:N	3:C:1002:AGS:O2B	2.33	0.56
1:D:305:LEU:HB3	1:D:334:ARG:HG3	1.87	0.56
1:D:785:ASP:OD2	1:D:789:LYS:NZ	2.38	0.56
1:A:765:ARG:NH2	3:B:1002:AGS:O3B	2.37	0.56
1:B:334:ARG:NH1	3:C:1001:AGS:S1G	2.79	0.56
1:D:302:LYS:C	1:D:302:LYS:HD3	2.31	0.56
1:E:333:ARG:HH11	1:F:215:GLY:CA	1.80	0.56
1:A:665:TYR:O	1:A:667:GLU:N	2.36	0.56
1:B:704:ASP:HB2	1:B:765:ARG:HE	1.70	0.56
1:E:680:TYR:CD1	1:E:680:TYR:C	2.83	0.56
1:D:213:GLU:CB	1:D:214:PRO:HD2	2.35	0.56
1:E:286:ILE:HD12	1:E:286:ILE:O	2.05	0.56
1:C:294:LYS:O	1:C:296:ASP:N	2.39	0.56
1:C:583:GLN:OE1	1:C:583:GLN:CA	2.51	0.56
1:A:202:ARG:CZ	1:A:205:LYS:HB2	2.37	0.55
1:B:660:ALA:HB3	1:C:658:THR:CG2	2.37	0.55
1:D:665:TYR:HE1	1:D:712:GLN:CG	1.70	0.55
1:D:880:LEU:HB2	1:D:881:PRO:HD2	1.87	0.55
1:E:662:TYR:CD1	1:E:662:TYR:N	2.73	0.55
1:B:205:LYS:HE3	1:B:333:ARG:HH21	1.64	0.55
1:C:856:ASN:OD1	1:C:856:ASN:C	2.49	0.55
1:C:256:LYS:HD2	1:C:256:LYS:H	1.70	0.55
1:C:659:THR:CG2	1:D:650:TYR:CD1	2.90	0.55
1:E:305:LEU:CB	1:E:334:ARG:HG2	2.35	0.55
1:C:645:GLU:OE1	1:C:654:LYS:NZ	2.39	0.55
1:B:306:SER:CB	1:B:334:ARG:NH2	2.63	0.55
1:C:668:GLY:O	1:C:669:GLY:C	2.50	0.55
1:F:264:ARG:HA	1:F:264:ARG:NE	2.22	0.55
1:F:562:SER:HB2	1:F:568:LYS:HE2	1.88	0.54
1:B:606:GLN:OE1	1:B:606:GLN:HA	2.06	0.54
1:E:712:GLN:HG2	1:E:714:LYS:HZ2	1.70	0.54
1:B:333:ARG:NH1	1:B:333:ARG:HG3	2.22	0.54
1:E:305:LEU:HD13	1:E:334:ARG:HB3	1.89	0.54
1:C:659:THR:HG22	1:D:650:TYR:HB3	1.89	0.53
1:C:680:TYR:CD1	1:C:680:TYR:C	2.84	0.53
1:E:765:ARG:HH11	1:E:765:ARG:HG2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:797:GLN:OE1	1:F:797:GLN:C	2.51	0.53
1:C:716:ILE:HD12	1:C:716:ILE:N	2.23	0.53
1:B:665:TYR:HD1	1:B:667:GLU:OE2	1.91	0.53
1:C:333:ARG:CD	3:D:1001:AGS:S1G	2.97	0.53
1:B:665:TYR:C	1:B:666:ASP:OD1	2.52	0.53
1:F:387:ARG:HA	1:F:387:ARG:NE	2.24	0.53
1:D:583:GLN:OE1	1:D:583:GLN:CA	2.57	0.53
1:D:805:ASN:O	1:D:806:LEU:C	2.49	0.53
1:C:336:GLN:O	1:C:336:GLN:OE1	2.26	0.53
1:D:319:ASN:OD1	1:D:319:ASN:N	2.42	0.53
1:E:333:ARG:HD3	1:E:334:ARG:HH22	1.70	0.53
1:D:662:TYR:CD1	1:D:662:TYR:N	2.73	0.53
1:F:184:ASP:OD1	1:F:358:LYS:NZ	2.42	0.53
3:A:1001:AGS:O1B	3:A:1001:AGS:S1G	2.61	0.52
1:E:665:TYR:C	1:E:667:GLU:N	2.58	0.52
1:B:387:ARG:HA	1:B:387:ARG:NE	2.24	0.52
1:C:333:ARG:HD2	3:D:1001:AGS:S1G	2.49	0.52
1:C:617:GLY:CA	3:C:1002:AGS:O2A	2.57	0.52
1:B:660:ALA:C	1:C:658:THR:CG2	2.83	0.52
1:C:617:GLY:HA2	3:C:1002:AGS:O2A	2.10	0.52
1:C:663:VAL:N	2:P:21:UNK:O	2.43	0.52
1:A:665:TYR:CZ	1:A:712:GLN:HG2	2.44	0.52
3:E:1003:AGS:H8	3:E:1003:AGS:H5'2	1.91	0.52
1:E:247:ASP:OD1	1:E:248:LEU:N	2.42	0.52
1:D:258:LYS:NZ	1:E:296:ASP:OD2	2.42	0.52
1:B:700:LEU:HD22	1:B:765:ARG:HD2	1.92	0.52
1:C:295:ASP:OD2	1:D:327:LYS:NZ	2.44	0.51
1:D:732:GLU:HA	1:D:732:GLU:OE1	2.09	0.51
1:A:765:ARG:NH1	3:B:1002:AGS:O3B	2.42	0.51
1:B:662:TYR:HE2	1:C:649:LYS:CB	2.23	0.51
1:A:333:ARG:HD3	1:B:215:GLY:HA2	1.92	0.51
3:A:1002:AGS:O1B	3:A:1002:AGS:O3G	2.28	0.51
1:C:333:ARG:NH2	1:C:333:ARG:CB	2.73	0.51
1:C:659:THR:CG2	1:D:650:TYR:HD1	2.23	0.51
1:E:165:GLU:OE2	1:E:276:LYS:NZ	2.44	0.51
1:E:189:ARG:HG2	1:E:189:ARG:NH1	2.26	0.51
1:B:317:THR:O	1:B:318:ASN:C	2.53	0.51
1:B:809:GLU:CD	1:B:809:GLU:H	2.19	0.51
1:C:616:SER:CB	3:C:1002:AGS:S1G	2.97	0.51
1:B:205:LYS:NZ	1:C:390:ASP:CG	2.69	0.51
1:B:660:ALA:C	1:C:658:THR:HG21	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:LEU:N	1:C:246:LEU:HD12	2.25	0.51
1:C:561:LEU:O	1:C:561:LEU:HG	2.11	0.51
1:A:202:ARG:NH1	1:A:205:LYS:HB2	2.26	0.51
1:C:205:LYS:HZ2	1:C:333:ARG:HE	1.59	0.51
1:D:165:GLU:N	1:D:168:SER:HG	2.08	0.51
1:E:645:GLU:O	1:E:645:GLU:CG	2.53	0.51
1:C:806:LEU:O	1:C:807:THR:C	2.50	0.50
1:E:825:ALA:C	1:E:827:PRO:HD2	2.36	0.50
1:C:333:ARG:CZ	1:C:333:ARG:CB	2.86	0.50
1:B:260:ASP:OD2	1:B:264:ARG:NH1	2.44	0.50
1:B:761:GLU:O	1:B:765:ARG:HG3	2.11	0.50
1:C:568:LYS:O	1:C:572:MET:N	2.43	0.50
1:C:704:ASP:O	1:C:705:ASP:CB	2.59	0.50
3:C:1003:AGS:PA	1:D:826:ARG:NH2	2.84	0.50
1:E:851:ASP:OD2	1:E:852:LYS:NZ	2.44	0.50
1:D:659:THR:HG21	1:E:650:TYR:HB3	1.93	0.50
1:A:625:LYS:NZ	1:A:636:ASP:OD1	2.44	0.50
1:E:642:ASP:OD1	1:E:642:ASP:C	2.53	0.50
1:E:662:TYR:HD2	1:F:650:TYR:HE1	0.57	0.50
1:A:765:ARG:HD3	1:B:826:ARG:NE	2.26	0.50
1:E:205:LYS:NZ	1:F:390:ASP:CG	2.70	0.50
1:B:666:ASP:OD1	1:B:666:ASP:N	2.45	0.50
1:C:299:ASN:OD1	1:C:299:ASN:C	2.54	0.50
1:E:323:SER:O	1:E:324:ILE:C	2.54	0.50
1:D:662:TYR:HD2	1:E:650:TYR:HE1	0.73	0.50
1:F:568:LYS:O	1:F:630:PHE:HE2	1.95	0.50
1:A:333:ARG:NE	1:B:390:ASP:CG	2.68	0.49
1:E:761:GLU:H	1:E:761:GLU:CD	2.11	0.49
3:E:1003:AGS:C8	3:E:1003:AGS:H5'1	2.42	0.49
1:A:765:ARG:HH11	1:B:826:ARG:NE	2.09	0.49
1:C:555:GLY:O	1:C:556:ILE:C	2.56	0.49
1:C:667:GLU:HB2	1:C:712:GLN:CD	2.37	0.49
1:F:569:LEU:O	1:F:572:MET:HB3	2.11	0.49
1:E:817:TYR:N	1:E:817:TYR:CD1	2.81	0.49
1:C:851:ASP:OD1	1:C:851:ASP:C	2.54	0.49
1:E:668:GLY:O	1:E:669:GLY:C	2.55	0.49
1:E:789:LYS:NZ	1:E:793:GLU:OE2	2.46	0.49
1:B:294:LYS:O	1:B:296:ASP:N	2.45	0.49
1:B:629:GLY:O	1:B:633:ASN:N	2.45	0.49
1:C:255:ALA:O	1:C:256:LYS:C	2.54	0.49
1:B:660:ALA:CB	1:C:658:THR:HG21	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:880:LEU:CB	1:E:881:PRO:CD	2.91	0.49
1:F:216:ILE:O	1:F:216:ILE:CG2	2.49	0.49
1:C:406:ALA:O	1:C:410:LYS:N	2.45	0.49
1:B:819:TYR:CD1	1:B:819:TYR:C	2.90	0.49
1:D:660:ALA:HB2	1:D:665:TYR:CZ	2.48	0.48
1:E:258:LYS:NZ	1:F:295:ASP:OD2	2.46	0.48
1:F:663:VAL:HG23	2:P:17:UNK:CB	2.43	0.48
1:B:660:ALA:HB1	1:C:658:THR:HG21	1.95	0.48
1:D:213:GLU:CG	1:D:214:PRO:CD	2.62	0.48
1:A:665:TYR:CD1	1:A:712:GLN:NE2	2.64	0.48
1:E:699:MET:HE2	1:E:699:MET:HA	1.96	0.48
3:E:1003:AGS:C5'	3:E:1003:AGS:C8	2.91	0.48
1:A:300:ILE:HG13	1:A:300:ILE:O	2.13	0.48
1:D:662:TYR:HE1	1:F:650:TYR:CZ	2.30	0.48
1:F:610:PHE:CD1	1:F:610:PHE:N	2.81	0.48
1:B:333:ARG:CG	1:B:333:ARG:NH1	2.73	0.48
1:D:390:ASP:OD1	1:D:390:ASP:O	2.32	0.48
1:D:819:TYR:CG	1:D:819:TYR:O	2.64	0.48
1:E:387:ARG:NE	1:E:387:ARG:CA	2.77	0.48
1:A:812:ASP:O	1:A:816:LYS:N	2.46	0.48
1:B:187:ILE:H	3:B:1001:AGS:HN62	1.62	0.48
1:B:665:TYR:O	1:B:667:GLU:HA	2.14	0.48
1:B:662:TYR:N	1:B:662:TYR:CD1	2.79	0.48
1:E:294:LYS:O	1:E:295:ASP:C	2.57	0.48
3:D:1002:AGS:C8	3:D:1002:AGS:C5'	2.92	0.48
1:A:563:GLU:OE1	1:A:563:GLU:N	2.27	0.48
3:D:1002:AGS:H8	3:D:1002:AGS:C5'	2.43	0.48
1:B:333:ARG:HD2	1:C:390:ASP:OD2	2.13	0.47
1:F:568:LYS:O	1:F:630:PHE:CE2	2.67	0.47
1:F:668:GLY:O	1:F:669:GLY:C	2.57	0.47
1:B:310:LEU:O	1:B:311:LYS:C	2.53	0.47
1:B:804:LEU:C	1:B:805:ASN:O	2.51	0.47
1:C:256:LYS:H	1:C:256:LYS:CD	2.27	0.47
1:E:324:ILE:HG13	1:E:325:VAL:N	2.26	0.47
1:B:330:ALA:O	1:B:334:ARG:HD2	2.15	0.47
1:C:386:ARG:HD3	1:C:390:ASP:CG	2.39	0.47
1:D:333:ARG:NE	1:E:215:GLY:H	2.08	0.47
1:D:662:TYR:HE2	1:E:649:LYS:O	1.96	0.47
1:E:274:GLU:O	1:E:274:GLU:HG3	2.14	0.47
1:E:333:ARG:NH1	1:F:215:GLY:C	2.68	0.47
1:E:629:GLY:O	1:E:633:ASN:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:LYS:NZ	1:B:328:ASP:OD1	2.46	0.46
1:E:255:ALA:O	1:E:256:LYS:C	2.57	0.46
1:A:257:TYR:N	1:A:257:TYR:CD1	2.79	0.46
1:C:322:ARG:NH2	1:D:666:ASP:OD1	2.49	0.46
1:E:765:ARG:NH1	1:E:765:ARG:CG	2.73	0.46
1:F:555:GLY:O	1:F:556:ILE:HB	2.16	0.46
1:A:680:TYR:CD2	1:A:680:TYR:N	2.81	0.46
1:D:333:ARG:NH1	3:D:1002:AGS:O3A	2.48	0.46
1:B:583:GLN:OE1	1:B:583:GLN:CA	2.64	0.46
1:C:336:GLN:C	1:C:336:GLN:OE1	2.59	0.46
1:E:249:ALA:O	1:E:250:ALA:C	2.59	0.46
1:D:585:ASP:OD2	1:D:741:LYS:NZ	2.49	0.46
1:D:668:GLY:O	1:D:669:GLY:C	2.58	0.46
1:A:333:ARG:CD	1:B:215:GLY:HA2	2.43	0.46
1:D:216:ILE:HD12	1:D:342:GLU:N	2.31	0.46
1:D:305:LEU:CD1	1:D:334:ARG:HG2	2.45	0.46
3:B:1001:AGS:O3A	3:B:1001:AGS:O2G	2.33	0.46
1:F:775:LEU:N	1:F:775:LEU:HD22	2.30	0.46
1:F:877:LEU:O	1:F:879:VAL:N	2.49	0.46
1:A:331:PHE:N	1:A:331:PHE:CD1	2.84	0.46
1:B:660:ALA:CB	1:C:658:THR:HG23	2.39	0.46
1:B:771:ILE:HD12	1:B:771:ILE:N	2.31	0.46
1:C:663:VAL:HG23	2:P:23:UNK:CA	2.44	0.46
1:D:294:LYS:NZ	1:D:328:ASP:OD1	2.47	0.46
1:B:333:ARG:CD	1:C:390:ASP:OD2	2.64	0.46
1:E:333:ARG:HD2	1:F:215:GLY:N	2.30	0.46
1:F:665:TYR:CZ	1:F:712:GLN:OE1	2.69	0.46
1:A:326:GLU:OE2	1:B:712:GLN:NE2	2.40	0.45
1:B:205:LYS:CE	1:B:333:ARG:CZ	2.78	0.45
1:D:216:ILE:CD1	1:D:341:ALA:O	2.64	0.45
1:D:667:GLU:OE2	1:D:712:GLN:OE1	2.34	0.45
1:C:665:TYR:CE2	1:C:712:GLN:NE2	2.84	0.45
1:C:825:ALA:HB3	3:C:1002:AGS:C8	2.47	0.45
1:E:585:ASP:OD2	1:E:741:LYS:NZ	2.49	0.45
1:B:249:ALA:O	1:B:250:ALA:C	2.59	0.45
1:D:333:ARG:NH2	3:D:1002:AGS:C5'	2.73	0.45
1:F:562:SER:CB	1:F:568:LYS:HE2	2.47	0.45
1:E:712:GLN:HG2	1:E:712:GLN:O	2.17	0.45
1:A:186:VAL:HA	3:A:1001:AGS:HN62	1.81	0.45
1:C:256:LYS:N	1:C:256:LYS:CD	2.80	0.45
1:B:661:GLY:O	2:P:23:UNK:HA	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:880:LEU:CB	1:D:881:PRO:CD	2.95	0.45
1:C:247:ASP:OD1	1:C:248:LEU:N	2.50	0.45
1:D:213:GLU:HB3	1:D:216:ILE:HG22	1.99	0.45
1:F:566:ASN:HA	1:F:570:ILE:HB	1.97	0.45
1:B:826:ARG:N	1:B:827:PRO:HD2	2.31	0.45
1:C:165:GLU:OE2	1:C:276:LYS:NZ	2.45	0.45
1:D:222:ILE:HD12	1:D:222:ILE:HA	1.79	0.45
1:D:305:LEU:HB3	1:D:334:ARG:CG	2.47	0.45
1:D:317:THR:O	1:D:318:ASN:C	2.60	0.45
1:E:333:ARG:CZ	1:F:215:GLY:CA	2.49	0.45
1:F:204:ILE:O	1:F:204:ILE:HG13	2.17	0.44
1:A:580:VAL:O	1:A:580:VAL:HG12	2.17	0.44
1:D:333:ARG:CZ	1:E:215:GLY:HA2	2.29	0.44
1:C:237:ILE:H	1:C:237:ILE:HD13	1.81	0.44
1:F:294:LYS:NZ	1:F:296:ASP:OD1	2.48	0.44
1:F:806:LEU:C	1:F:807:THR:O	2.60	0.44
1:E:284:ASP:O	1:E:285:GLU:C	2.60	0.44
1:E:299:ASN:O	1:E:300:ILE:C	2.53	0.44
1:B:843:ARG:HB3	1:B:849:ILE:HG12	1.99	0.44
1:C:222:ILE:HD13	1:C:222:ILE:HA	1.58	0.44
1:C:310:LEU:O	1:C:311:LYS:C	2.57	0.44
1:E:326:GLU:OE1	1:F:714:LYS:NZ	2.48	0.44
1:F:772:PHE:N	1:F:772:PHE:CD1	2.86	0.44
1:D:294:LYS:O	1:D:296:ASP:N	2.50	0.44
1:B:662:TYR:N	1:B:662:TYR:HD1	2.15	0.44
1:C:665:TYR:CD2	1:C:712:GLN:NE2	2.86	0.44
1:D:662:TYR:CD1	1:F:650:TYR:OH	2.67	0.44
1:C:637:MET:HE3	1:C:637:MET:HB3	1.85	0.44
1:E:661:GLY:HA2	1:F:662:TYR:HB3	1.98	0.44
1:A:326:GLU:CD	1:B:712:GLN:NE2	2.76	0.43
1:E:299:ASN:O	1:E:301:LEU:N	2.52	0.43
1:E:645:GLU:OE2	1:E:654:LYS:NZ	2.51	0.43
1:E:817:TYR:N	1:E:817:TYR:HD1	2.15	0.43
1:A:326:GLU:OE1	1:B:712:GLN:OE1	2.36	0.43
1:F:569:LEU:HD13	1:F:595:ARG:HG3	2.00	0.43
1:D:214:PRO:O	3:D:1001:AGS:O3B	2.35	0.43
1:B:165:GLU:OE2	1:B:276:LYS:NZ	2.51	0.43
1:B:261:PHE:CD1	1:B:261:PHE:O	2.71	0.43
1:D:385:TYR:CD2	1:D:385:TYR:N	2.86	0.43
1:C:826:ARG:N	1:C:827:PRO:CD	2.81	0.43
1:E:333:ARG:CD	1:F:215:GLY:HA2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:629:GLY:O	1:C:633:ASN:N	2.51	0.43
1:D:542:ASP:OD1	1:D:542:ASP:C	2.59	0.43
1:E:203:ARG:HG3	1:F:362:HIS:HB3	2.00	0.43
1:A:261:PHE:CD1	1:A:261:PHE:C	2.93	0.43
1:E:732:GLU:OE1	1:E:732:GLU:N	2.49	0.43
1:F:302:LYS:HB2	1:F:303:PRO:HD3	2.01	0.43
1:A:685:PHE:CD1	1:A:685:PHE:N	2.86	0.43
1:A:761:GLU:O	1:A:765:ARG:HG3	2.19	0.43
1:B:333:ARG:HH11	1:B:333:ARG:HG3	1.79	0.43
1:D:216:ILE:HD12	1:D:341:ALA:O	2.18	0.43
1:E:309:GLN:O	1:E:310:LEU:C	2.59	0.43
1:F:658:THR:HG21	1:F:662:TYR:HB2	2.01	0.43
1:F:665:TYR:CE1	1:F:712:GLN:NE2	2.86	0.43
1:A:661:GLY:N	1:B:663:VAL:O	2.51	0.43
1:C:246:LEU:N	1:C:246:LEU:CD1	2.82	0.43
1:D:772:PHE:N	1:D:772:PHE:CD1	2.85	0.43
1:A:331:PHE:N	1:A:331:PHE:HD1	2.17	0.42
1:B:849:ILE:HD13	1:B:880:LEU:H	1.83	0.42
1:C:821:ASP:OD1	1:C:821:ASP:N	2.51	0.42
1:D:388:LEU:O	1:D:389:PRO:C	2.62	0.42
1:D:390:ASP:OD1	1:D:394:ASP:CG	2.62	0.42
1:B:702:MET:HE2	1:B:702:MET:HB3	1.76	0.42
1:D:659:THR:CG2	1:E:650:TYR:HB3	2.49	0.42
1:E:772:PHE:N	1:E:772:PHE:CD1	2.85	0.42
1:A:222:ILE:HD13	1:A:222:ILE:HA	1.82	0.42
1:E:324:ILE:CG1	1:E:325:VAL:H	2.26	0.42
1:A:812:ASP:O	1:A:813:PHE:C	2.61	0.42
1:A:826:ARG:N	1:A:827:PRO:HD2	2.34	0.42
1:C:387:ARG:NE	1:C:387:ARG:CA	2.77	0.42
1:E:714:LYS:N	1:E:714:LYS:HD2	2.33	0.42
1:B:704:ASP:O	1:B:705:ASP:CB	2.68	0.42
1:D:393:LEU:HD23	1:D:393:LEU:HA	1.91	0.42
1:D:539:ASN:OD1	1:D:539:ASN:N	2.44	0.42
1:A:294:LYS:O	1:A:295:ASP:C	2.62	0.42
1:B:205:LYS:HZ1	1:B:333:ARG:NH2	1.98	0.42
1:C:299:ASN:O	1:C:300:ILE:C	2.60	0.42
1:D:666:ASP:C	1:D:667:GLU:O	2.59	0.42
3:D:1002:AGS:O2B	3:D:1002:AGS:O2A	2.37	0.42
1:E:333:ARG:HD2	1:F:215:GLY:HA2	2.01	0.42
3:A:1001:AGS:H3'	3:A:1001:AGS:N3	2.35	0.42
1:C:835:GLU:OE1	1:C:835:GLU:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:665:TYR:CE2	1:D:712:GLN:CD	2.95	0.42
1:E:320:GLU:O	1:E:324:ILE:HG12	2.20	0.42
3:E:1001:AGS:O2B	3:E:1001:AGS:O3G	2.37	0.42
1:C:659:THR:CG2	1:D:650:TYR:CB	2.92	0.42
1:B:222:ILE:HD13	1:B:222:ILE:HA	1.76	0.41
1:B:242:LYS:HB3	1:B:242:LYS:HE3	1.86	0.41
3:B:1001:AGS:O2B	3:B:1001:AGS:O2A	2.36	0.41
1:C:249:ALA:O	1:C:250:ALA:C	2.63	0.41
1:D:663:VAL:HG23	2:P:20:UNK:O	2.20	0.41
1:E:823:MET:HE2	1:E:823:MET:HB3	1.91	0.41
1:F:772:PHE:N	1:F:772:PHE:HD1	2.18	0.41
1:C:333:ARG:HD3	1:C:334:ARG:NH1	2.35	0.41
1:D:333:ARG:O	1:D:333:ARG:HG2	2.20	0.41
1:A:882:ASN:OD1	1:A:882:ASN:C	2.63	0.41
1:B:662:TYR:CE2	1:C:649:LYS:CB	3.00	0.41
1:C:299:ASN:O	1:C:299:ASN:CG	2.59	0.41
1:C:849:ILE:HG23	1:C:849:ILE:O	2.20	0.41
1:D:216:ILE:HD12	1:D:342:GLU:HA	2.02	0.41
1:A:626:LYS:HD3	1:A:626:LYS:HA	1.90	0.41
1:C:368:LEU:HD12	1:C:368:LEU:N	2.34	0.41
1:A:382:TYR:CD2	1:A:383:LEU:HG	2.55	0.41
1:B:609:SER:OG	1:B:767:SER:N	2.53	0.41
1:C:606:GLN:O	1:C:607:PRO:C	2.63	0.41
1:B:701:GLN:CG	1:C:642:ASP:OD2	2.69	0.41
1:F:165:GLU:OE2	1:F:276:LYS:NZ	2.53	0.41
1:C:702:MET:SD	1:C:702:MET:C	3.03	0.41
1:D:299:ASN:O	1:D:299:ASN:CG	2.64	0.41
1:D:794:ARG:O	1:D:795:PHE:C	2.61	0.41
1:B:772:PHE:N	1:B:772:PHE:CD1	2.87	0.41
1:C:667:GLU:CD	1:C:712:GLN:OE1	2.55	0.41
1:F:647:SER:O	1:F:648:GLU:C	2.64	0.41
1:B:333:ARG:HD3	1:C:215:GLY:CA	2.50	0.40
1:B:659:THR:HG21	1:C:650:TYR:O	2.21	0.40
1:D:704:ASP:O	1:D:705:ASP:CB	2.69	0.40
1:F:665:TYR:C	1:F:667:GLU:N	2.78	0.40
1:B:566:ASN:O	1:B:567:GLU:C	2.63	0.40
1:B:675:LEU:HD23	1:B:675:LEU:HA	1.90	0.40
1:C:387:ARG:HA	1:C:387:ARG:HE	1.82	0.40
1:D:305:LEU:HD13	1:D:334:ARG:HG2	2.03	0.40
1:F:555:GLY:O	1:F:556:ILE:CB	2.69	0.40
1:B:651:ALA:O	1:B:652:VAL:C	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:ASN:O	1:C:301:LEU:N	2.54	0.40
3:C:1003:AGS:H8	3:C:1003:AGS:O2A	2.21	0.40
1:D:629:GLY:O	1:D:633:ASN:N	2.53	0.40
1:A:333:ARG:CZ	1:B:390:ASP:OD1	2.69	0.40
1:C:331:PHE:HD1	1:C:331:PHE:HA	1.69	0.40
1:C:356:GLN:N	1:C:357:PRO:HD2	2.36	0.40
1:D:777:ARG:O	1:D:778:LYS:C	2.64	0.40
1:F:282:PHE:CD1	1:F:282:PHE:N	2.90	0.40
1:A:765:ARG:CZ	3:B:1002:AGS:O3B	2.69	0.40
1:B:568:LYS:O	1:B:572:MET:N	2.54	0.40
1:E:763:LEU:HD23	1:E:763:LEU:HA	1.89	0.40
1:F:317:THR:O	1:F:318:ASN:C	2.63	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	573/908 (63%)	530 (92%)	31 (5%)	12 (2%)	5	32
1	B	573/908 (63%)	544 (95%)	23 (4%)	6 (1%)	12	45
1	C	573/908 (63%)	548 (96%)	21 (4%)	4 (1%)	18	54
1	D	573/908 (63%)	541 (94%)	27 (5%)	5 (1%)	14	48
1	E	573/908 (63%)	542 (95%)	26 (4%)	5 (1%)	14	48
1	F	573/908 (63%)	529 (92%)	29 (5%)	15 (3%)	4	29
All	All	3438/5448 (63%)	3234 (94%)	157 (5%)	47 (1%)	11	39

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	290	MET

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Mol	Chain	Res	Type
1	B	295	ASP
1	B	666	ASP
1	C	295	ASP
1	C	705	ASP
1	E	324	ILE
1	E	667	GLU
1	F	247	ASP
1	F	666	ASP
1	F	853	GLU
1	A	277	THR
1	A	561	LEU
1	A	706	GLY
1	A	819	TYR
1	B	274	GLU
1	B	277	THR
1	C	274	GLU
1	D	277	THR
1	D	717	ASP
1	D	880	LEU
1	E	274	GLU
1	F	277	THR
1	F	669	GLY
1	F	796	GLU
1	F	878	GLU
1	A	801	HIS
1	D	705	ASP
1	F	255	ALA
1	F	257	TYR
1	F	309	GLN
1	A	666	ASP
1	A	877	LEU
1	A	878	GLU
1	D	166	TYR
1	F	556	ILE
1	F	663	VAL
1	A	298	ALA
1	A	556	ILE
1	B	665	TYR
1	B	705	ASP
1	E	880	LEU
1	F	879	VAL
1	A	879	VAL

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Mol	Chain	Res	Type
1	F	295	ASP
1	C	556	ILE
1	E	302	LYS
1	F	216	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	497/783 (64%)	495 (100%)	2 (0%)	84	84
1	B	497/783 (64%)	493 (99%)	4 (1%)	73	77
1	C	497/783 (64%)	493 (99%)	4 (1%)	73	77
1	D	497/783 (64%)	493 (99%)	4 (1%)	73	77
1	E	497/783 (64%)	491 (99%)	6 (1%)	63	73
1	F	497/783 (64%)	494 (99%)	3 (1%)	78	81
All	All	2982/4698 (64%)	2959 (99%)	23 (1%)	70	77

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	333	ARG
1	A	665	TYR
1	B	333	ARG
1	B	659	THR
1	B	665	TYR
1	B	765	ARG
1	C	333	ARG
1	C	659	THR
1	C	663	VAL
1	C	765	ARG
1	D	216	ILE
1	D	256	LYS
1	D	659	THR
1	D	826	ARG

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Mol	Chain	Res	Type
1	E	286	ILE
1	E	334	ARG
1	E	665	TYR
1	E	666	ASP
1	E	765	ARG
1	E	831	LEU
1	F	333	ARG
1	F	568	LYS
1	F	665	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	735	ASN
1	B	737	GLN
1	B	801	HIS
1	C	177	GLN
1	C	239	GLN
1	C	356	GLN
1	D	177	GLN
1	D	676	GLN
1	D	712	GLN
1	D	720	ASN
1	D	808	GLN
1	D	856	ASN
1	E	712	GLN
1	F	362	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 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	C	1002	-	32,33,33	2.18	9 (28%)	45,52,52	2.31	15 (33%)
3	AGS	B	1001	-	32,33,33	2.23	9 (28%)	45,52,52	2.25	15 (33%)
3	AGS	D	1002	-	32,33,33	2.29	10 (31%)	45,52,52	2.13	14 (31%)
3	AGS	A	1001	-	32,33,33	2.10	7 (21%)	45,52,52	2.15	13 (28%)
3	AGS	E	1002	-	32,33,33	2.23	12 (37%)	45,52,52	2.22	13 (28%)
3	AGS	A	1002	-	32,33,33	1.98	5 (15%)	45,52,52	2.18	15 (33%)
3	AGS	E	1003	-	32,33,33	2.37	10 (31%)	45,52,52	2.34	14 (31%)
3	AGS	B	1002	-	32,33,33	2.18	9 (28%)	45,52,52	2.31	15 (33%)
3	AGS	D	1001	-	32,33,33	2.54	10 (31%)	45,52,52	2.16	14 (31%)
3	AGS	E	1001	-	32,33,33	2.20	9 (28%)	45,52,52	2.44	17 (37%)
3	AGS	C	1001	-	32,33,33	2.47	9 (28%)	45,52,52	2.26	15 (33%)
3	AGS	C	1003	-	32,33,33	2.21	9 (28%)	45,52,52	2.42	17 (37%)

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	C	1002	-	-	2/21/38/38	0/3/3/3
3	AGS	B	1001	-	-	10/21/38/38	0/3/3/3
3	AGS	D	1002	-	-	7/21/38/38	0/3/3/3
3	AGS	A	1001	-	-	9/21/38/38	0/3/3/3
3	AGS	E	1002	-	-	7/21/38/38	0/3/3/3
3	AGS	A	1002	-	-	8/21/38/38	0/3/3/3
3	AGS	E	1003	-	-	2/21/38/38	0/3/3/3
3	AGS	B	1002	-	-	2/21/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AGS	D	1001	-	-	7/21/38/38	0/3/3/3
3	AGS	E	1001	-	-	5/21/38/38	0/3/3/3
3	AGS	C	1001	-	-	2/21/38/38	0/3/3/3
3	AGS	C	1003	-	-	5/21/38/38	0/3/3/3

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	AGS	PG-S1G	7.44	2.06	1.90
3	A	1002	AGS	PG-S1G	7.40	2.06	1.90
3	D	1002	AGS	PG-S1G	7.22	2.06	1.90
3	B	1001	AGS	PG-S1G	7.01	2.05	1.90
3	E	1002	AGS	PG-S1G	6.84	2.05	1.90
3	D	1001	AGS	PG-S1G	6.65	2.05	1.90
3	E	1003	AGS	PG-S1G	6.63	2.05	1.90
3	B	1002	AGS	PG-S1G	6.46	2.04	1.90
3	C	1002	AGS	PG-S1G	6.39	2.04	1.90
3	D	1001	AGS	PA-O3A	-6.34	1.52	1.59
3	C	1001	AGS	PG-S1G	6.20	2.04	1.90
3	C	1003	AGS	PG-S1G	6.04	2.03	1.90
3	D	1001	AGS	PB-O3A	-6.04	1.53	1.59
3	E	1001	AGS	PG-S1G	5.99	2.03	1.90
3	C	1001	AGS	PB-O3A	-5.79	1.53	1.59
3	C	1001	AGS	PA-O3A	-5.49	1.53	1.59
3	E	1003	AGS	PB-O3A	-5.23	1.53	1.59
3	A	1002	AGS	C5-C4	5.00	1.48	1.39
3	C	1003	AGS	PB-O3B	-4.97	1.54	1.59
3	E	1001	AGS	PB-O3B	-4.93	1.54	1.59
3	E	1003	AGS	C5-C4	4.68	1.47	1.39
3	C	1001	AGS	PB-O3B	-4.67	1.54	1.59
3	D	1002	AGS	PB-O3B	-4.67	1.54	1.59
3	C	1002	AGS	C5-C4	4.64	1.47	1.39
3	B	1002	AGS	C5-C4	4.61	1.47	1.39
3	E	1003	AGS	PA-O3A	-4.61	1.54	1.59
3	A	1001	AGS	C5-C4	4.59	1.47	1.39
3	B	1001	AGS	PB-O3A	-4.47	1.54	1.59
3	E	1001	AGS	C5-C4	4.43	1.47	1.39
3	E	1002	AGS	C5-C4	4.41	1.47	1.39
3	C	1003	AGS	C5-C4	4.37	1.46	1.39
3	C	1003	AGS	C5-N7	-4.35	1.31	1.39
3	E	1002	AGS	PB-O3B	-4.35	1.54	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1002	AGS	C5-C4	4.33	1.46	1.39
3	D	1001	AGS	PB-O3B	-4.31	1.54	1.59
3	E	1001	AGS	C5-N7	-4.31	1.31	1.39
3	B	1002	AGS	C5-N7	-4.26	1.31	1.39
3	C	1002	AGS	C5-N7	-4.24	1.31	1.39
3	E	1003	AGS	PB-O3B	-4.18	1.55	1.59
3	C	1002	AGS	PB-O3B	-4.17	1.55	1.59
3	B	1002	AGS	PB-O3B	-4.13	1.55	1.59
3	B	1001	AGS	PB-O3B	-4.11	1.55	1.59
3	D	1001	AGS	C5-C4	4.10	1.46	1.39
3	C	1001	AGS	C5-C4	3.84	1.45	1.39
3	E	1001	AGS	PB-O3A	-3.84	1.55	1.59
3	C	1003	AGS	PB-O3A	-3.82	1.55	1.59
3	E	1002	AGS	PB-O3A	-3.77	1.55	1.59
3	E	1003	AGS	C5-N7	-3.72	1.32	1.39
3	E	1002	AGS	PA-O3A	-3.72	1.55	1.59
3	B	1001	AGS	C5-C4	3.72	1.45	1.39
3	B	1001	AGS	C5-N7	-3.58	1.32	1.39
3	D	1002	AGS	C5-N7	-3.58	1.32	1.39
3	C	1001	AGS	C5-N7	-3.56	1.32	1.39
3	D	1002	AGS	PA-O3A	-3.43	1.55	1.59
3	D	1001	AGS	C5-N7	-3.36	1.32	1.39
3	B	1002	AGS	PB-O3A	-3.36	1.55	1.59
3	A	1001	AGS	C5-N7	-3.35	1.33	1.39
3	C	1002	AGS	PB-O3A	-3.32	1.55	1.59
3	A	1001	AGS	PA-O3A	-3.28	1.56	1.59
3	C	1001	AGS	C4-N9	-3.28	1.30	1.37
3	D	1002	AGS	PB-O3A	-3.27	1.56	1.59
3	A	1002	AGS	C5-N7	-3.20	1.33	1.39
3	E	1002	AGS	C5-N7	-3.09	1.33	1.39
3	B	1001	AGS	PA-O3A	-3.05	1.56	1.59
3	A	1001	AGS	PB-O3A	-2.95	1.56	1.59
3	D	1001	AGS	C4-N9	-2.88	1.31	1.37
3	C	1002	AGS	PA-O3A	-2.82	1.56	1.59
3	E	1001	AGS	PA-O3A	-2.82	1.56	1.59
3	C	1003	AGS	PA-O3A	-2.81	1.56	1.59
3	B	1002	AGS	PA-O3A	-2.80	1.56	1.59
3	D	1002	AGS	C4-N9	-2.63	1.32	1.37
3	B	1001	AGS	C4-N9	-2.62	1.32	1.37
3	C	1003	AGS	C8-N9	-2.54	1.33	1.37
3	E	1001	AGS	C8-N9	-2.54	1.33	1.37
3	B	1001	AGS	C8-N9	-2.48	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1001	AGS	C8-N9	-2.39	1.33	1.37
3	B	1001	AGS	PG-O3G	-2.38	1.47	1.54
3	D	1002	AGS	PG-O3G	-2.38	1.47	1.54
3	C	1001	AGS	PG-O3G	-2.36	1.47	1.54
3	E	1001	AGS	PG-O3G	-2.35	1.47	1.54
3	A	1001	AGS	PG-O2G	2.34	1.62	1.54
3	C	1003	AGS	PG-O3G	-2.33	1.47	1.54
3	E	1002	AGS	C4-N9	-2.32	1.32	1.37
3	C	1002	AGS	C8-N9	-2.32	1.33	1.37
3	B	1002	AGS	C8-N9	-2.29	1.33	1.37
3	B	1002	AGS	C4-N9	-2.29	1.32	1.37
3	C	1002	AGS	C4-N9	-2.29	1.32	1.37
3	D	1001	AGS	PG-O3G	-2.28	1.47	1.54
3	A	1002	AGS	PG-O2G	2.25	1.62	1.54
3	E	1002	AGS	PG-O2G	2.23	1.61	1.54
3	B	1002	AGS	PG-O3G	-2.21	1.47	1.54
3	E	1003	AGS	PG-O2G	2.18	1.61	1.54
3	D	1002	AGS	C8-N7	2.18	1.35	1.31
3	E	1002	AGS	C5-C6	2.17	1.47	1.41
3	C	1002	AGS	PG-O3G	-2.17	1.47	1.54
3	D	1002	AGS	PG-O2G	2.16	1.61	1.54
3	D	1001	AGS	PG-O2G	2.14	1.61	1.54
3	E	1002	AGS	C8-N7	2.12	1.35	1.31
3	A	1002	AGS	C5-C6	2.12	1.46	1.41
3	E	1003	AGS	PG-O3G	-2.11	1.47	1.54
3	E	1003	AGS	C4-N9	-2.11	1.33	1.37
3	E	1001	AGS	C4-N9	-2.08	1.33	1.37
3	A	1001	AGS	PB-O3B	-2.07	1.57	1.59
3	D	1001	AGS	C8-N9	-2.06	1.34	1.37
3	C	1003	AGS	C4-N9	-2.05	1.33	1.37
3	E	1002	AGS	C8-N9	-2.05	1.34	1.37
3	E	1003	AGS	C8-N9	-2.04	1.34	1.37
3	E	1002	AGS	PG-O3G	-2.03	1.48	1.54

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1001	AGS	PB-O3B-PG	-8.10	103.52	133.17
3	C	1003	AGS	PB-O3B-PG	-8.09	103.56	133.17
3	C	1001	AGS	PB-O3B-PG	-7.94	104.12	133.17
3	C	1002	AGS	PB-O3B-PG	-7.53	105.63	133.17
3	B	1002	AGS	PB-O3B-PG	-7.52	105.66	133.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1003	AGS	PB-O3B-PG	-7.52	105.67	133.17
3	E	1002	AGS	PB-O3B-PG	-7.38	106.18	133.17
3	D	1002	AGS	PB-O3B-PG	-6.71	108.60	133.17
3	B	1001	AGS	PB-O3B-PG	-6.56	109.18	133.17
3	E	1001	AGS	C5-C4-N3	-6.45	117.84	126.72
3	A	1002	AGS	C5-C4-N3	-6.39	117.92	126.72
3	C	1003	AGS	C5-C4-N3	-6.38	117.93	126.72
3	E	1003	AGS	C5-C4-N3	-6.26	118.10	126.72
3	B	1002	AGS	C5-C4-N3	-6.25	118.11	126.72
3	C	1002	AGS	C5-C4-N3	-6.24	118.12	126.72
3	A	1001	AGS	C5-C4-N3	-6.13	118.28	126.72
3	B	1001	AGS	C5-C4-N3	-6.09	118.33	126.72
3	E	1002	AGS	C5-C4-N3	-5.99	118.47	126.72
3	D	1002	AGS	C5-C4-N3	-5.98	118.49	126.72
3	E	1001	AGS	N3-C4-N9	5.94	137.26	127.17
3	D	1001	AGS	PB-O3B-PG	-5.90	111.58	133.17
3	C	1003	AGS	N3-C4-N9	5.87	137.15	127.17
3	A	1002	AGS	N3-C4-N9	5.79	137.01	127.17
3	D	1001	AGS	C5-C4-N3	-5.75	118.80	126.72
3	A	1001	AGS	PB-O3B-PG	-5.65	112.48	133.17
3	B	1001	AGS	N3-C4-N9	5.65	136.77	127.17
3	C	1001	AGS	C5-C4-N3	-5.58	119.03	126.72
3	E	1003	AGS	N3-C4-N9	5.50	136.53	127.17
3	A	1001	AGS	N3-C4-N9	5.39	136.33	127.17
3	C	1002	AGS	N3-C4-N9	5.31	136.21	127.17
3	B	1002	AGS	N3-C4-N9	5.31	136.20	127.17
3	A	1002	AGS	PB-O3B-PG	-5.27	113.88	133.17
3	E	1002	AGS	N3-C4-N9	4.82	135.36	127.17
3	D	1001	AGS	N3-C4-N9	4.74	135.24	127.17
3	C	1001	AGS	N3-C4-N9	4.73	135.22	127.17
3	D	1002	AGS	N3-C4-N9	4.64	135.06	127.17
3	E	1001	AGS	N6-C6-N1	3.66	126.54	118.38
3	C	1003	AGS	N6-C6-N1	3.66	126.52	118.38
3	B	1001	AGS	C4-N9-C8	3.55	109.47	105.74
3	A	1001	AGS	O3A-PA-O1A	-3.39	100.50	110.70
3	B	1001	AGS	C2-N3-C4	3.34	120.00	111.83
3	D	1001	AGS	O3A-PA-O1A	-3.33	100.67	110.70
3	A	1002	AGS	C2-N3-C4	3.29	119.86	111.83
3	C	1003	AGS	O2G-PG-O3B	3.28	115.61	104.64
3	A	1001	AGS	C2-N3-C4	3.28	119.85	111.83
3	E	1001	AGS	O2G-PG-O3B	3.27	115.57	104.64
3	E	1002	AGS	C4-C5-N7	-3.25	106.87	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1002	AGS	C2-N3-C4	3.24	119.75	111.83
3	E	1002	AGS	C2-N3-C4	3.23	119.73	111.83
3	E	1003	AGS	O3A-PA-O1A	-3.19	101.11	110.70
3	D	1001	AGS	C2-N3-C4	3.16	119.54	111.83
3	E	1003	AGS	C2-N3-C4	3.11	119.44	111.83
3	C	1002	AGS	N6-C6-N1	3.10	125.29	118.38
3	E	1001	AGS	C2-N3-C4	3.10	119.39	111.83
3	B	1002	AGS	N6-C6-N1	3.10	125.27	118.38
3	C	1001	AGS	O3A-PA-O1A	-3.08	101.45	110.70
3	C	1001	AGS	C4-N9-C8	3.07	108.97	105.74
3	C	1003	AGS	C2-N3-C4	3.07	119.33	111.83
3	A	1002	AGS	N6-C6-N1	3.05	125.18	118.38
3	D	1002	AGS	O2G-PG-O3B	3.04	114.79	104.64
3	C	1001	AGS	C2-N3-C4	3.02	119.21	111.83
3	A	1002	AGS	O2G-PG-O3B	3.00	114.66	104.64
3	B	1002	AGS	C2-N3-C4	2.98	119.12	111.83
3	E	1003	AGS	O2G-PG-O3B	2.98	114.57	104.64
3	C	1001	AGS	N6-C6-N1	2.97	124.99	118.38
3	C	1002	AGS	C2-N3-C4	2.96	119.07	111.83
3	B	1002	AGS	O2G-PG-O3B	2.93	114.41	104.64
3	C	1002	AGS	O2G-PG-O3B	2.93	114.41	104.64
3	D	1002	AGS	C4-C5-N7	-2.92	107.24	110.58
3	E	1002	AGS	O2B-PB-O1B	2.91	125.97	112.44
3	E	1003	AGS	O2B-PB-O1B	2.88	125.84	112.44
3	D	1001	AGS	C4-C5-N7	-2.88	107.29	110.58
3	C	1002	AGS	C4-C5-N7	-2.87	107.31	110.58
3	C	1001	AGS	O2G-PG-O3B	2.85	114.16	104.64
3	C	1003	AGS	O2B-PB-O1B	2.83	125.61	112.44
3	B	1002	AGS	C4-C5-N7	-2.83	107.35	110.58
3	E	1002	AGS	O2G-PG-O3B	2.82	114.07	104.64
3	E	1001	AGS	O2B-PB-O1B	2.82	125.58	112.44
3	D	1001	AGS	O2G-PG-O3B	2.82	114.04	104.64
3	E	1003	AGS	N6-C6-N1	2.80	124.61	118.38
3	D	1001	AGS	N6-C6-N1	2.79	124.60	118.38
3	D	1002	AGS	N6-C6-N1	2.78	124.58	118.38
3	B	1001	AGS	N3-C2-N1	-2.78	124.37	128.58
3	A	1002	AGS	C5'-C4'-C3'	-2.77	105.23	115.21
3	A	1001	AGS	O5'-C5'-C4'	-2.76	99.60	108.99
3	C	1001	AGS	C4-C5-N7	-2.75	107.44	110.58
3	A	1001	AGS	O2G-PG-O3B	2.74	113.80	104.64
3	B	1001	AGS	N6-C6-N1	2.70	124.40	118.38
3	B	1001	AGS	O2G-PG-O3B	2.68	113.59	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	AGS	O3A-PA-O1A	-2.67	102.69	110.70
3	A	1001	AGS	N3-C2-N1	-2.65	124.56	128.58
3	D	1001	AGS	O2B-PB-O1B	2.65	124.75	112.44
3	E	1003	AGS	C4-C5-N7	-2.64	107.56	110.58
3	D	1001	AGS	C4-N9-C8	2.64	108.51	105.74
3	E	1002	AGS	C4-N9-C8	2.61	108.48	105.74
3	B	1001	AGS	O2B-PB-O1B	2.57	124.41	112.44
3	D	1001	AGS	C5'-C4'-C3'	-2.56	105.99	115.21
3	A	1002	AGS	O4'-C4'-C5'	2.55	117.52	109.33
3	E	1001	AGS	O3A-PA-O1A	-2.53	103.08	110.70
3	C	1003	AGS	O3A-PA-O1A	-2.53	103.08	110.70
3	E	1002	AGS	O3A-PA-O1A	-2.53	103.09	110.70
3	E	1001	AGS	C4-C5-N7	-2.53	107.69	110.58
3	B	1002	AGS	C2'-C3'-C4'	2.53	107.50	102.61
3	A	1001	AGS	C4-C5-N7	-2.53	107.69	110.58
3	E	1001	AGS	C4-N9-C8	2.53	108.39	105.74
3	C	1002	AGS	C2'-C3'-C4'	2.53	107.49	102.61
3	C	1003	AGS	C4-N9-C8	2.49	108.35	105.74
3	B	1001	AGS	C4-C5-N7	-2.47	107.75	110.58
3	E	1001	AGS	C5-N7-C8	2.47	107.34	103.45
3	C	1003	AGS	C4-C5-N7	-2.45	107.78	110.58
3	C	1003	AGS	C5-C6-N6	-2.44	117.25	123.29
3	C	1003	AGS	C5-N7-C8	2.43	107.28	103.45
3	E	1001	AGS	C5-C6-N6	-2.42	117.31	123.29
3	E	1002	AGS	C5-N7-C8	2.41	107.23	103.45
3	E	1002	AGS	N3-C2-N1	-2.41	124.94	128.58
3	C	1003	AGS	N3-C2-N1	-2.40	124.94	128.58
3	E	1001	AGS	N3-C2-N1	-2.40	124.95	128.58
3	C	1002	AGS	C5-N7-C8	2.39	107.20	103.45
3	B	1002	AGS	O5'-C5'-C4'	-2.38	100.88	108.99
3	C	1002	AGS	O5'-C5'-C4'	-2.38	100.90	108.99
3	B	1002	AGS	C5-N7-C8	2.37	107.18	103.45
3	E	1003	AGS	C4-N9-C8	2.36	108.22	105.74
3	A	1002	AGS	C4-C5-N7	-2.35	107.89	110.58
3	D	1002	AGS	O3A-PA-O1A	-2.35	103.65	110.70
3	A	1002	AGS	N3-C2-N1	-2.34	125.04	128.58
3	E	1003	AGS	N3-C2-N1	-2.34	125.05	128.58
3	B	1001	AGS	C5-N7-C8	2.33	107.12	103.45
3	D	1002	AGS	C5'-C4'-C3'	-2.33	106.82	115.21
3	E	1001	AGS	C6-C5-C4	2.32	120.35	117.18
3	A	1002	AGS	C1'-N9-C8	-2.32	121.95	127.09
3	A	1001	AGS	C4-N9-C8	2.32	108.17	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1002	AGS	N6-C6-N1	2.32	123.54	118.38
3	B	1002	AGS	N3-C2-N1	-2.31	125.08	128.58
3	C	1001	AGS	N3-C2-N1	-2.30	125.10	128.58
3	E	1001	AGS	O3B-PB-O1B	-2.30	103.80	110.70
3	D	1002	AGS	O2A-PA-O1A	2.29	123.11	112.44
3	A	1001	AGS	N6-C6-N1	2.29	123.47	118.38
3	E	1003	AGS	C5-N7-C8	2.29	107.04	103.45
3	C	1003	AGS	O3B-PB-O1B	-2.28	103.83	110.70
3	C	1003	AGS	C6-C5-C4	2.27	120.27	117.18
3	B	1001	AGS	N9-C8-N7	-2.26	110.72	113.94
3	B	1002	AGS	O3B-PB-O1B	-2.26	103.91	110.70
3	B	1001	AGS	C5-C6-N6	-2.26	117.70	123.29
3	C	1002	AGS	N3-C2-N1	-2.25	125.18	128.58
3	D	1001	AGS	N3-C2-N1	-2.25	125.18	128.58
3	E	1003	AGS	C5'-C4'-C3'	-2.24	107.16	115.21
3	C	1002	AGS	O3B-PB-O1B	-2.24	103.98	110.70
3	E	1002	AGS	O3B-PB-O1B	-2.23	104.00	110.70
3	A	1002	AGS	C4-N9-C8	2.22	108.07	105.74
3	A	1001	AGS	C5-N7-C8	2.20	106.91	103.45
3	C	1002	AGS	C6-C5-C4	2.20	120.19	117.18
3	B	1002	AGS	C6-C5-C4	2.20	120.18	117.18
3	C	1001	AGS	O5'-C5'-C4'	-2.18	101.56	108.99
3	A	1002	AGS	C5-C6-N6	-2.18	117.88	123.29
3	C	1003	AGS	C1'-N9-C8	-2.16	122.30	127.09
3	E	1001	AGS	C1'-N9-C8	-2.15	122.31	127.09
3	B	1001	AGS	O3A-PA-O1A	-2.14	104.27	110.70
3	B	1002	AGS	O2B-PB-O1B	2.12	122.31	112.44
3	D	1001	AGS	C5-N7-C8	2.12	106.78	103.45
3	B	1001	AGS	O2A-PA-O1A	2.12	122.29	112.44
3	C	1002	AGS	O2B-PB-O1B	2.12	122.29	112.44
3	C	1001	AGS	C5-C6-N6	-2.10	118.08	123.29
3	C	1001	AGS	O3B-PB-O1B	-2.09	104.41	110.70
3	D	1002	AGS	C5-N7-C8	2.07	106.71	103.45
3	A	1001	AGS	O2B-PB-O1B	2.07	122.09	112.44
3	B	1002	AGS	O3A-PA-O1A	-2.06	104.50	110.70
3	A	1002	AGS	O2A-PA-O1A	2.06	122.04	112.44
3	C	1002	AGS	O3A-PA-O1A	-2.06	104.52	110.70
3	D	1001	AGS	O5'-C5'-C4'	-2.04	102.03	108.99
3	C	1001	AGS	C5-N7-C8	2.04	106.66	103.45
3	E	1003	AGS	O5'-C5'-C4'	-2.03	102.06	108.99
3	D	1002	AGS	N3-C2-N1	-2.03	125.51	128.58
3	C	1003	AGS	C5'-C4'-C3'	-2.03	107.91	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1002	AGS	C4-N9-C8	2.03	107.87	105.74
3	E	1001	AGS	C5'-C4'-C3'	-2.02	107.95	115.21
3	D	1002	AGS	O2B-PB-O1B	2.01	121.79	112.44
3	C	1001	AGS	C5'-C4'-C3'	-2.01	107.99	115.21

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	AGS	C5'-O5'-PA-O2A
3	A	1001	AGS	O4'-C4'-C5'-O5'
3	A	1002	AGS	C5'-O5'-PA-O3A
3	B	1001	AGS	C5'-O5'-PA-O1A
3	B	1001	AGS	C5'-O5'-PA-O2A
3	B	1001	AGS	C5'-O5'-PA-O3A
3	B	1001	AGS	O4'-C1'-N9-C8
3	B	1001	AGS	O4'-C1'-N9-C4
3	B	1002	AGS	O4'-C4'-C5'-O5'
3	B	1002	AGS	C3'-C4'-C5'-O5'
3	C	1002	AGS	O4'-C4'-C5'-O5'
3	C	1002	AGS	C3'-C4'-C5'-O5'
3	C	1003	AGS	C5'-O5'-PA-O2A
3	C	1003	AGS	C5'-O5'-PA-O3A
3	D	1001	AGS	C5'-O5'-PA-O2A
3	D	1001	AGS	C5'-O5'-PA-O3A
3	D	1002	AGS	PB-O3B-PG-O2G
3	D	1002	AGS	C5'-O5'-PA-O1A
3	E	1001	AGS	C5'-O5'-PA-O2A
3	E	1001	AGS	C5'-O5'-PA-O3A
3	E	1002	AGS	C5'-O5'-PA-O3A
3	A	1001	AGS	C3'-C4'-C5'-O5'
3	E	1002	AGS	C3'-C4'-C5'-O5'
3	B	1001	AGS	O4'-C4'-C5'-O5'
3	C	1001	AGS	O4'-C4'-C5'-O5'
3	D	1002	AGS	O4'-C4'-C5'-O5'
3	D	1002	AGS	C3'-C4'-C5'-O5'
3	E	1002	AGS	O4'-C4'-C5'-O5'
3	B	1001	AGS	C3'-C4'-C5'-O5'
3	D	1001	AGS	C3'-C4'-C5'-O5'
3	A	1002	AGS	C2'-C1'-N9-C4
3	C	1001	AGS	C3'-C4'-C5'-O5'
3	D	1001	AGS	C2'-C1'-N9-C4

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Mol	Chain	Res	Type	Atoms
3	A	1002	AGS	PA-O3A-PB-O1B
3	C	1003	AGS	PA-O3A-PB-O1B
3	E	1001	AGS	PA-O3A-PB-O1B
3	E	1002	AGS	PA-O3A-PB-O1B
3	E	1003	AGS	PA-O3A-PB-O1B
3	A	1002	AGS	C2'-C1'-N9-C8
3	D	1001	AGS	C2'-C1'-N9-C8
3	A	1001	AGS	C5'-O5'-PA-O1A
3	A	1001	AGS	C5'-O5'-PA-O3A
3	A	1002	AGS	C5'-O5'-PA-O1A
3	E	1002	AGS	C5'-O5'-PA-O1A
3	A	1001	AGS	C4'-C5'-O5'-PA
3	D	1002	AGS	C4'-C5'-O5'-PA
3	D	1001	AGS	O4'-C4'-C5'-O5'
3	D	1002	AGS	PB-O3A-PA-O2A
3	E	1003	AGS	PA-O3A-PB-O2B
3	B	1001	AGS	PB-O3B-PG-O2G
3	D	1002	AGS	PB-O3B-PG-O3G
3	C	1003	AGS	C4'-C5'-O5'-PA
3	E	1001	AGS	C4'-C5'-O5'-PA
3	B	1001	AGS	C4'-C5'-O5'-PA
3	A	1001	AGS	C2'-C1'-N9-C8
3	A	1001	AGS	O4'-C1'-N9-C8
3	D	1001	AGS	PG-O3B-PB-O1B
3	A	1002	AGS	PA-O3A-PB-O2B
3	A	1002	AGS	PB-O3A-PA-O1A
3	B	1001	AGS	PB-O3A-PA-O2A
3	A	1001	AGS	C2'-C1'-N9-C4
3	E	1002	AGS	C4'-C5'-O5'-PA
3	A	1002	AGS	PB-O3A-PA-O2A
3	C	1003	AGS	PA-O3A-PB-O2B
3	E	1001	AGS	PA-O3A-PB-O2B
3	E	1002	AGS	PA-O3A-PB-O2B

There are no ring outliers.

12 monomers are involved in 73 short contacts:

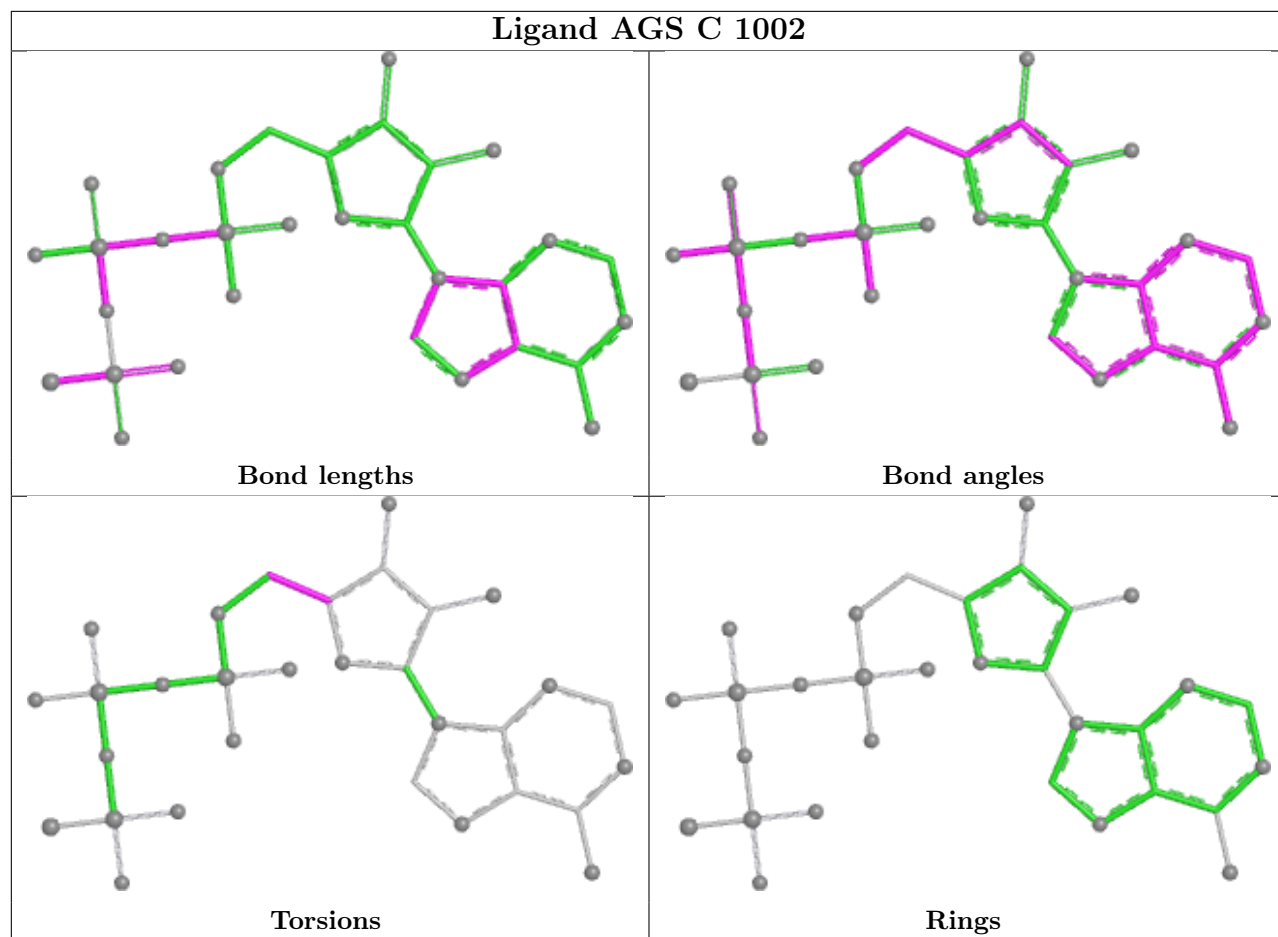
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1002	AGS	8	0
3	B	1001	AGS	4	0
3	D	1002	AGS	16	0
3	A	1001	AGS	5	0

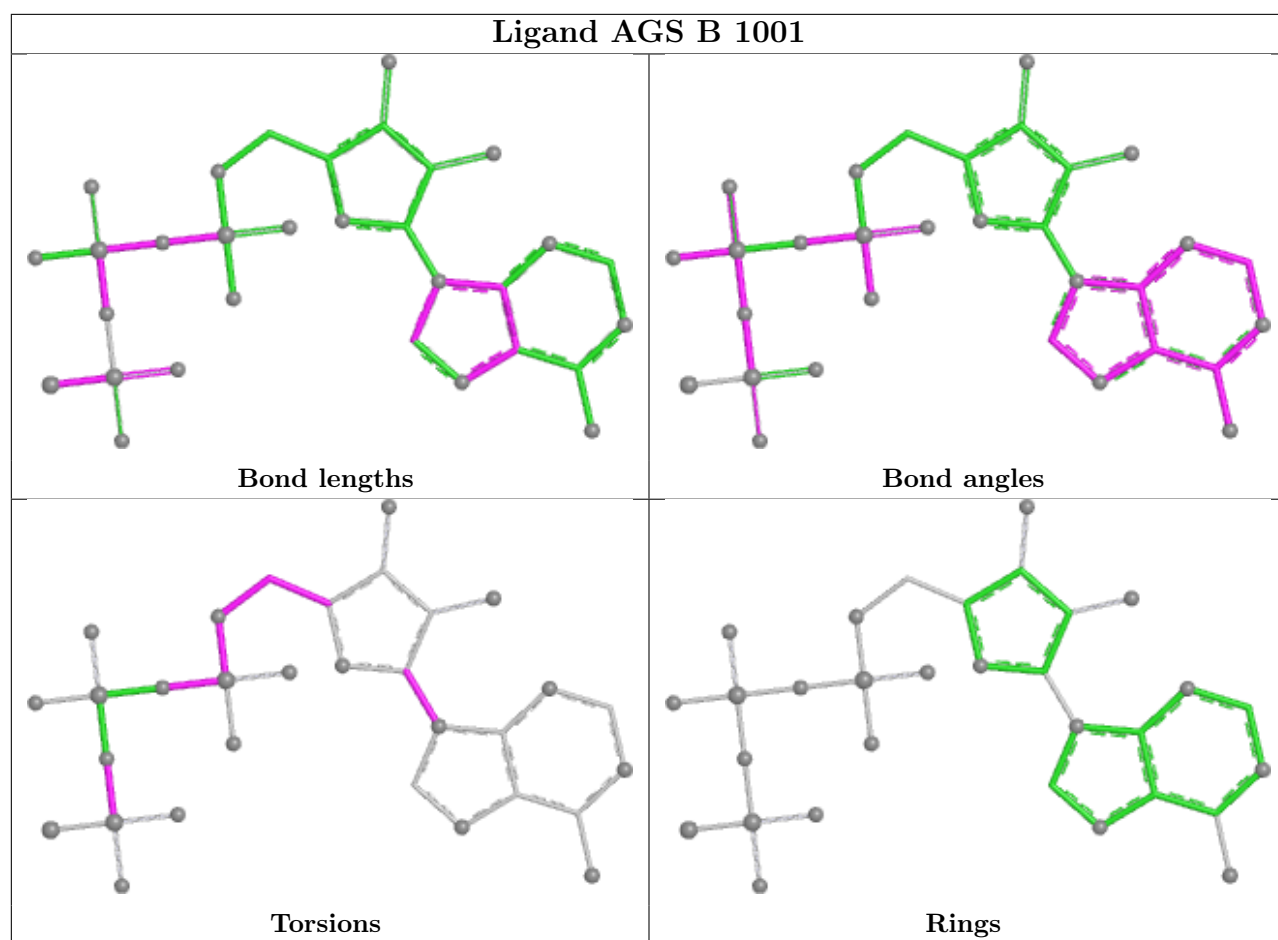
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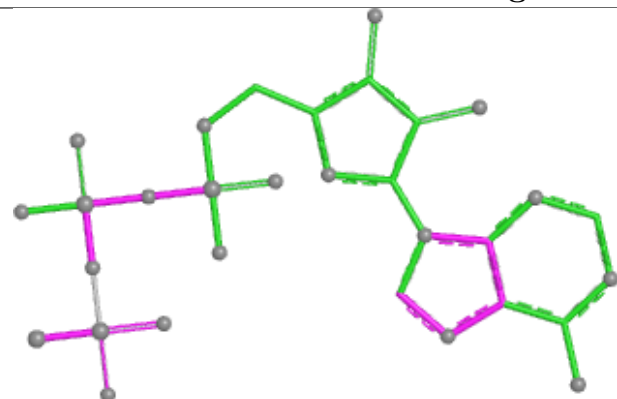
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1002	AGS	4	0
3	A	1002	AGS	2	0
3	E	1003	AGS	5	0
3	B	1002	AGS	9	0
3	D	1001	AGS	5	0
3	E	1001	AGS	4	0
3	C	1001	AGS	2	0
3	C	1003	AGS	9	0

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.

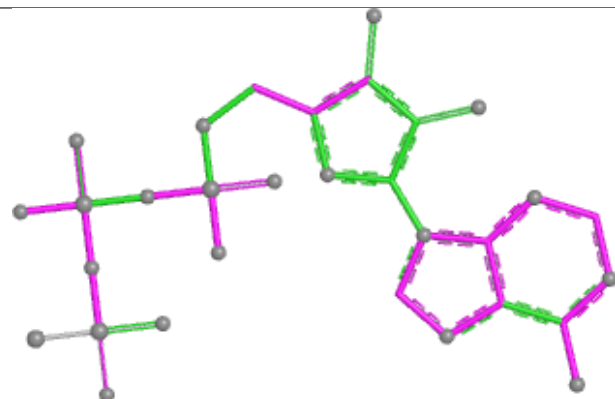




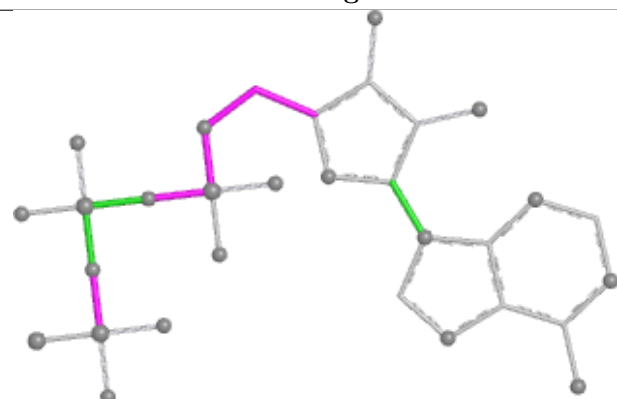
Ligand AGS D 1002



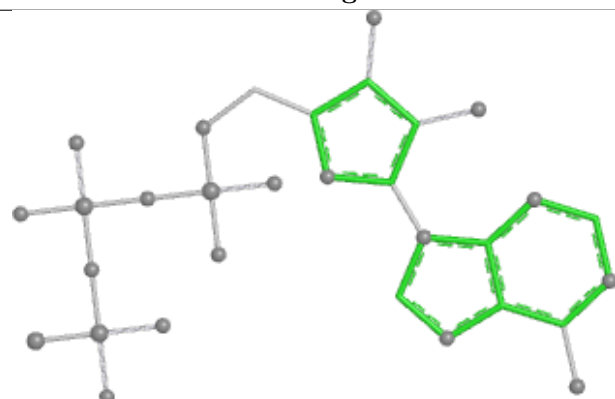
Bond lengths



Bond angles

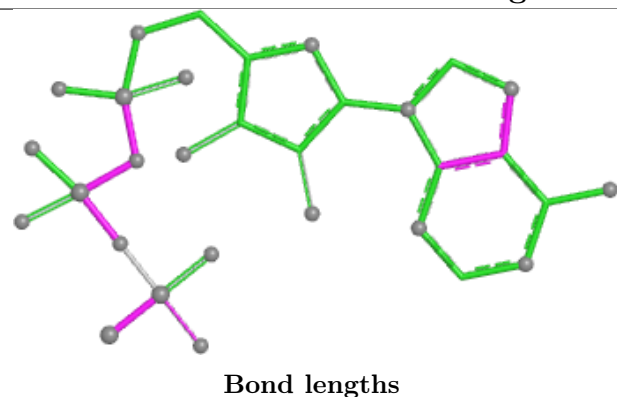


Torsions

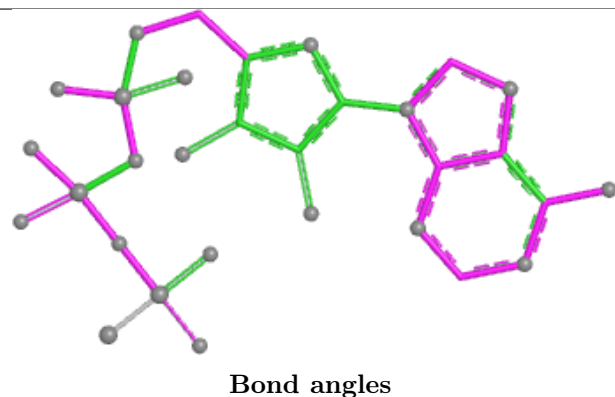


Rings

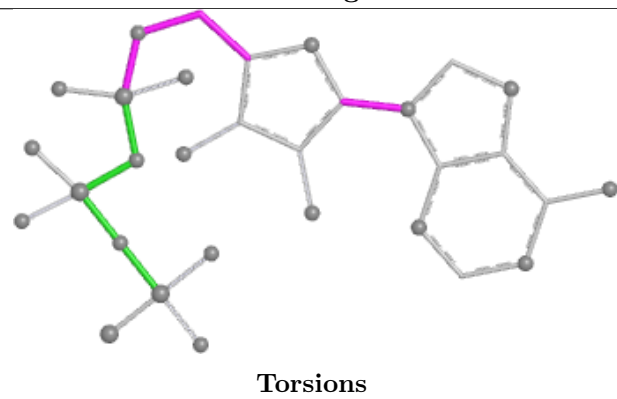
Ligand AGS A 1001



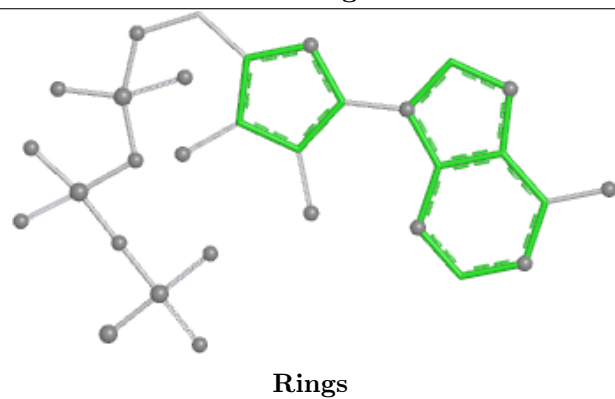
Bond lengths



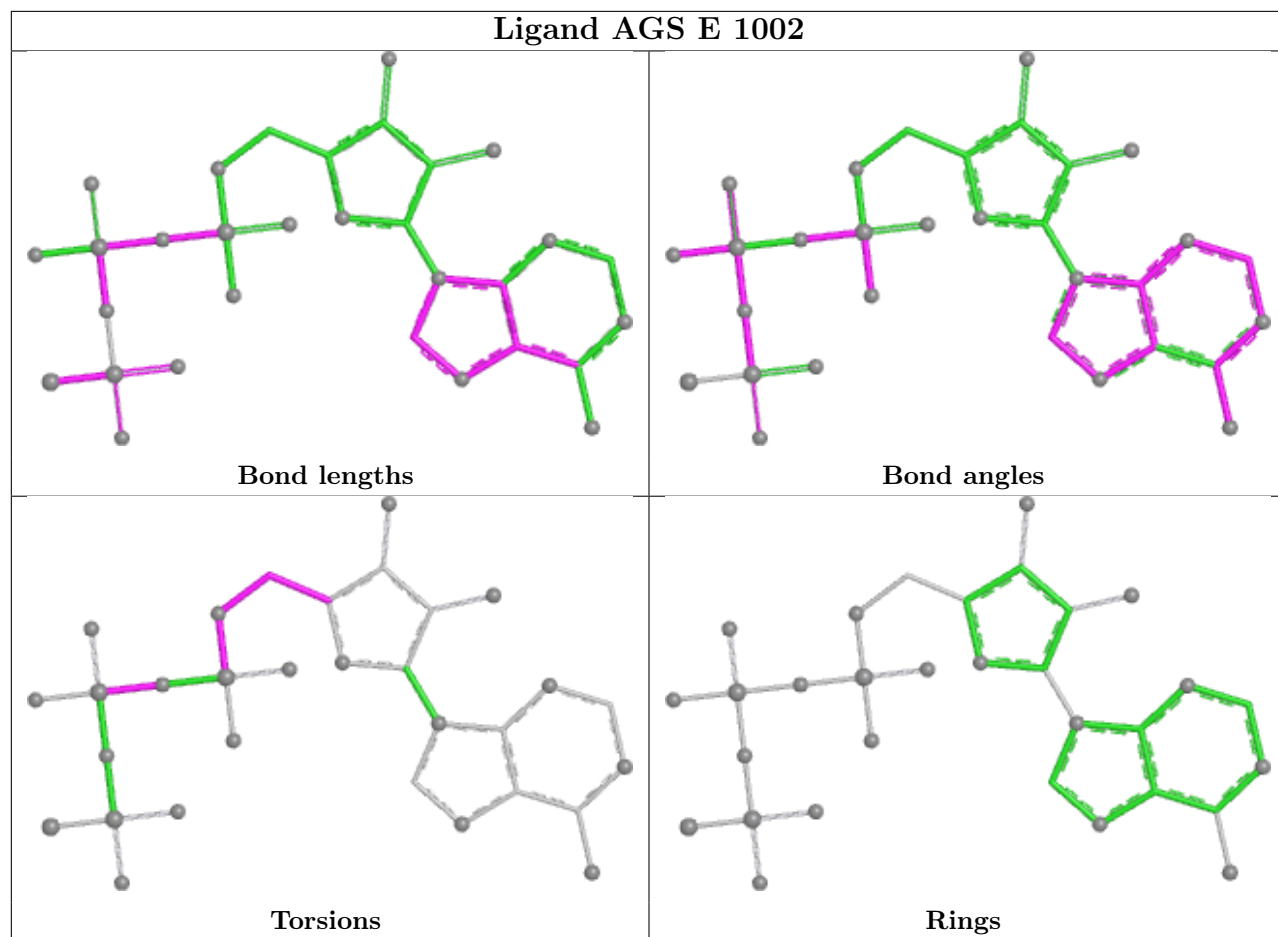
Bond angles

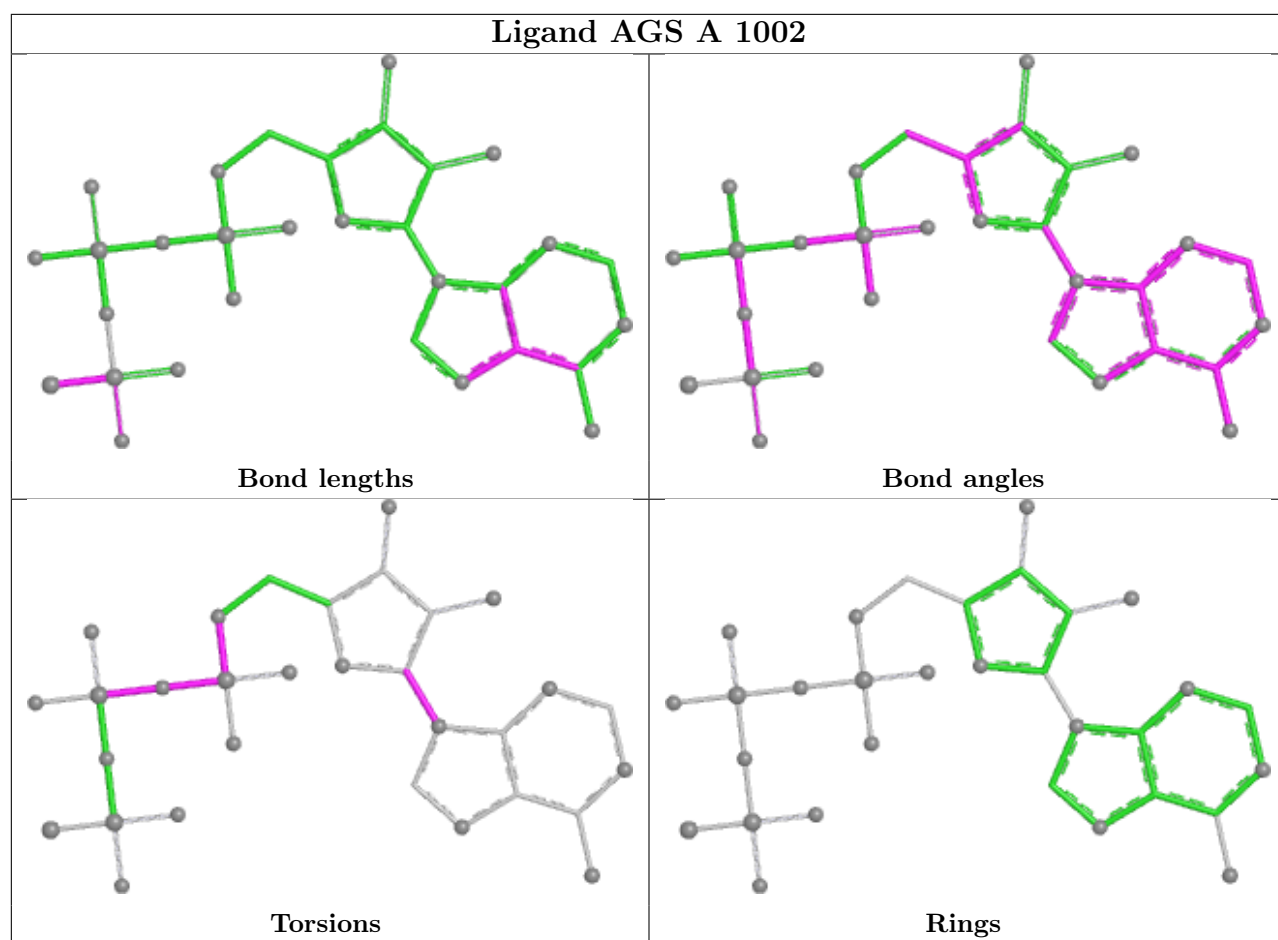


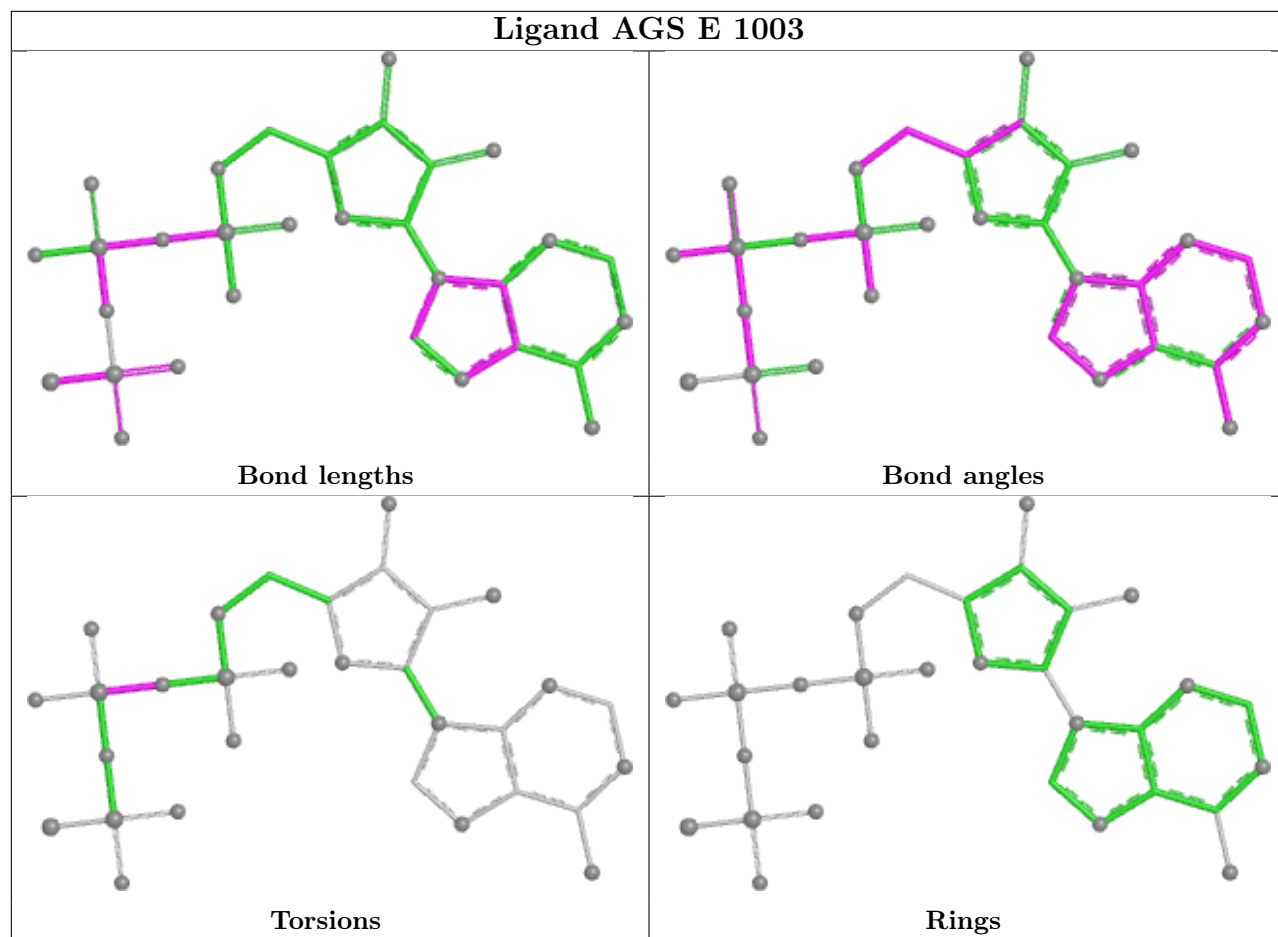
Torsions

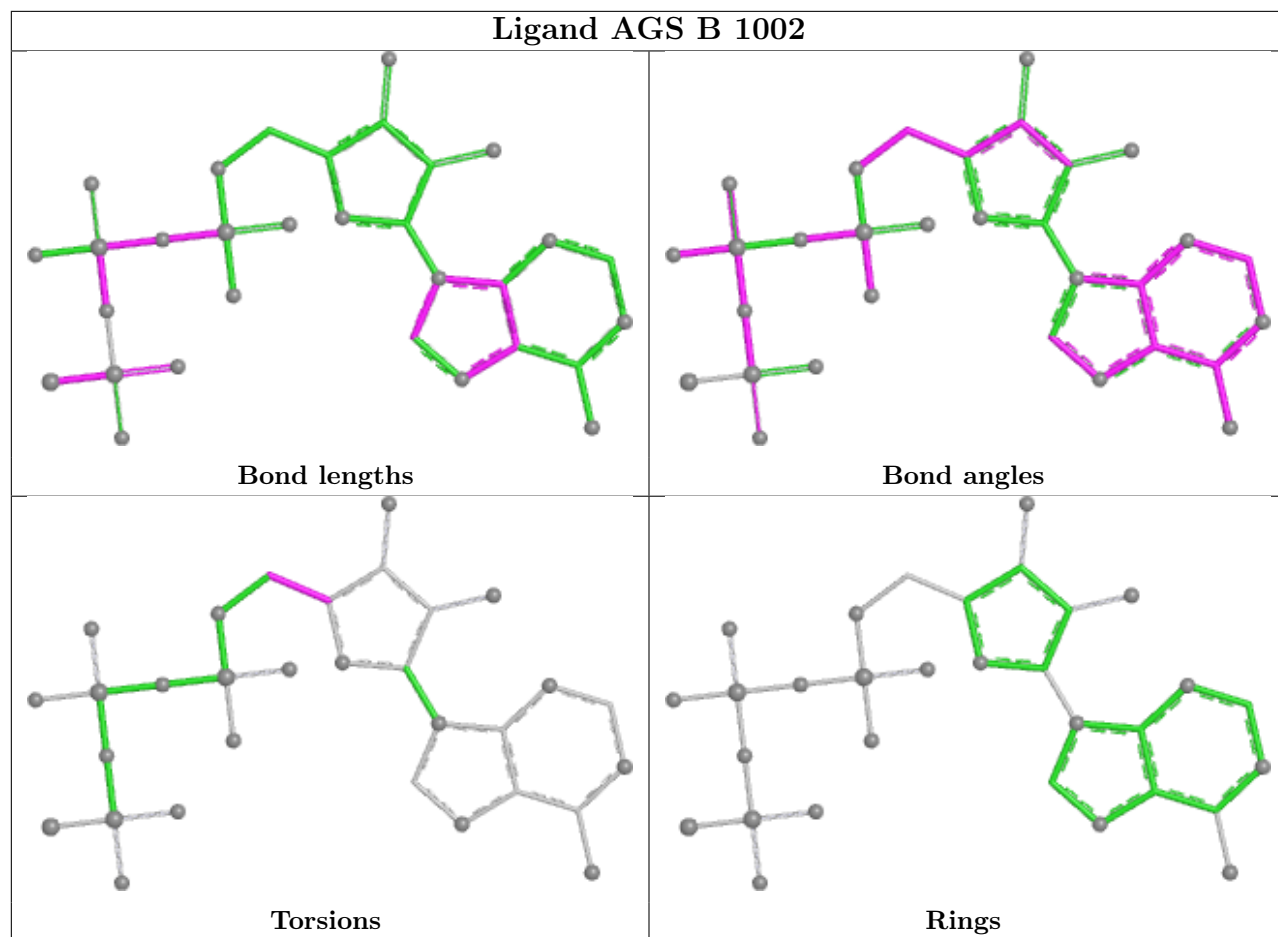


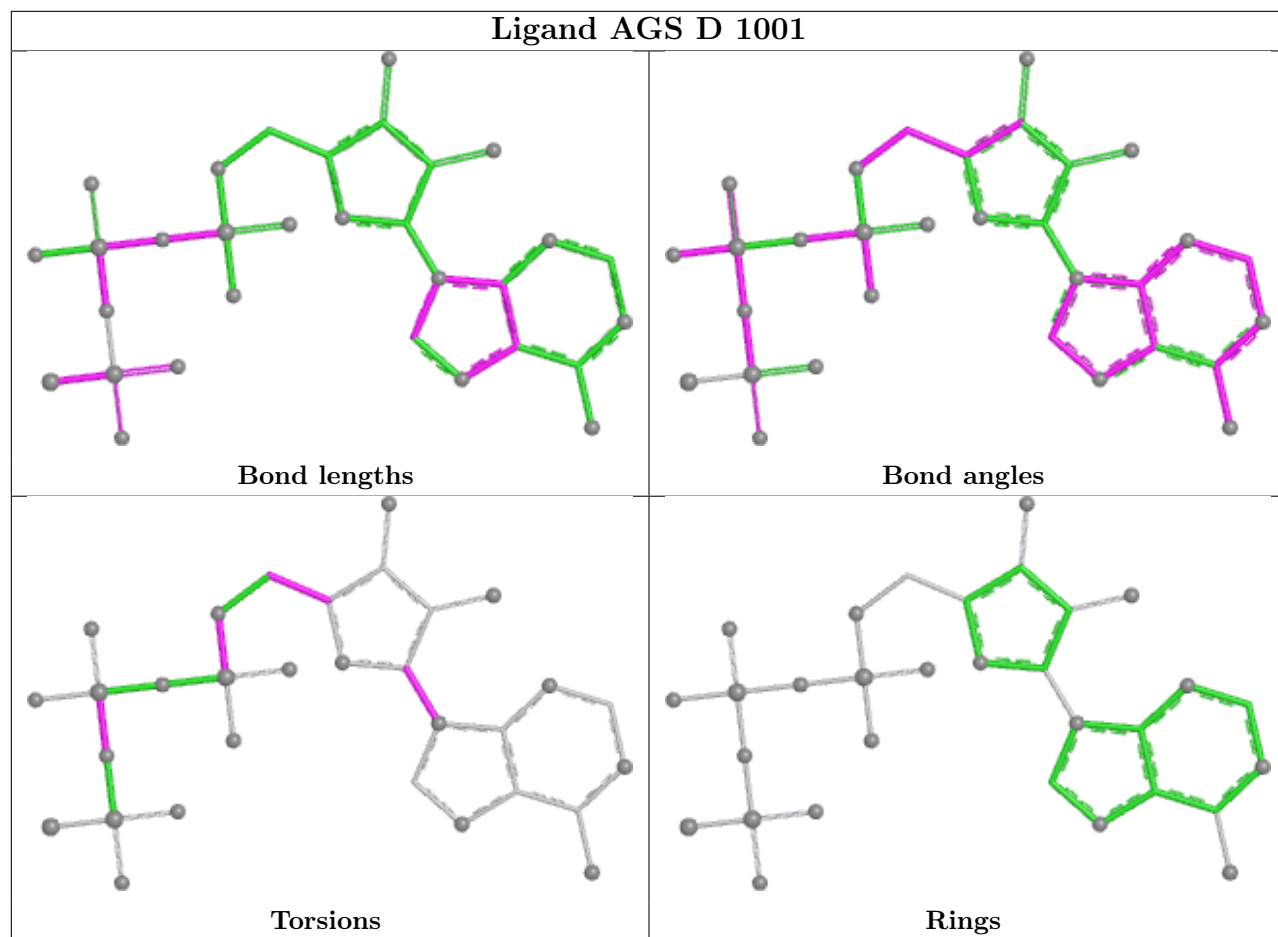
Rings

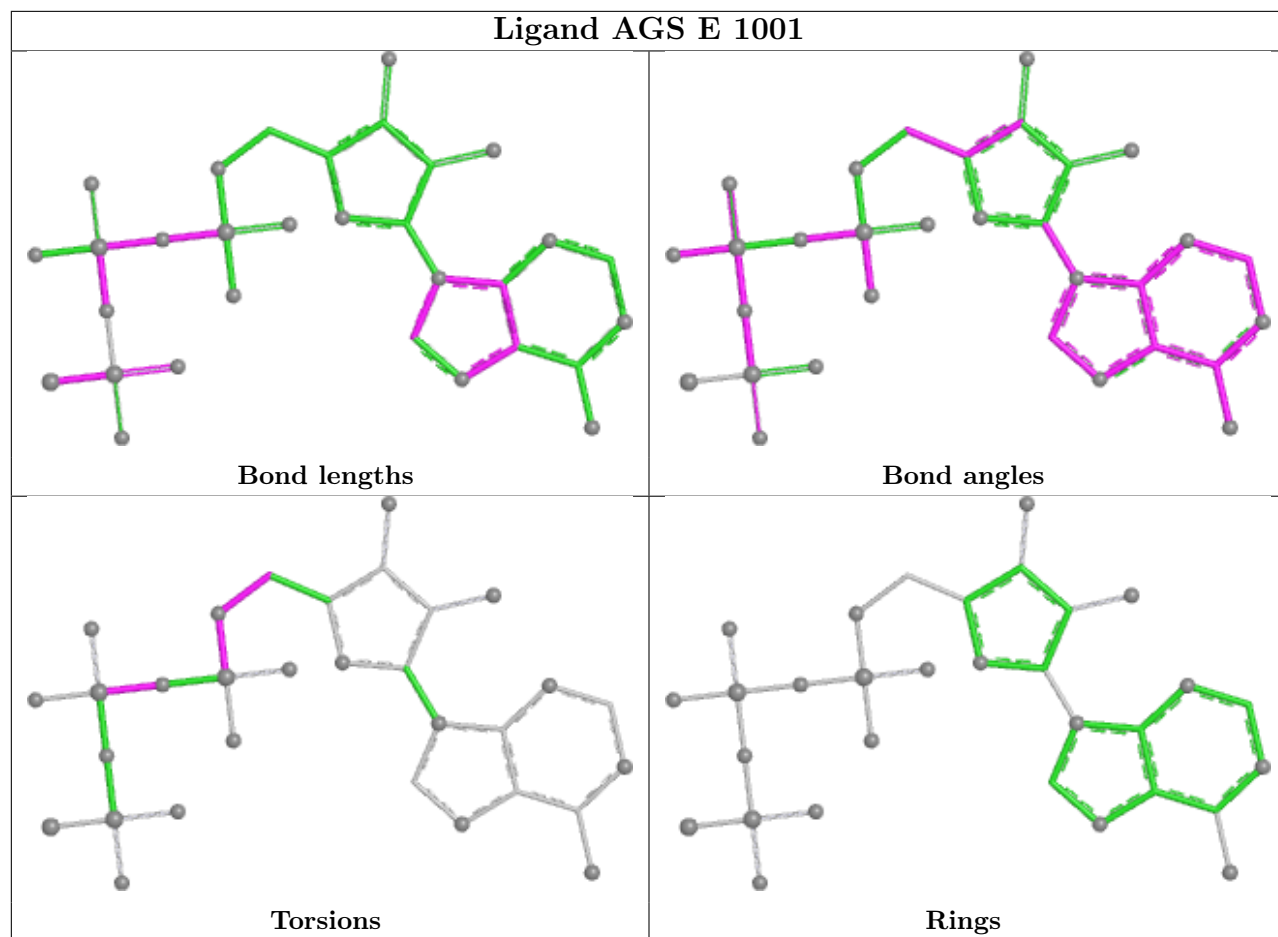


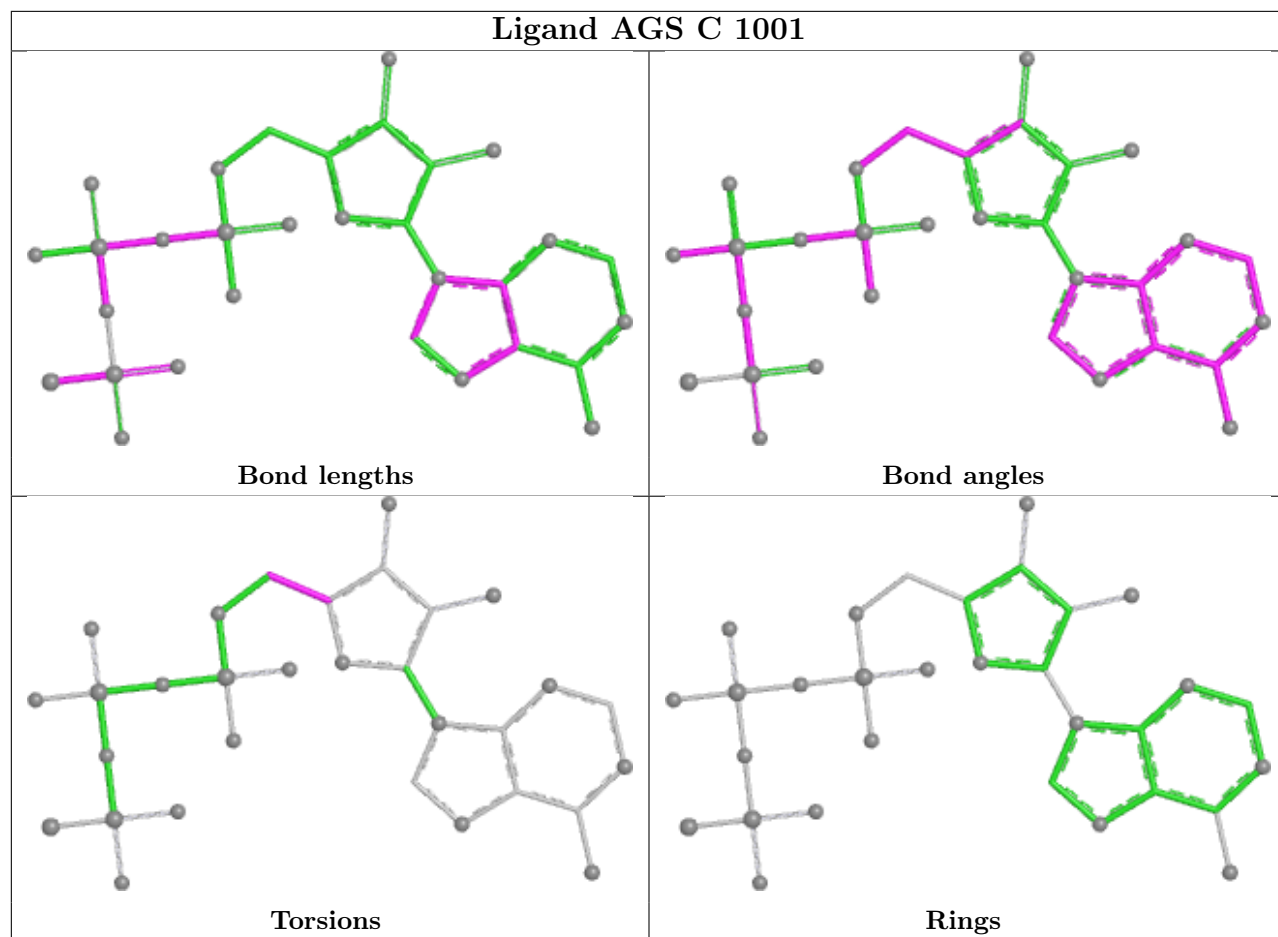


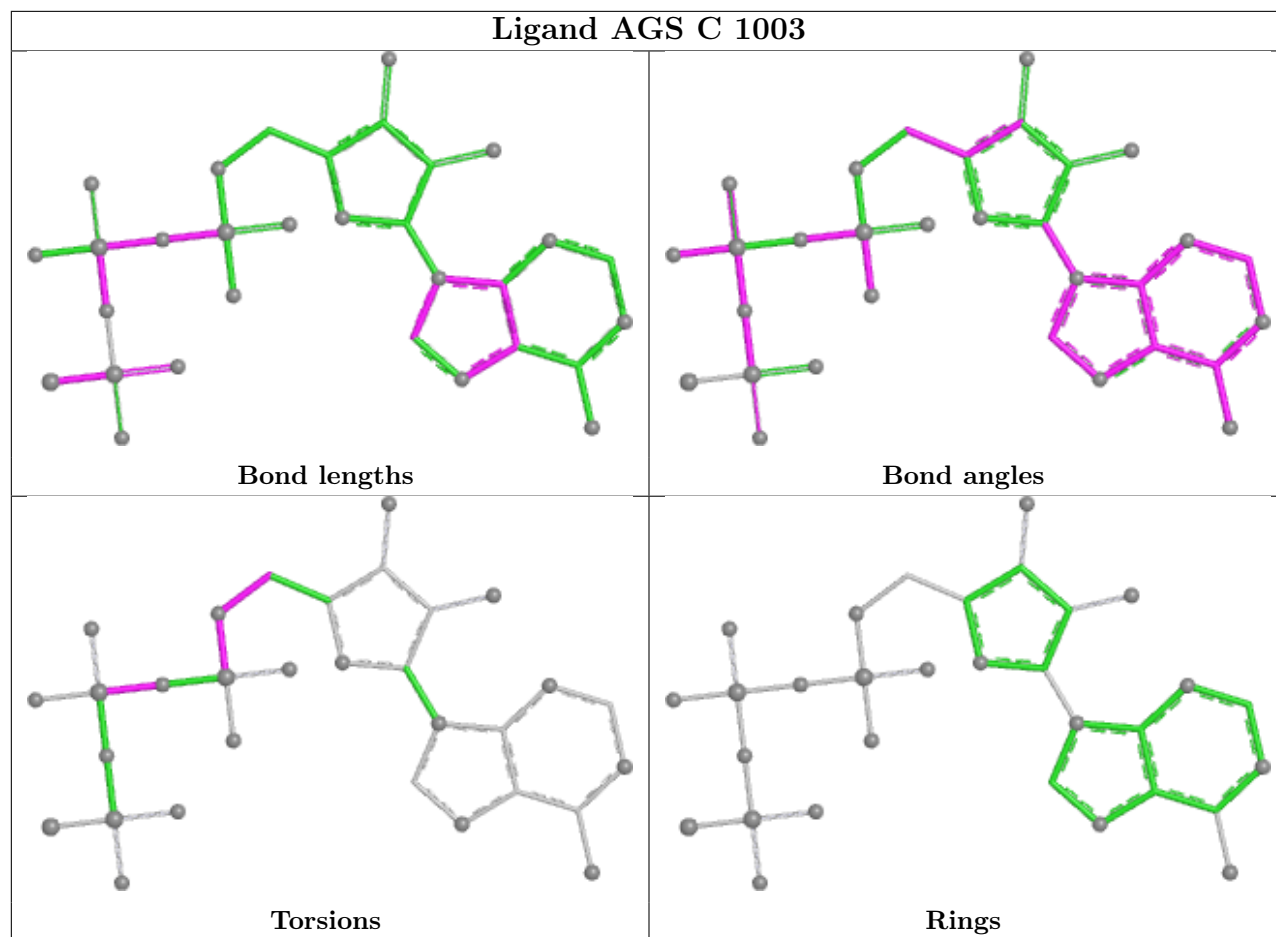












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

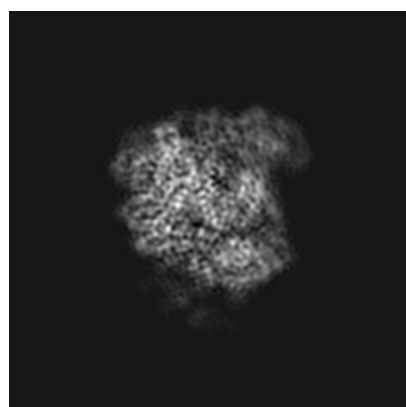
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8746. These allow visual inspection of the internal detail of the map and identification of artifacts.

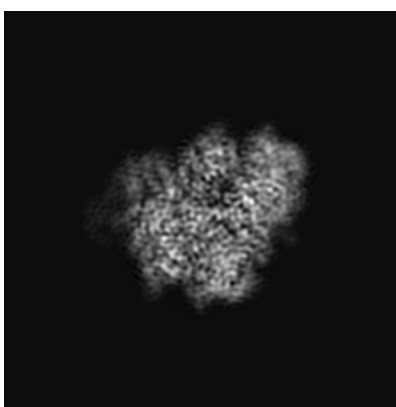
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

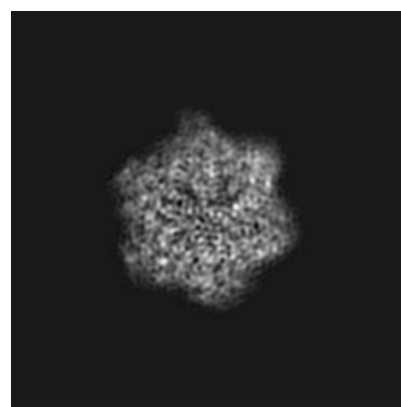
6.1.1 Primary map



X



Y

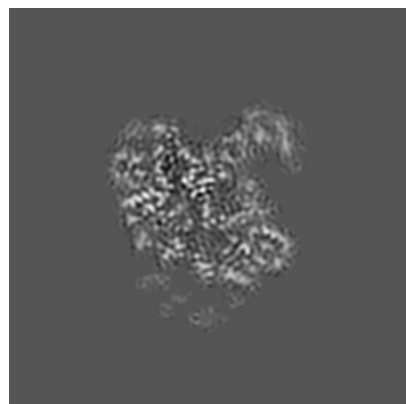


Z

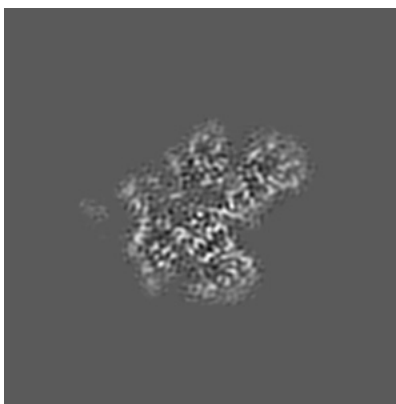
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

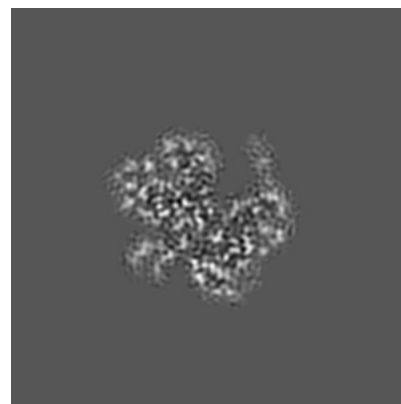
6.2.1 Primary map



X Index: 128



Y Index: 128

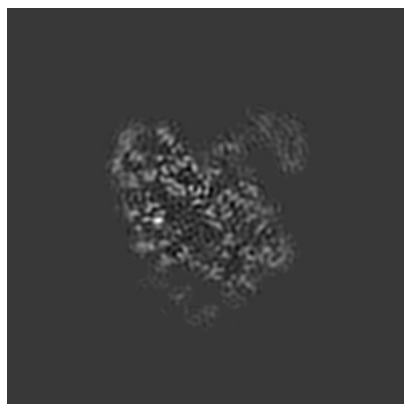


Z Index: 128

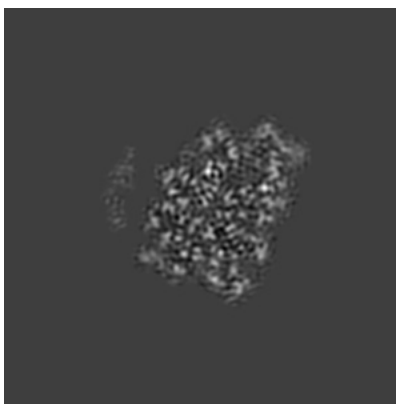
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

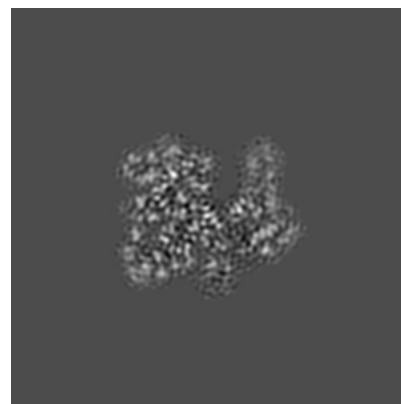
6.3.1 Primary map



X Index: 124



Y Index: 107

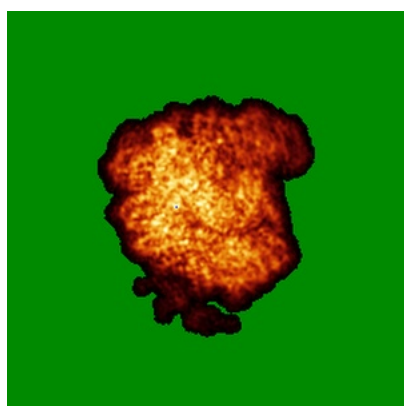


Z Index: 138

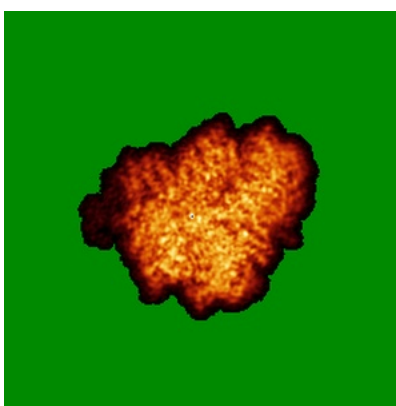
The images above show the largest variance slices of the map in three orthogonal directions.

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

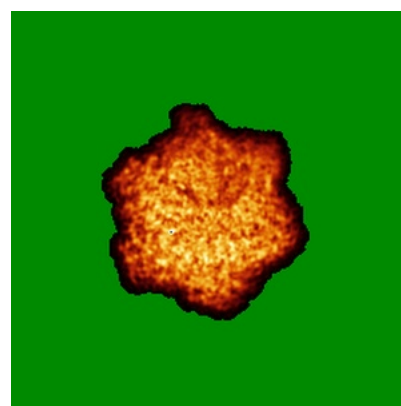
6.4.1 Primary map



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.

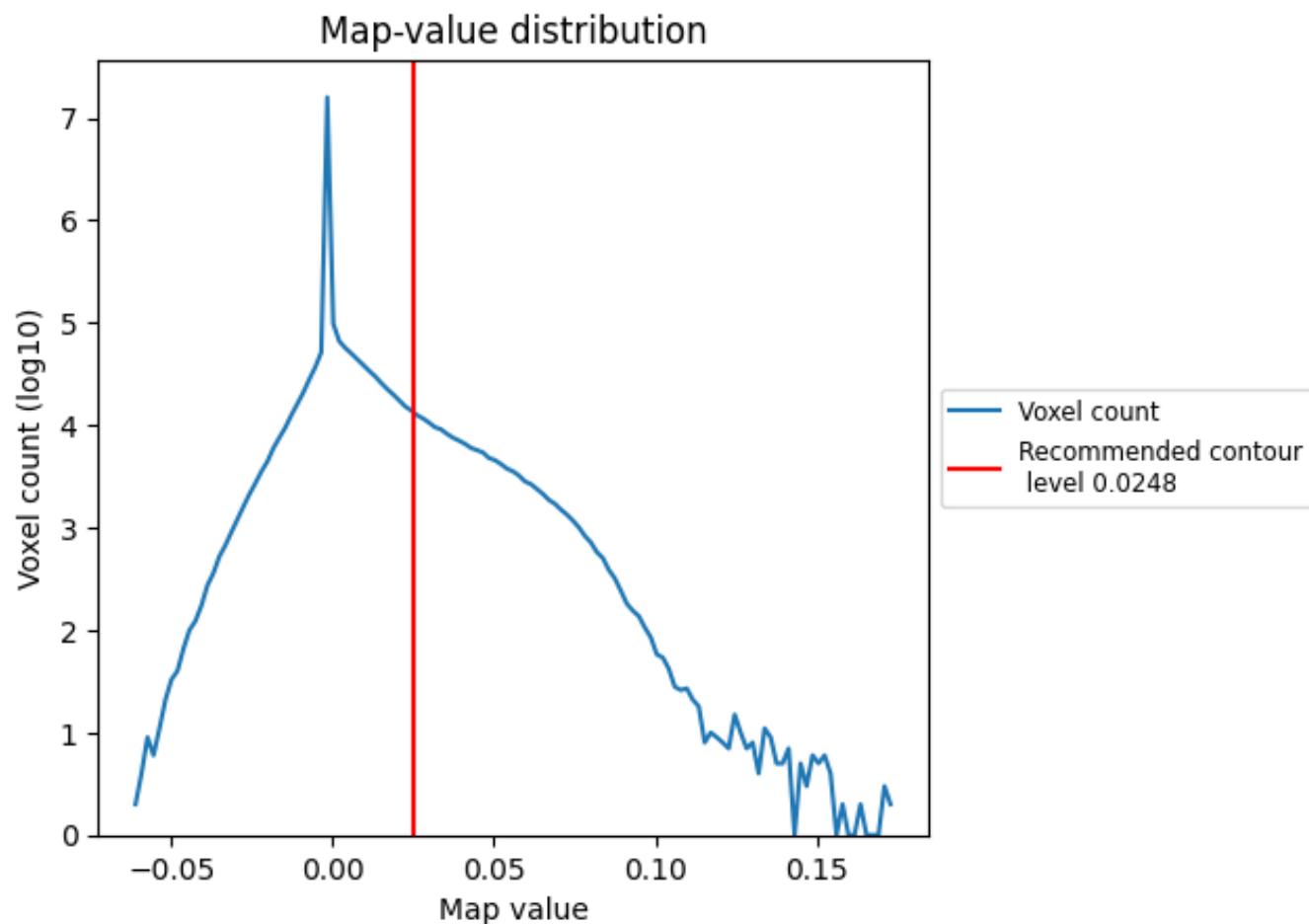
6.6 Mask visualisation

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

7 Map analysis [i](#)

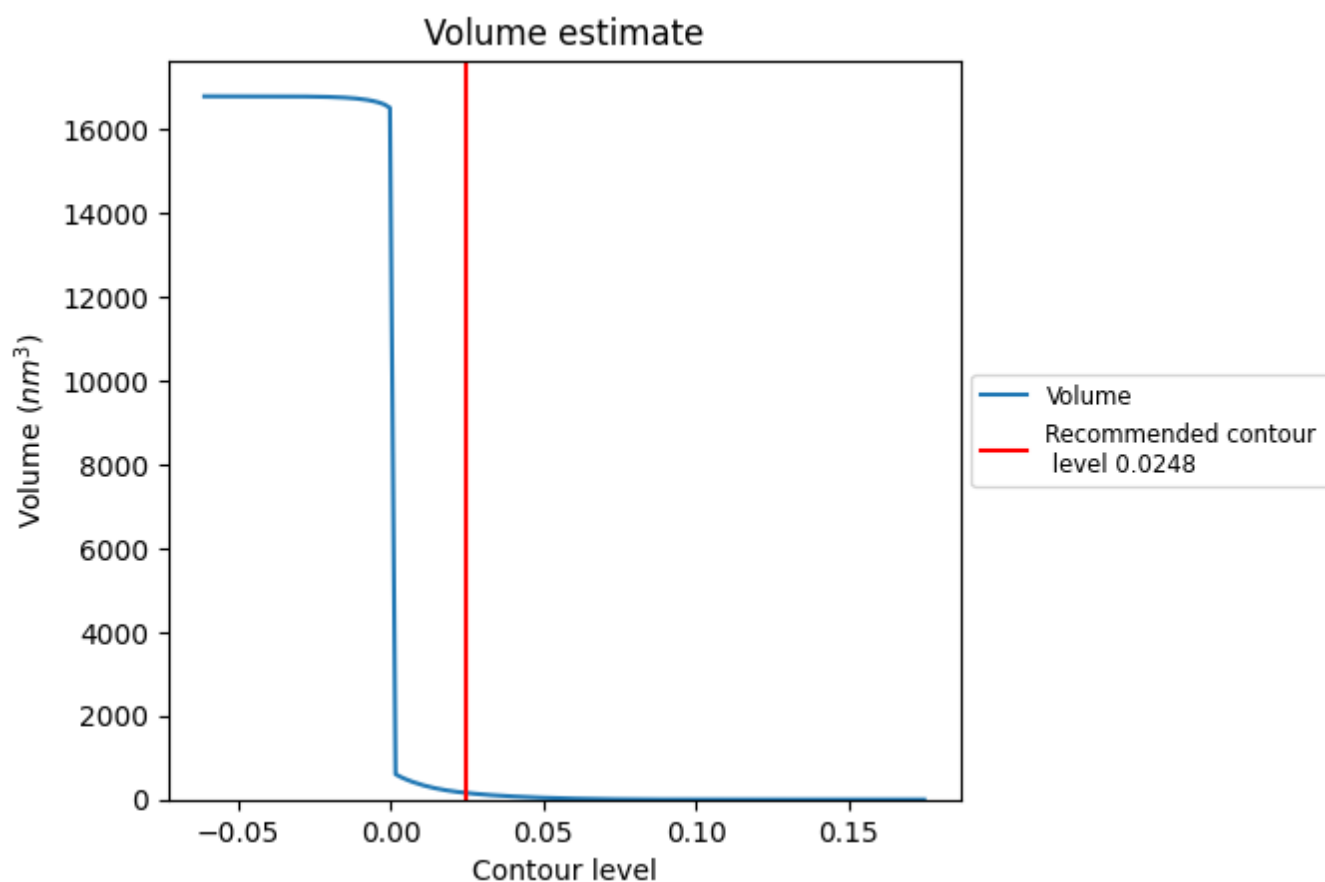
This section contains the results of statistical analysis of the map.

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.

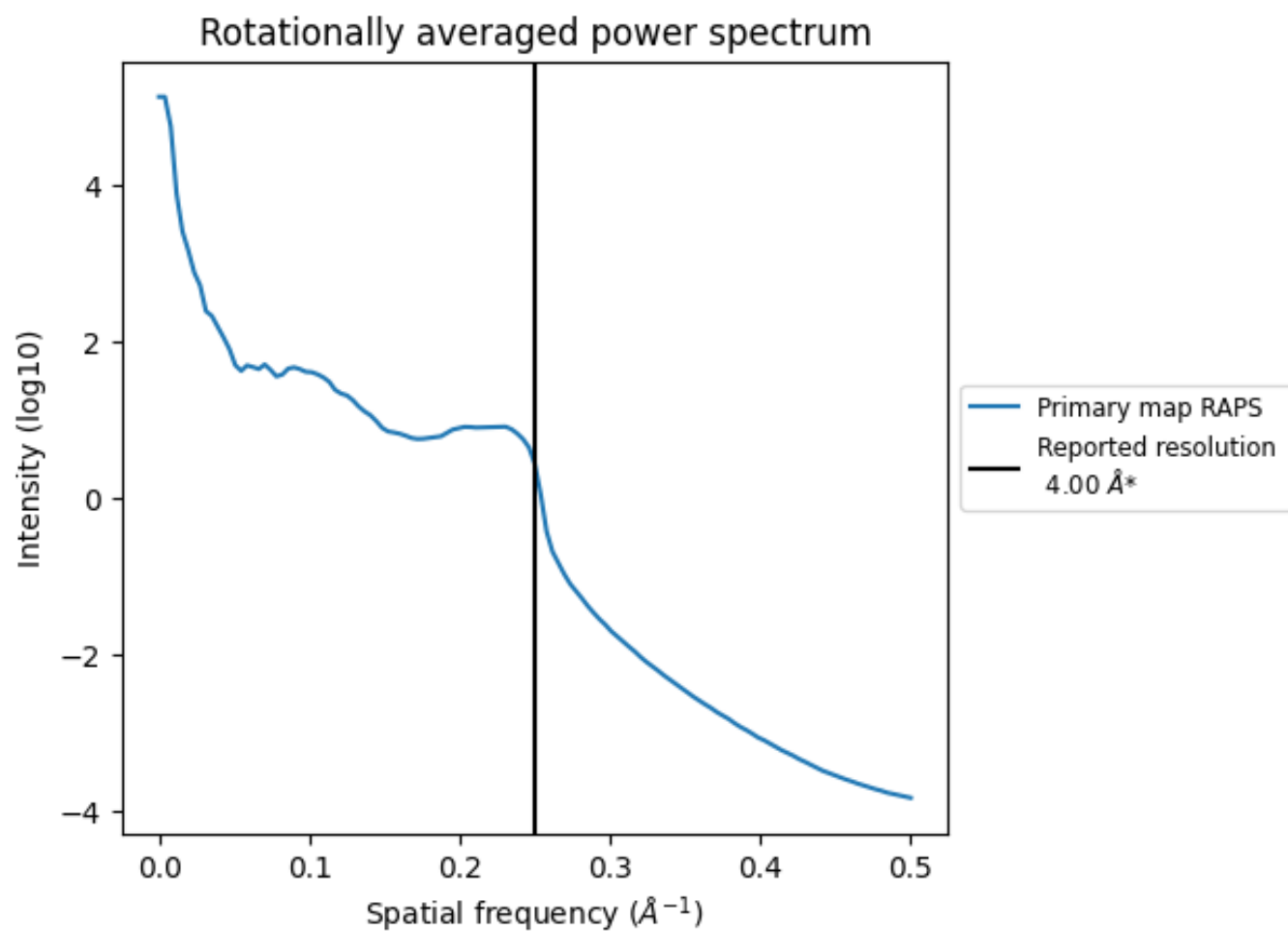
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 158 nm^3 ; this corresponds to an approximate mass of 143 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 0.250 Å⁻¹

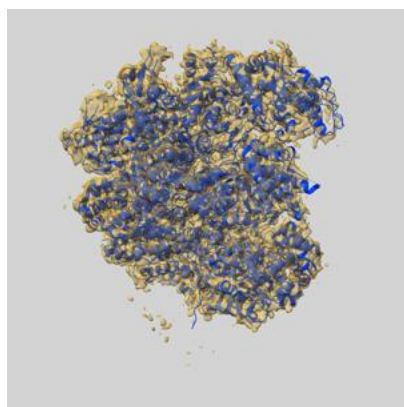
8 Fourier-Shell correlation

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

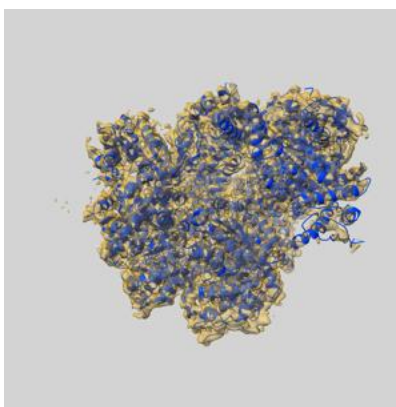
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8746 and PDB model 5VYA. Per-residue inclusion information can be found in section [3](#) on page [6](#).

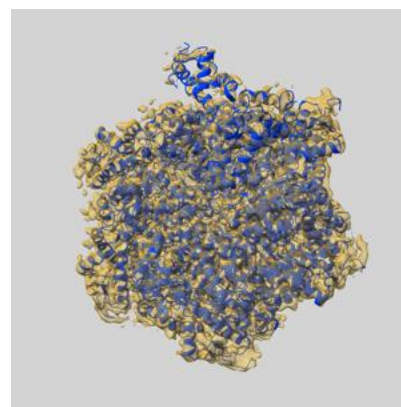
9.1 Map-model overlay [i](#)



X



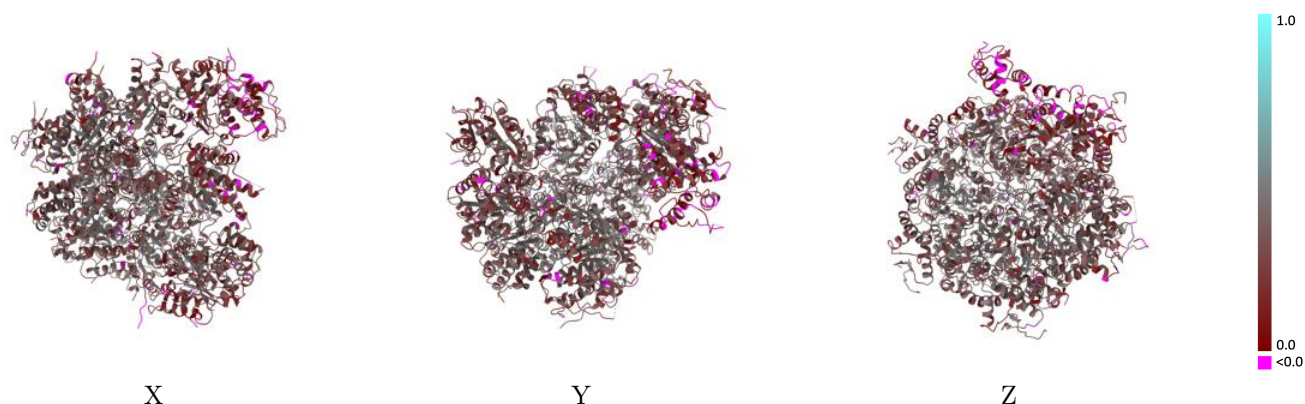
Y



Z

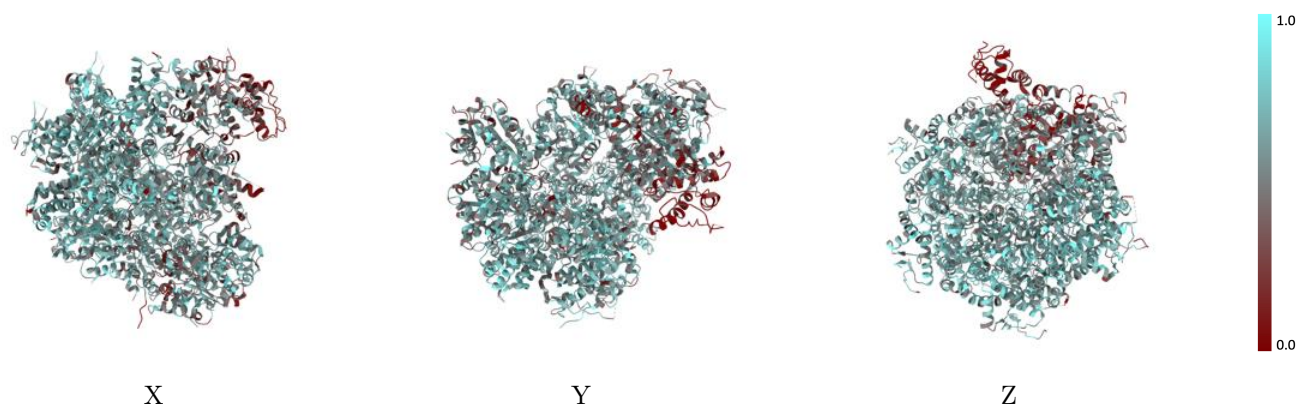
The images above show the 3D surface view of the map at the recommended contour level 0.0248 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



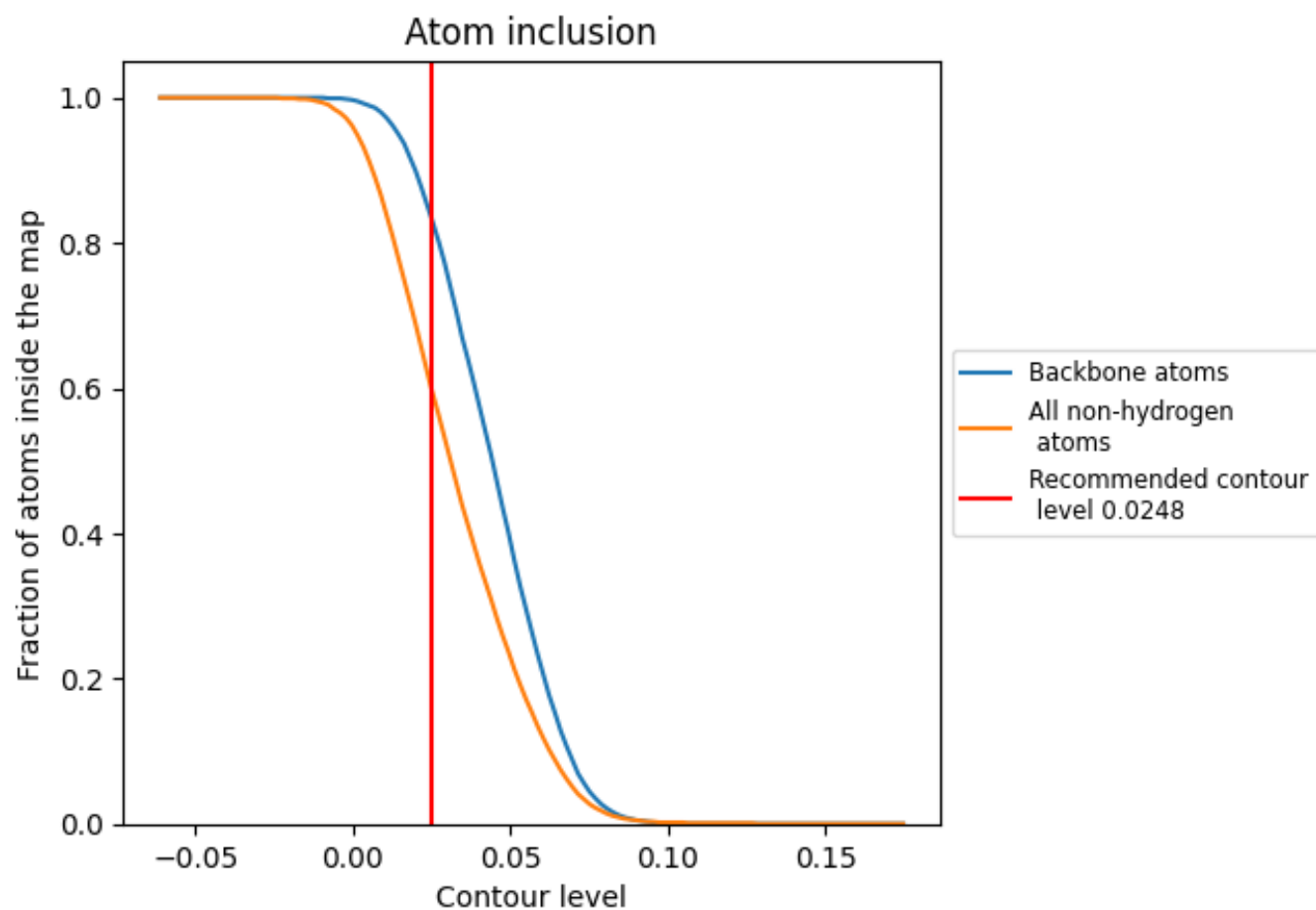
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0248).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0248) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6020	0.3130
A	0.4320	0.2290
B	0.6230	0.3160
C	0.6650	0.3480
D	0.6660	0.3540
E	0.6510	0.3370
F	0.5750	0.2920
P	0.6260	0.3260

1.0

0.0

<0.0