



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 04:22 AM UTC

PDB ID : 8XJ6 / pdb_00008xj6
EMDB ID : EMD-38394
Title : The Cryo-EM structure of MPXV E5 apo conformation
Authors : Zhang, W.; Liu, Y.; Gao, H.; Gan, J.
Deposited on : 2023-12-20
Resolution : 3.32 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

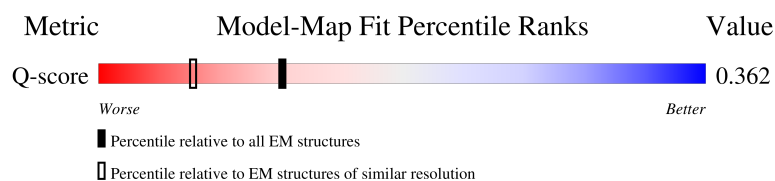
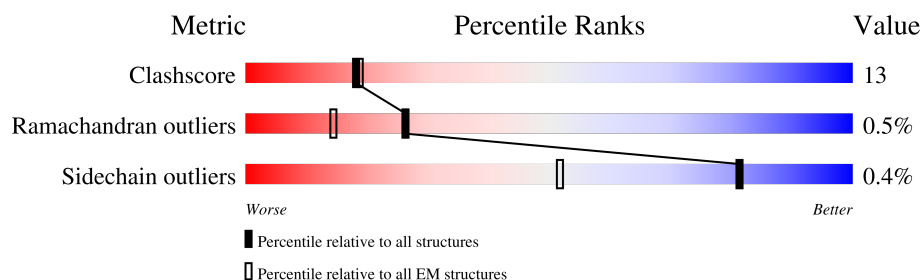
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.32 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	14518 (2.82 - 3.82)

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	785	 6% 30% 16% 54%
1	B	785	 6% 31% 14% 55%
1	C	785	 5% 33% 13% 54%
1	D	785	 8% 52% 23% 25%

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Mol	Chain	Length	Quality of chain
1	E	785	15% 44% 41%
1	F	785	15% 59% 26%

2 Entry composition [i](#)

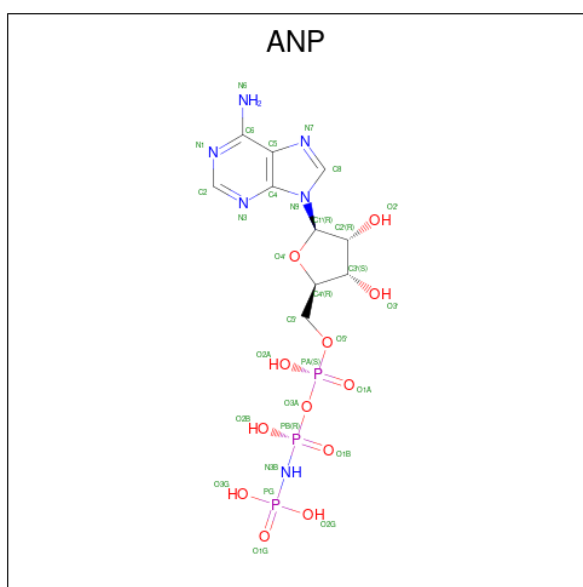
There are 4 unique types of molecules in this entry. The entry contains 22688 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Monkeypox virus E5.

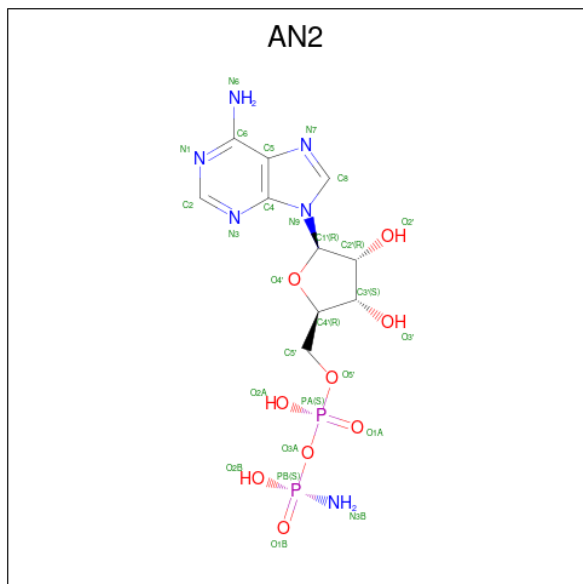
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	359	Total 2889	1840	489	546	14	0	0
1	B	357	Total 2865	1824	486	540	15	0	0
1	C	365	Total 2938	1878	499	546	15	0	0
1	D	589	Total 4752	3013	803	907	29	0	0
1	E	461	Total 3682	2350	630	684	18	0	0
1	F	676	Total 5386	3417	915	1023	31	0	0

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	C	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	D	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 3 is AMP PHOSPHORAMIDATE (CCD ID: AN2) (formula: $C_{10}H_{16}N_6O_9P_2$).

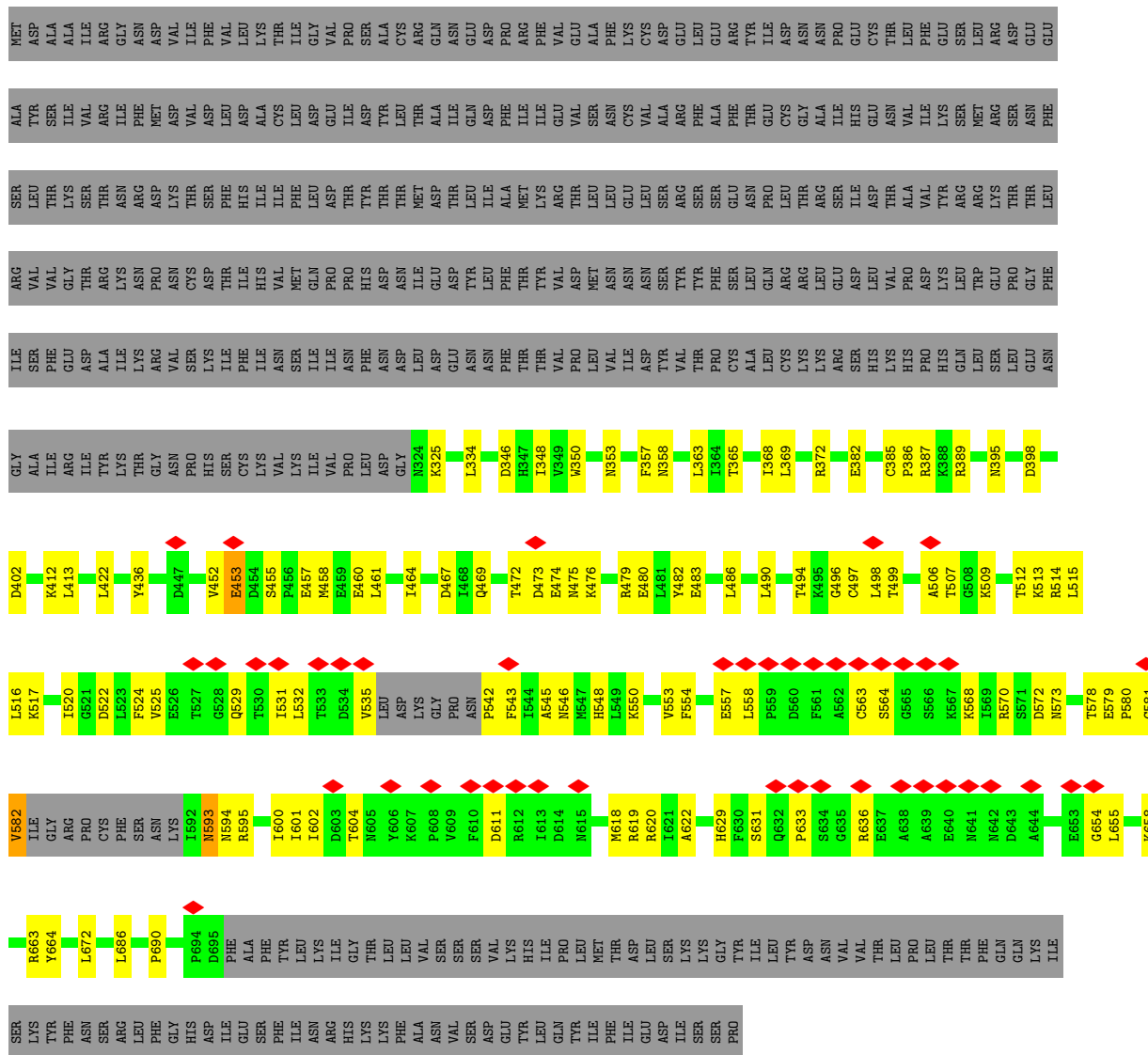


Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	N	O	P	0
			27	10	6	9	2	
3	E	1	Total	C	N	O	P	0
			27	10	6	9	2	
3	F	1	Total	C	N	O	P	0
			27	10	6	9	2	

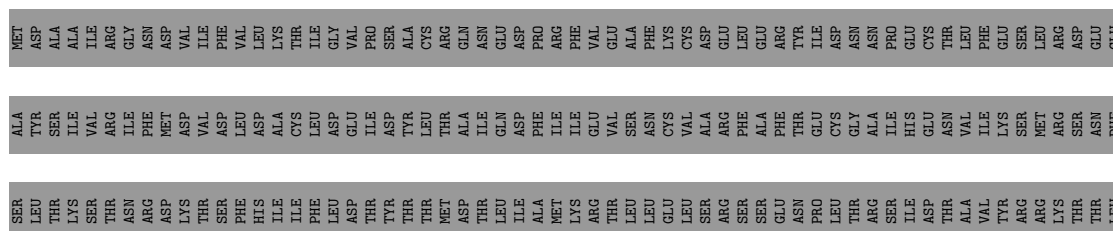
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

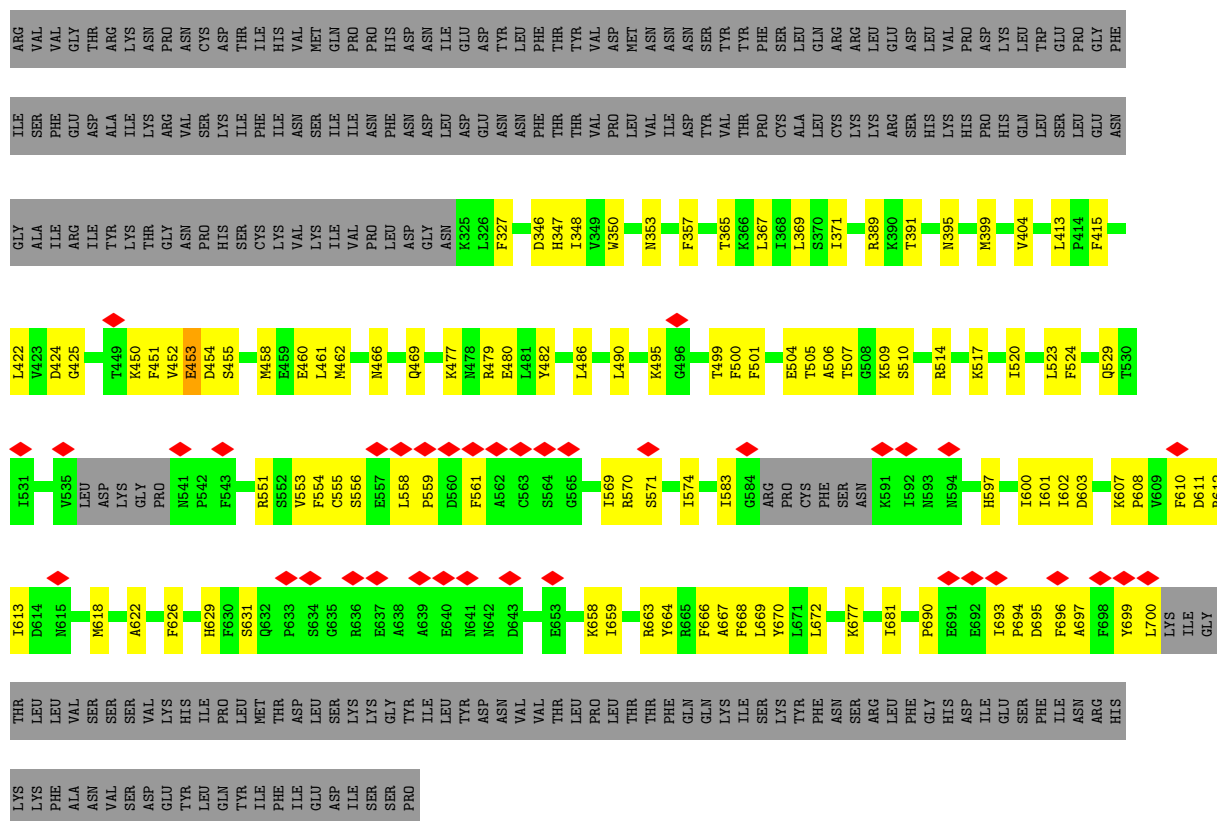
Mol	Chain	Residues	Atoms		AltConf
4	E	1	Total	Zn	0
			1	1	
4	F	1	Total	Zn	0
			1	1	

Chain B: 6% 31% 14% 55%

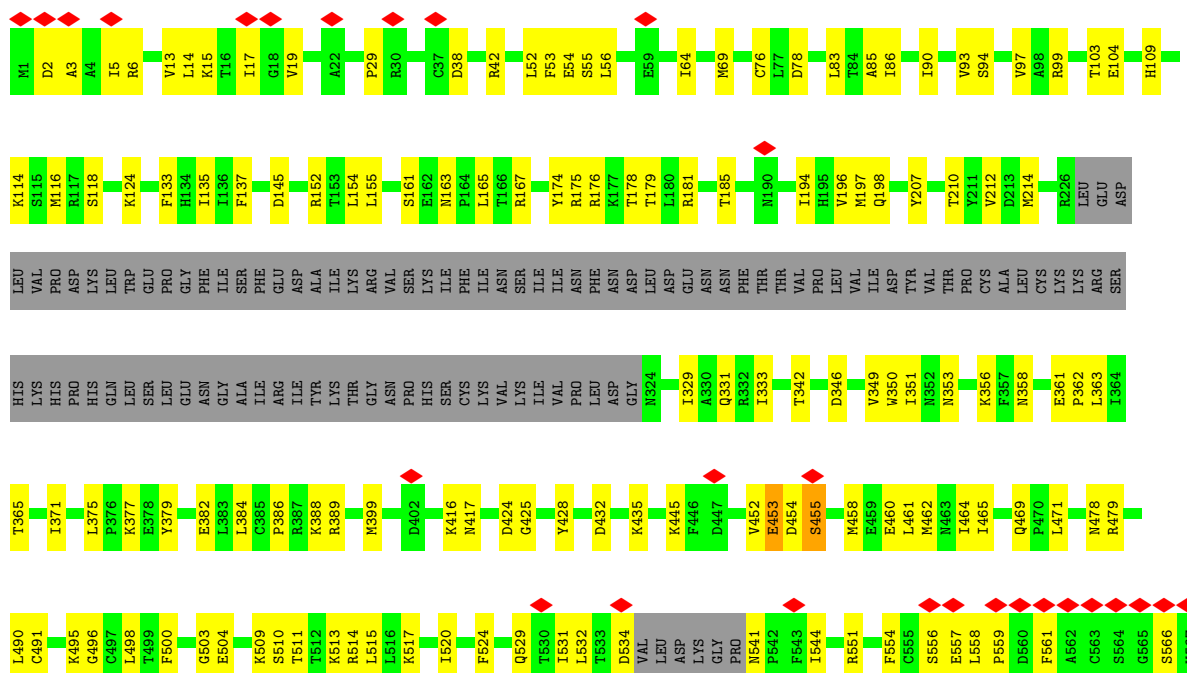


Chain C: 5% 33% 13% 54%





• Molecule 1: Monkeypox virus E5



THR	PHE	P633	P559	P470	N300	L208	T143	I67
ASP	ILE	S634	D560	E474	L321	F209	MI44	F68
LEU	GLU	G635	F561	N475	D322	T210	DI45	M69
SER	ASP	R636	A562	R479	K325	M214	M150	D70
LYS	ILE	E637	C563	T485	L326	N215	K151	V71
GLY	SER	A638	S564	L334	L340	N216	R152	D72
TYR	SER	A639	G565	L490	H347	N217	T153	L73
ILE	PRO	D643	S566	C491	L340	Q224	L154	D74
LEU			K567	T494	H347	R225	L155	A75
TYR			K568	K495	G496	R226	E156	C76
ASP			N573	G496	W350	LEU	L157	L77
ASN			L574	T499	I351	ASP	S158	D78
VAL			K575	G503	H352	LEU	R159	E79
VAL			K576	G504	N353	PRO	S160	I80
THR			L577	E505	N358	LYS	S161	D81
LEU			L578	T507	S359	LEU	E162	Y82
LEU			E579	G508	E360	VAL	N163	L83
THR			V582	K509	L363	ASP	P164	T84
PHE			L583	S510	K366	LEU	L165	A85
GLN			ARG	T511	L375	F240	T166	I86
GLN			PRO	R514	L379	I241	R167	Q87
LYS			CYS	V525	Y379	D245	I169	D88
ILE			PHE	G528	L384	K248	D170	F89
SER			ASN	Q529	C385	I255	Y174	I90
SER			LYS	T530	R387	I259	K177	I91
ARG			T592	I531	K388	N260	T178	E92
LEU			N593	L532	R389	D263	T179	V93
LEU			N594	L533	K390	L264	L180	S94
PHE			R595	T534	D398	D265	R181	F100
GLY			H597	V535	M399	N268	V182	A101
HIS			A598	LEU	V404	V272	V183	T103
ASP			T599	ASP	N417	P273	G184	G106
ILE			A600	LYS	N417	L274	T185	A107
GLU			I601	PRO	K445	V275	N186	M111
SER			I602	GLY	V452	D277	N187	V112
PHE			I602	ASP	E453	Y278	P188	I113
ILE			N605	LYS	S455	V279	N189	K114
ASN				PRO	M458	THR	C191	S115
ARG				LYS	E459	PRO	D192	M116
HIS				ASN	L461	C282	T193	R117
LYS				GLY	F554	C285	I194	M118
LYS				PRO	C555	K286	H195	S118
PHE				LYS	S556	K287	V196	N119
ALA				ILE	E557	K291	M197	F120
ASN				VAL	L558		Q198	K124
VAL				LEU			P199	S125
SER				GLU			T200	T126
GLU				TYR			H201	N127
TYR				LEU			D202	R128
LEU				SER			N203	D129
SER				VAL			I204	L138
TYR				GLN			E205	D139
GLN				LYS				
TYR				HIS				
ILE				ILE				
PRO				PRO				
LEU				LEU				
MET				MET				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60606	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.981	Depositor
Minimum map value	-1.337	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.336	Depositor
Map size ($\text{\AA}$)	301.64398, 301.64398, 301.64398	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0773, 1.0773, 1.0773	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ANP, AN2, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.17	0/2945	0.41	0/3974
1	B	0.21	0/2921	0.42	0/3944
1	C	0.21	0/2997	0.41	0/4046
1	D	0.18	0/4843	0.39	0/6549
1	E	0.21	0/3758	0.43	2/5080 (0.0%)
1	F	0.20	0/5490	0.40	0/7431
All	All	0.20	0/22954	0.41	2/31024 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	321	LEU	CA-C-N	-5.42	114.81	122.94
1	E	321	LEU	C-N-CA	-5.42	114.81	122.94

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2889	0	2876	98	0
1	B	2865	0	2865	87	0
1	C	2938	0	2952	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4752	0	4704	129	0
1	E	3682	0	3684	88	0
1	F	5386	0	5288	139	0
2	A	31	0	13	4	0
2	C	31	0	13	1	0
2	D	31	0	13	0	0
3	B	27	0	14	3	0
3	E	27	0	14	1	0
3	F	27	0	14	1	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
All	All	22688	0	22450	594	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 13.

All (594) 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:E:570:ARG:HE	1:E:573:ASN:HD21	1.26	0.81
1:F:158:SER:HA	1:F:166:THR:HG22	1.65	0.78
1:F:677:LYS:HA	1:F:681:ILE:HD12	1.65	0.77
1:A:568:LYS:HD2	1:A:611:ASP:HB3	1.68	0.76
1:B:348:ILE:HG22	1:B:357:PHE:HB2	1.68	0.75
1:D:38:ASP:HB2	1:D:42:ARG:HH12	1.52	0.74
1:D:469:GLN:O	1:D:479:ARG:NH1	2.21	0.73
1:A:470:PRO:HD2	1:A:475:ASN:HD22	1.54	0.72
1:B:522:ASP:O	1:B:550:LYS:NZ	2.22	0.72
1:B:570:ARG:HH11	1:B:572:ASP:HB3	1.55	0.72
1:F:514:ARG:NH2	1:F:660:GLN:OE1	2.22	0.72
1:C:555:CYS:HB2	1:C:602:ILE:HG12	1.72	0.71
1:E:255:ILE:HG12	1:E:283:ALA:HB2	1.70	0.71
1:F:83:LEU:O	1:F:87:GLN:NE2	2.24	0.71
1:C:490:LEU:O	1:C:551:ARG:NH1	2.24	0.71
1:E:455:SER:HB3	1:E:458:MET:HB2	1.73	0.70
1:E:290:HIS:HE1	1:E:314:CYS:HB2	1.57	0.70
1:D:181:ARG:HH12	1:D:194:ILE:HA	1.57	0.70
1:D:531:ILE:HG13	1:D:532:LEU:HD12	1.75	0.69
1:E:569:ILE:HD11	1:E:608:PRO:HB2	1.74	0.69
1:B:413:LEU:HD23	1:B:422:LEU:HD21	1.75	0.69
1:F:455:SER:HB3	1:F:458:MET:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:LEU:O	1:B:573:ASN:ND2	2.26	0.68
1:A:346:ASP:OD1	1:A:347:HIS:N	2.27	0.68
1:A:461:LEU:HD11	1:A:664:TYR:HB3	1.73	0.68
1:F:161:SER:O	1:F:167:ARG:NH1	2.27	0.68
1:A:340:LEU:HD13	1:A:404:VAL:HG21	1.76	0.67
1:F:470:PRO:HD2	1:F:475:ASN:HD22	1.59	0.67
1:A:497:CYS:HB2	1:A:686:LEU:HG	1.77	0.67
1:A:531:ILE:HG13	1:A:532:LEU:HD12	1.78	0.66
1:B:469:GLN:OE1	1:B:479:ARG:NH1	2.27	0.66
1:D:99:ARG:NH1	1:E:337:ASN:OD1	2.28	0.66
1:E:385:CYS:SG	1:E:387:ARG:NH1	2.68	0.66
1:E:458:MET:HE1	1:E:671:LEU:HG	1.78	0.65
1:E:510:SER:OG	1:E:514:ARG:NH1	2.29	0.65
1:D:38:ASP:HB2	1:D:42:ARG:NH1	2.10	0.65
1:D:677:LYS:HA	1:D:681:ILE:HD12	1.79	0.65
1:E:555:CYS:HB3	1:E:602:ILE:HG12	1.79	0.65
1:D:97:VAL:HB	1:D:116:MET:HE1	1.79	0.65
1:D:514:ARG:HG2	1:D:517:LYS:HE3	1.79	0.65
1:F:490:LEU:O	1:F:551:ARG:NH1	2.30	0.65
1:F:529:GLN:HE22	1:F:559:PRO:HD3	1.62	0.65
1:F:14:LEU:HD23	1:F:32:VAL:HG12	1.79	0.64
1:D:532:LEU:O	1:D:573:ASN:ND2	2.31	0.64
1:D:619:ARG:HA	1:D:688:PRO:HG3	1.79	0.64
1:F:531:ILE:HG13	1:F:532:LEU:HD12	1.80	0.64
1:D:529:GLN:NE2	1:D:557:GLU:O	2.30	0.63
1:E:389:ARG:NH2	1:F:398:ASP:OD2	2.30	0.63
1:B:455:SER:O	1:B:458:MET:N	2.22	0.63
1:B:520:ILE:HD11	1:B:524:PHE:HB2	1.81	0.63
1:A:351:ILE:O	1:A:356:LYS:NZ	2.32	0.63
1:B:542:PRO:O	1:B:546:ASN:ND2	2.24	0.63
1:F:461:LEU:HD12	1:F:664:TYR:HB3	1.80	0.62
1:F:573:ASN:HA	1:F:576:LYS:HG2	1.81	0.62
1:B:545:ALA:O	1:B:548:HIS:ND1	2.30	0.62
1:A:504:GLU:O	1:A:509:LYS:NZ	2.32	0.62
1:D:69:MET:HE1	1:D:93:VAL:HG11	1.81	0.62
1:A:532:LEU:O	1:A:573:ASN:ND2	2.33	0.61
1:C:529:GLN:HE22	1:C:556:SER:H	1.48	0.61
1:A:611:ASP:OD1	1:A:612:ARG:N	2.33	0.61
1:C:501:PHE:HB2	1:C:603:ASP:HA	1.82	0.61
1:D:558:LEU:HD12	1:D:604:THR:HG22	1.81	0.61
1:A:561:PHE:HD1	1:A:566:SER:HB3	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:612:ARG:NH1	1:A:613:ILE:O	2.33	0.61
1:B:506:ALA:HA	3:B:801:AN2:H5'1	1.82	0.61
1:C:348:ILE:HG22	1:C:357:PHE:HB2	1.83	0.61
1:D:455:SER:HB3	1:D:458:MET:HB2	1.82	0.61
1:A:511:THR:HG21	2:A:801:ANP:H8	1.81	0.61
1:D:490:LEU:O	1:D:551:ARG:NH1	2.34	0.61
1:A:514:ARG:HE	1:A:659:ILE:HD11	1.65	0.60
1:B:499:THR:HG22	1:B:622:ALA:HB3	1.82	0.60
1:A:574:ILE:O	1:A:620:ARG:NH2	2.34	0.60
1:B:467:ASP:OD1	3:B:801:AN2:N6	2.34	0.60
1:E:452:VAL:O	1:E:453:GLU:HB2	2.02	0.60
1:D:17:ILE:HG12	1:D:53:PHE:HE2	1.67	0.60
1:D:452:VAL:O	1:D:453:GLU:HB2	2.02	0.59
1:B:455:SER:HB3	1:B:458:MET:HB2	1.84	0.59
1:A:389:ARG:NH2	1:B:395:ASN:OD1	2.35	0.59
1:E:469:GLN:O	1:E:479:ARG:NH1	2.35	0.59
1:F:35:PHE:HB3	1:F:40:LEU:HB2	1.84	0.59
1:F:532:LEU:O	1:F:573:ASN:ND2	2.33	0.59
1:C:413:LEU:HG	1:C:422:LEU:HD21	1.84	0.59
1:A:572:ASP:HA	1:A:575:LYS:HG2	1.83	0.59
1:B:554:PHE:CD1	1:B:601:ILE:HB	2.37	0.59
1:D:2:ASP:H	1:D:5:ILE:HD12	1.68	0.59
1:E:459:GLU:HA	1:E:462:MET:HE2	1.85	0.59
1:F:14:LEU:HB2	1:F:53:PHE:HB2	1.83	0.59
1:D:495:LYS:NZ	1:D:597:HIS:O	2.36	0.59
1:B:593:ASN:O	1:B:595:ARG:NH1	2.36	0.59
1:B:460:GLU:OE1	1:B:663:ARG:NH1	2.34	0.59
1:A:469:GLN:O	1:A:479:ARG:NH1	2.37	0.58
1:F:544:ILE:HD11	1:F:582:VAL:HG21	1.86	0.58
1:F:568:LYS:HE3	1:F:611:ASP:HA	1.84	0.58
1:D:491:CYS:O	1:D:495:LYS:NZ	2.36	0.58
1:B:479:ARG:NE	1:B:483:GLU:OE2	2.27	0.58
1:D:496:GLY:HA2	1:D:578:THR:HG23	1.86	0.58
1:F:452:VAL:HG23	1:F:453:GLU:H	1.69	0.58
1:E:263:ASP:O	1:E:268:ASN:ND2	2.33	0.58
1:F:162:GLU:HA	1:F:167:ARG:HH12	1.69	0.58
1:C:461:LEU:HD12	1:C:664:TYR:HB3	1.85	0.58
1:E:575:LYS:HA	1:E:620:ARG:HH22	1.68	0.58
1:F:120:PHE:O	1:F:201:HIS:NE2	2.37	0.58
1:F:260:ASN:ND2	1:F:273:PRO:O	2.37	0.58
1:F:611:ASP:OD1	1:F:612:ARG:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:334:LEU:HD12	1:F:399:MET:HE2	1.85	0.58
1:F:469:GLN:O	1:F:479:ARG:NH1	2.36	0.58
1:C:469:GLN:O	1:C:479:ARG:NH1	2.36	0.57
1:A:389:ARG:NH1	1:B:398:ASP:OD2	2.36	0.57
1:D:504:GLU:O	1:D:509:LYS:NZ	2.37	0.57
1:D:510:SER:HA	1:D:513:LYS:HE2	1.84	0.57
1:A:573:ASN:O	1:A:577:LEU:HD23	2.04	0.57
1:D:161:SER:O	1:D:167:ARG:NH2	2.36	0.57
1:F:6:ARG:NH2	1:F:214:MET:O	2.37	0.57
1:F:68:PHE:O	1:F:69:MET:HE2	2.04	0.57
1:F:496:GLY:HA2	1:F:578:THR:HG23	1.87	0.57
1:F:627:ARG:NH2	1:F:643:ASP:O	2.34	0.57
1:F:240:PHE:HD1	1:F:241:ILE:HG12	1.69	0.57
1:C:658:LYS:HB3	1:C:663:ARG:HD2	1.86	0.57
1:D:520:ILE:HD11	1:D:524:PHE:HB2	1.85	0.57
1:F:197:MET:O	1:F:198:GLN:NE2	2.36	0.57
1:C:559:PRO:HD2	1:C:561:PHE:HE1	1.69	0.57
1:D:53:PHE:HB3	1:D:179:THR:HB	1.87	0.57
1:D:351:ILE:O	1:D:356:LYS:NZ	2.38	0.57
1:D:424:ASP:OD1	1:D:425:GLY:N	2.34	0.57
1:A:532:LEU:HD21	1:A:602:ILE:HG12	1.86	0.56
1:F:152:ARG:NH2	1:F:155:LEU:HD22	2.21	0.56
1:D:428:TYR:HB3	1:D:432:ASP:HB2	1.88	0.56
1:A:515:LEU:HG	1:A:668:PHE:CD2	2.40	0.56
1:F:12:PHE:HB2	1:F:57:ARG:HD2	1.88	0.56
1:E:529:GLN:NE2	1:E:557:GLU:O	2.39	0.56
1:C:514:ARG:HG2	1:C:517:LYS:HZ3	1.69	0.56
1:B:531:ILE:HG13	1:B:532:LEU:HD12	1.86	0.56
1:A:358:ASN:HB3	1:A:363:LEU:HD11	1.88	0.56
1:B:578:THR:HG21	1:B:620:ARG:HE	1.69	0.56
1:F:452:VAL:O	1:F:453:GLU:HB2	2.04	0.56
1:B:358:ASN:HB3	1:B:363:LEU:HD11	1.87	0.56
1:E:556:SER:HA	1:E:603:ASP:OD1	2.05	0.55
1:D:342:THR:OG1	1:D:346:ASP:OD1	2.23	0.55
1:B:452:VAL:O	1:B:453:GLU:HB2	2.05	0.55
1:E:334:LEU:HD21	1:E:396:ILE:HG23	1.89	0.55
1:D:416:LYS:HE3	1:D:445:LYS:HG2	1.88	0.55
1:D:365:THR:HG23	1:D:389:ARG:HG2	1.88	0.55
1:D:377:LYS:NZ	1:E:239:GLY:O	2.40	0.55
1:F:36:LYS:O	1:F:40:LEU:N	2.26	0.55
1:F:66:ARG:HB2	1:F:209:PHE:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:THR:HG23	1:D:104:GLU:HG2	1.88	0.55
1:D:571:SER:HB3	1:D:617:LEU:HD13	1.89	0.55
1:B:568:LYS:HE3	1:B:611:ASP:HA	1.88	0.55
1:C:495:LYS:NZ	1:C:597:HIS:O	2.40	0.55
1:C:607:LYS:HE3	1:C:694:PRO:HD2	1.89	0.55
1:D:167:ARG:NH1	1:E:302:ALA:HB2	2.22	0.55
1:F:529:GLN:NE2	1:F:557:GLU:O	2.40	0.55
1:A:495:LYS:NZ	1:A:597:HIS:O	2.40	0.54
1:F:90:ILE:HA	1:F:93:VAL:HG12	1.89	0.54
1:F:554:PHE:CE1	1:F:601:ILE:HD12	2.42	0.54
1:A:401:VAL:HG21	1:F:351:ILE:HG21	1.90	0.54
1:F:655:LEU:HA	1:F:658:LYS:HD3	1.88	0.54
1:A:542:PRO:O	1:A:546:ASN:ND2	2.38	0.54
1:F:150:MET:HG3	1:F:154:LEU:HG	1.89	0.54
1:B:460:GLU:O	1:B:464:ILE:HG12	2.07	0.54
1:C:514:ARG:HE	1:C:659:ILE:HD11	1.73	0.54
1:D:611:ASP:OD1	1:D:612:ARG:N	2.41	0.54
1:F:673:VAL:HG12	1:F:677:LYS:HE3	1.90	0.54
1:F:21:SER:O	1:F:24:ARG:N	2.40	0.54
1:D:52:LEU:HB2	1:D:185:THR:HG21	1.87	0.54
1:D:64:ILE:HD12	1:D:212:VAL:HG11	1.90	0.54
1:D:351:ILE:HD12	1:D:363:LEU:HD23	1.89	0.54
1:E:377:LYS:HD2	1:F:300:ASN:HD21	1.73	0.54
1:E:458:MET:HE3	1:E:462:MET:SD	2.48	0.54
1:C:514:ARG:HG2	1:C:517:LYS:NZ	2.23	0.54
1:B:469:GLN:HG2	1:B:475:ASN:HD21	1.72	0.53
1:B:496:GLY:HA2	1:B:578:THR:HG23	1.90	0.53
1:D:109:HIS:CG	1:E:337:ASN:HD22	2.26	0.53
1:F:359:SER:OG	1:F:360:GLU:N	2.40	0.53
1:C:611:ASP:OD1	1:C:612:ARG:N	2.40	0.53
1:A:346:ASP:OD2	1:A:359:SER:OG	2.23	0.53
1:A:474:GLU:HG2	1:A:475:ASN:H	1.74	0.53
1:C:611:ASP:OD1	1:C:612:ARG:HD3	2.09	0.53
1:D:331:GLN:HG2	1:D:399:MET:HE1	1.89	0.53
1:E:618:MET:HE1	1:E:696:PHE:CD1	2.43	0.53
1:E:259:ILE:HB	1:E:275:VAL:HG23	1.90	0.53
1:F:101:ALA:O	1:F:106:GLY:N	2.41	0.53
1:B:452:VAL:HG23	1:B:453:GLU:H	1.74	0.53
1:F:151:LYS:HB2	1:F:174:TYR:HD2	1.73	0.53
1:F:152:ARG:HH21	1:F:155:LEU:HD22	1.74	0.53
1:D:124:LYS:O	1:D:196:VAL:N	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:655:LEU:O	1:D:659:ILE:HG12	2.08	0.53
1:F:508:GLY:O	1:F:511:THR:OG1	2.22	0.53
1:C:693:ILE:HG22	1:C:696:PHE:H	1.74	0.53
1:D:461:LEU:HD12	1:D:664:TYR:HD2	1.73	0.53
1:D:69:MET:CE	1:D:93:VAL:HG11	2.39	0.52
1:D:15:LYS:NZ	1:D:29:PRO:O	2.37	0.52
1:F:461:LEU:HD13	1:F:667:ALA:HB3	1.91	0.52
1:B:402:ASP:OD1	1:B:402:ASP:N	2.42	0.52
1:B:497:CYS:HB3	1:B:686:LEU:HG	1.92	0.52
1:B:513:LYS:HG2	1:B:554:PHE:HD2	1.74	0.52
1:F:460:GLU:HG3	1:F:664:TYR:HE1	1.74	0.52
1:F:554:PHE:CE1	1:F:601:ILE:HB	2.45	0.52
1:A:334:LEU:HD11	1:A:400:LEU:HD21	1.92	0.52
1:C:451:PHE:HE1	1:C:670:TYR:HA	1.73	0.52
1:C:501:PHE:HB3	1:C:626:PHE:HE2	1.75	0.52
1:F:264:LEU:HD11	1:F:274:LEU:HD11	1.92	0.52
1:D:452:VAL:HG23	1:D:453:GLU:H	1.73	0.52
1:F:494:THR:OG1	1:F:596:ASN:O	2.27	0.52
1:C:460:GLU:HG3	1:C:664:TYR:HE1	1.75	0.51
1:D:386:PRO:HG2	1:E:391:THR:HG23	1.93	0.51
1:D:568:LYS:HE3	1:D:611:ASP:HB3	1.92	0.51
1:C:613:ILE:HB	1:C:699:TYR:CE2	2.45	0.51
1:E:629:HIS:O	1:E:649:LYS:N	2.33	0.51
1:D:582:VAL:HG23	1:D:596:ASN:HB2	1.91	0.51
1:E:462:MET:HA	1:E:465:ILE:HG22	1.91	0.51
1:D:14:LEU:HD12	1:D:19:VAL:HG21	1.93	0.51
1:C:523:LEU:HD13	1:C:551:ARG:HD2	1.93	0.51
1:F:575:LYS:HZ1	1:F:617:LEU:HB2	1.75	0.51
1:B:460:GLU:OE1	1:B:664:TYR:OH	2.26	0.51
1:B:507:THR:OG1	3:B:801:AN2:O2B	2.20	0.51
1:C:553:VAL:HB	1:C:600:ILE:HD13	1.93	0.51
1:E:611:ASP:OD1	1:E:612:ARG:N	2.44	0.51
1:F:186:ARG:HA	1:F:194:ILE:HG12	1.93	0.51
1:C:346:ASP:OD1	1:C:347:HIS:N	2.44	0.51
1:B:498:LEU:O	1:B:622:ALA:N	2.42	0.50
1:E:290:HIS:CE1	1:E:314:CYS:HB2	2.41	0.50
1:E:677:LYS:HA	1:E:681:ILE:HD12	1.93	0.50
1:F:485:THR:HG21	1:F:499:THR:HG21	1.92	0.50
1:F:514:ARG:NH1	1:F:656:ASP:OD1	2.44	0.50
1:B:529:GLN:NE2	1:B:557:GLU:O	2.43	0.50
1:C:452:VAL:O	1:C:453:GLU:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:457:GLU:HA	1:E:460:GLU:OE2	2.11	0.50
1:F:325:LYS:HZ1	1:F:379:TYR:HE1	1.58	0.50
1:A:494:THR:OG1	1:A:596:ASN:O	2.26	0.50
1:F:529:GLN:NE2	1:F:559:PRO:HD3	2.27	0.50
1:A:629:HIS:CE1	1:A:631:SER:HB3	2.46	0.50
1:D:656:ASP:O	1:D:659:ILE:N	2.43	0.50
1:D:333:ILE:HG12	1:D:371:ILE:HD11	1.94	0.50
1:D:554:PHE:CZ	1:D:603:ASP:HB2	2.46	0.50
1:F:340:LEU:HD13	1:F:404:VAL:HG21	1.92	0.50
1:C:506:ALA:HB3	1:C:629:HIS:CD2	2.47	0.50
1:D:511:THR:O	1:D:515:LEU:HG	2.11	0.50
1:F:326:LEU:HD11	1:F:388:LYS:HB3	1.93	0.50
1:B:482:TYR:CZ	1:B:486:LEU:HD11	2.46	0.50
1:A:631:SER:O	1:A:651:LEU:N	2.39	0.50
1:B:513:LYS:HG2	1:B:554:PHE:CD2	2.47	0.49
1:C:556:SER:HA	1:C:603:ASP:OD1	2.12	0.49
1:F:10:VAL:HG22	1:F:57:ARG:HH22	1.77	0.49
1:D:76:CYS:SG	1:E:312:HIS:NE2	2.84	0.49
1:E:570:ARG:O	1:E:570:ARG:HG3	2.11	0.49
1:D:627:ARG:NH2	1:D:643:ASP:O	2.32	0.49
1:A:453:GLU:OE1	1:A:670:TYR:OH	2.24	0.49
1:D:500:PHE:HB2	1:D:623:VAL:HG22	1.94	0.49
1:A:533:THR:HB	1:A:567:LYS:HD2	1.94	0.49
1:E:534:ASP:O	1:E:570:ARG:NH2	2.46	0.49
1:F:375:LEU:HD21	1:F:379:TYR:HD2	1.78	0.49
1:B:386:PRO:HG2	1:C:391:THR:HG23	1.95	0.49
1:B:516:LEU:HD13	1:B:554:PHE:HZ	1.76	0.49
1:C:350:TRP:CZ2	1:C:353:ASN:HA	2.47	0.49
1:B:461:LEU:HD11	1:B:664:TYR:HB3	1.95	0.49
1:E:452:VAL:HG13	1:E:453:GLU:N	2.28	0.49
1:A:440:VAL:HG21	1:A:549:LEU:HB3	1.96	0.48
1:C:477:LYS:HA	1:C:480:GLU:HG2	1.94	0.48
1:D:558:LEU:HD22	1:D:561:PHE:HE2	1.78	0.48
1:E:495:LYS:HE3	1:E:599:THR:OG1	2.13	0.48
1:E:459:GLU:HG2	1:E:460:GLU:N	2.28	0.48
1:A:520:ILE:HD11	1:A:524:PHE:HB2	1.94	0.48
1:C:367:LEU:O	1:C:371:ILE:HG12	2.13	0.48
1:F:100:PHE:HB3	1:F:150:MET:HE1	1.96	0.48
1:F:495:LYS:NZ	1:F:597:HIS:O	2.41	0.48
1:A:385:CYS:SG	1:A:387:ARG:NH2	2.86	0.48
1:C:697:ALA:HA	1:C:700:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:ILE:HD11	1:D:137:PHE:HE1	1.78	0.48
1:F:240:PHE:CE1	1:F:321:LEU:HB3	2.49	0.48
1:D:154:LEU:HD12	1:D:174:TYR:HE2	1.77	0.48
1:D:361:GLU:O	1:D:363:LEU:HD12	2.13	0.48
1:D:375:LEU:HD21	1:D:379:TYR:HB2	1.96	0.48
1:A:413:LEU:HB2	1:A:422:LEU:HD21	1.96	0.48
1:E:247:ILE:HA	1:E:250:VAL:HG12	1.95	0.48
1:F:111:ASN:HA	1:F:114:LYS:HE3	1.95	0.48
1:A:508:GLY:O	1:A:511:THR:OG1	2.28	0.48
1:C:490:LEU:HD11	1:C:672:LEU:HB3	1.94	0.48
1:B:413:LEU:CD2	1:B:422:LEU:HD21	2.43	0.47
1:F:375:LEU:HD21	1:F:379:TYR:HB2	1.96	0.47
1:A:424:ASP:OD1	1:A:425:GLY:N	2.44	0.47
1:A:458:MET:HE1	1:A:670:TYR:CD2	2.49	0.47
1:A:461:LEU:O	1:A:464:ILE:HG22	2.15	0.47
1:A:549:LEU:HD21	1:A:595:ARG:NH2	2.30	0.47
1:C:520:ILE:HD11	1:C:524:PHE:HB2	1.95	0.47
1:D:471:LEU:HD23	1:D:479:ARG:HG2	1.96	0.47
1:F:241:ILE:HD11	1:F:321:LEU:HD13	1.95	0.47
1:D:2:ASP:O	1:D:6:ARG:N	2.43	0.47
1:E:358:ASN:OD1	1:E:359:SER:N	2.47	0.47
1:A:333:ILE:HG12	1:A:371:ILE:HD11	1.96	0.47
1:A:350:TRP:CZ2	1:A:353:ASN:HA	2.49	0.47
1:C:504:GLU:HG3	1:C:505:THR:H	1.78	0.47
1:D:109:HIS:CD2	1:E:337:ASN:HD22	2.33	0.47
1:D:175:ARG:O	1:D:178:THR:OG1	2.25	0.47
1:D:693:ILE:HB	1:D:696:PHE:HD2	1.79	0.47
1:F:94:SER:HB3	1:F:116:MET:SD	2.54	0.47
1:F:417:ASN:HB3	1:F:445:LYS:HD3	1.96	0.47
1:A:431:ASP:O	1:A:434:LYS:HG2	2.14	0.47
1:C:570:ARG:HG3	1:C:570:ARG:O	2.15	0.47
1:A:507:THR:N	2:A:801:ANP:O2A	2.48	0.47
1:C:369:LEU:HD21	1:C:389:ARG:NH1	2.29	0.47
1:D:556:SER:HB3	1:D:557:GLU:OE1	2.15	0.47
1:A:411:ASP:OD1	1:A:411:ASP:N	2.40	0.47
1:A:461:LEU:HA	1:A:464:ILE:HG22	1.97	0.47
1:B:369:LEU:O	1:B:372:ARG:HG2	2.15	0.47
1:D:78:ASP:OD1	1:D:78:ASP:N	2.47	0.47
1:A:561:PHE:CD1	1:A:566:SER:HB3	2.48	0.46
1:B:346:ASP:HB3	1:B:357:PHE:HE1	1.81	0.46
1:C:558:LEU:HD22	1:C:561:PHE:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:554:PHE:HD1	1:D:601:ILE:HB	1.81	0.46
1:E:305:ILE:HB	1:E:317:LYS:HB3	1.96	0.46
1:F:65:VAL:HG12	1:F:210:THR:HA	1.97	0.46
1:F:163:ASN:HB3	1:F:166:THR:OG1	2.15	0.46
1:B:325:LYS:NZ	1:B:382:GLU:OE2	2.47	0.46
1:D:460:GLU:O	1:D:464:ILE:HG12	2.15	0.46
1:B:350:TRP:CZ2	1:B:353:ASN:HA	2.50	0.46
1:C:327:PHE:CZ	1:C:399:MET:HE2	2.50	0.46
1:F:592:ILE:O	1:F:593:ASN:C	2.58	0.46
1:A:358:ASN:OD1	1:A:360:GLU:HG2	2.16	0.46
1:F:37:CYS:SG	1:F:38:ASP:N	2.88	0.46
1:E:575:LYS:HD3	1:E:620:ARG:HH22	1.80	0.46
1:E:250:VAL:HG23	1:E:305:ILE:HD11	1.96	0.46
1:F:67:ILE:HG23	1:F:137:PHE:HB2	1.96	0.46
1:F:161:SER:HB3	1:F:166:THR:HG21	1.97	0.46
1:F:633:PRO:HA	1:F:636:ARG:HD2	1.97	0.46
1:B:469:GLN:OE1	1:B:479:ARG:HD3	2.16	0.46
1:E:470:PRO:HD2	1:E:475:ASN:ND2	2.31	0.46
1:A:358:ASN:ND2	1:A:361:GLU:HG3	2.31	0.46
1:A:490:LEU:O	1:A:551:ARG:NH1	2.49	0.46
1:A:496:GLY:HA2	1:A:578:THR:HG23	1.97	0.46
1:D:382:GLU:OE1	1:D:388:LYS:NZ	2.38	0.46
1:A:452:VAL:HG23	1:A:453:GLU:H	1.81	0.46
1:C:365:THR:HG23	1:C:389:ARG:HG2	1.98	0.46
1:A:358:ASN:OD1	1:A:359:SER:N	2.49	0.45
1:A:404:VAL:O	1:A:405:GLU:HG3	2.15	0.45
1:D:145:ASP:OD1	1:D:145:ASP:N	2.49	0.45
1:D:554:PHE:CD1	1:D:601:ILE:HB	2.51	0.45
1:A:681:ILE:HD12	1:A:682:PRO:HA	1.97	0.45
1:B:619:ARG:HG3	1:B:620:ARG:HG3	1.98	0.45
1:C:507:THR:OG1	2:C:801:ANP:O1B	2.35	0.45
1:D:197:MET:HG2	1:D:207:TYR:CZ	2.50	0.45
1:F:350:TRP:CZ2	1:F:353:ASN:HA	2.52	0.45
1:E:473:ASP:OD1	1:E:473:ASP:N	2.49	0.45
1:F:363:LEU:HD23	1:F:366:LYS:HD3	1.99	0.45
1:A:500:PHE:HB2	1:A:623:VAL:HG22	1.99	0.45
1:B:368:ILE:HG21	1:B:389:ARG:HG3	1.97	0.45
1:D:569:ILE:HB	1:D:610:PHE:HD1	1.82	0.45
1:A:451:PHE:HZ	1:A:673:VAL:HG11	1.82	0.45
1:A:461:LEU:HD21	1:A:664:TYR:CG	2.52	0.45
1:B:553:VAL:HG23	1:B:600:ILE:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:ARG:NH1	1:D:214:MET:O	2.49	0.45
1:D:133:PHE:HE1	1:D:165:LEU:HD22	1.82	0.45
1:F:614:ASP:OD1	1:F:615:ASN:N	2.48	0.45
1:A:629:HIS:HB2	1:A:645:TYR:CG	2.51	0.45
1:A:674:LYS:O	1:A:677:LYS:HG2	2.16	0.45
1:D:417:ASN:HB3	1:D:445:LYS:HD2	1.98	0.45
1:F:548:HIS:HB2	1:F:594:ASN:CG	2.41	0.45
1:A:559:PRO:HD2	1:A:561:PHE:CE1	2.52	0.45
1:D:54:GLU:OE2	1:D:210:THR:OG1	2.27	0.45
1:D:55:SER:OG	1:D:56:LEU:N	2.50	0.45
1:B:461:LEU:HG	1:B:664:TYR:CD1	2.52	0.45
1:D:197:MET:O	1:D:198:GLN:NE2	2.48	0.45
1:D:350:TRP:CZ2	1:D:353:ASN:HA	2.52	0.45
1:D:462:MET:HA	1:D:465:ILE:HG12	1.99	0.45
1:D:514:ARG:HA	1:D:517:LYS:HG2	1.98	0.45
1:F:53:PHE:HE1	1:F:181:ARG:HG3	1.81	0.45
1:A:355:TRP:HE1	1:A:434:LYS:HA	1.82	0.44
1:A:508:GLY:N	2:A:801:ANP:O2A	2.47	0.44
1:B:469:GLN:HE21	1:B:475:ASN:CG	2.25	0.44
1:D:503:GLY:HA3	1:D:626:PHE:HB2	1.98	0.44
1:D:613:ILE:HB	1:D:699:TYR:CE2	2.52	0.44
1:F:268:ASN:HB2	1:F:272:VAL:HG23	1.99	0.44
1:C:514:ARG:HA	1:C:517:LYS:NZ	2.32	0.44
1:D:349:VAL:HG21	1:D:363:LEU:HB3	1.98	0.44
1:B:512:THR:HA	1:B:515:LEU:HG	2.00	0.44
1:A:582:VAL:HG23	1:A:596:ASN:OD1	2.17	0.44
1:D:561:PHE:CD1	1:D:566:SER:HB3	2.52	0.44
1:A:452:VAL:O	1:A:453:GLU:HB2	2.18	0.44
1:A:533:THR:O	1:A:567:LYS:NZ	2.38	0.44
1:C:415:PHE:HZ	1:C:669:LEU:HD21	1.81	0.44
1:C:501:PHE:HB3	1:C:626:PHE:CE2	2.53	0.44
1:D:94:SER:HA	1:D:116:MET:HE3	2.00	0.44
1:E:452:VAL:HG13	1:E:453:GLU:H	1.83	0.44
1:E:543:PHE:CZ	1:F:583:ILE:HG21	2.52	0.44
1:B:525:VAL:CG1	1:B:553:VAL:HG12	2.47	0.44
1:C:697:ALA:O	1:C:700:LEU:HB2	2.17	0.44
1:D:358:ASN:OD1	1:D:362:PRO:HA	2.17	0.44
1:E:520:ILE:HD11	1:E:524:PHE:HB2	2.00	0.44
1:F:85:ALA:HA	1:F:163:ASN:HD21	1.82	0.44
1:C:677:LYS:HA	1:C:681:ILE:HD12	2.00	0.44
1:D:570:ARG:CZ	1:D:573:ASN:HD21	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:570:ARG:O	1:D:572:ASP:N	2.50	0.44
1:E:384:LEU:O	1:E:389:ARG:NH1	2.51	0.44
1:F:375:LEU:CD2	1:F:379:TYR:HB2	2.47	0.44
1:F:506:ALA:H	3:F:801:AN2:H3B1	1.66	0.44
1:A:547:MET:HE1	1:A:596:ASN:HD22	1.83	0.44
1:B:469:GLN:NE2	1:B:479:ARG:HB2	2.33	0.44
1:B:593:ASN:HB2	1:B:595:ARG:HD3	1.99	0.44
1:B:629:HIS:CD2	1:B:631:SER:HB3	2.52	0.44
1:D:514:ARG:HA	1:D:517:LYS:HE3	1.98	0.44
1:E:576:LYS:O	1:E:579:GLU:HG3	2.18	0.44
1:A:462:MET:HE3	1:A:466:ASN:HD21	1.82	0.44
1:D:69:MET:HE3	1:D:135:ILE:HG21	2.00	0.44
1:D:541:ASN:HB3	1:D:544:ILE:HG22	2.00	0.44
1:C:570:ARG:HA	1:C:611:ASP:OD2	2.17	0.43
1:D:329:ILE:O	1:D:333:ILE:HG13	2.18	0.43
1:E:491:CYS:SG	1:E:684:MET:HE2	2.57	0.43
1:F:285:CYS:SG	1:F:287:LYS:CB	3.06	0.43
1:A:670:TYR:O	1:A:673:VAL:HG12	2.18	0.43
1:D:2:ASP:OD1	1:D:3:ALA:N	2.46	0.43
1:F:186:ARG:NH1	1:F:191:CYS:O	2.50	0.43
1:A:457:GLU:HB3	1:A:664:TYR:CE1	2.54	0.43
1:A:656:ASP:OD1	1:A:657:GLY:N	2.49	0.43
1:B:655:LEU:HA	1:B:658:LYS:HG2	2.00	0.43
1:C:569:ILE:HD11	1:C:608:PRO:HB3	2.00	0.43
1:D:432:ASP:HA	1:D:435:LYS:HE2	2.00	0.43
1:E:573:ASN:HB3	1:E:577:LEU:HD23	2.01	0.43
1:E:655:LEU:O	1:E:659:ILE:HG12	2.18	0.43
1:E:670:TYR:O	1:E:674:LYS:HG2	2.19	0.43
1:F:384:LEU:O	1:F:389:ARG:NH1	2.51	0.43
1:F:548:HIS:ND1	1:F:594:ASN:HA	2.33	0.43
1:A:657:GLY:O	1:A:661:ASN:ND2	2.52	0.43
1:B:480:GLU:HA	1:B:483:GLU:OE1	2.18	0.43
1:E:475:ASN:OD1	1:E:478:ASN:HB3	2.17	0.43
1:F:265:ASP:H	1:F:268:ASN:CG	2.23	0.43
1:F:554:PHE:HA	1:F:601:ILE:O	2.17	0.43
1:F:558:LEU:HA	1:F:559:PRO:HD3	1.86	0.43
1:C:395:ASN:O	1:C:399:MET:HG3	2.18	0.43
1:D:384:LEU:HD11	1:E:324:ASN:H	1.84	0.43
1:E:535:VAL:HA	1:E:570:ARG:HH22	1.83	0.43
1:E:541:ASN:HB3	1:E:544:ILE:HG22	1.98	0.43
1:F:693:ILE:HG22	1:F:696:PHE:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:ASP:OD1	1:A:615:ASN:N	2.47	0.43
1:B:506:ALA:HB3	1:B:629:HIS:CE1	2.54	0.43
1:D:175:ARG:NH1	1:D:178:THR:HA	2.33	0.43
1:E:570:ARG:HE	1:E:573:ASN:ND2	2.04	0.43
1:A:479:ARG:O	1:A:483:GLU:HG3	2.19	0.43
1:A:558:LEU:HD22	1:A:561:PHE:CE2	2.54	0.43
1:B:455:SER:O	1:B:457:GLU:N	2.52	0.43
1:B:472:THR:O	1:B:476:LYS:HE3	2.18	0.43
1:D:152:ARG:O	1:D:155:LEU:N	2.52	0.43
1:F:101:ALA:HB1	1:F:107:ALA:HB3	2.00	0.43
1:C:454:ASP:O	1:C:458:MET:HB3	2.19	0.43
1:C:500:PHE:CE1	1:C:602:ILE:HD12	2.54	0.43
1:A:471:LEU:HD23	1:A:479:ARG:HG2	2.00	0.43
1:B:385:CYS:SG	1:B:387:ARG:NH2	2.92	0.43
1:C:499:THR:HB	1:C:622:ALA:HB3	2.01	0.43
1:C:559:PRO:HD2	1:C:561:PHE:CE1	2.53	0.43
1:E:495:LYS:NZ	1:E:597:HIS:O	2.32	0.43
1:E:506:ALA:H	3:E:801:AN2:H3B1	1.66	0.43
1:F:83:LEU:HA	1:F:86:ILE:HG22	1.99	0.43
1:F:245:ASP:HA	1:F:248:LYS:HG2	2.01	0.43
1:F:277:ASP:O	1:F:279:VAL:N	2.50	0.43
1:B:593:ASN:H	1:B:595:ARG:NH1	2.17	0.43
1:B:654:GLY:C	1:B:658:LYS:HZ2	2.27	0.43
1:E:350:TRP:CZ2	1:E:353:ASN:HA	2.54	0.43
1:A:416:LYS:HB2	1:A:445:LYS:HE2	2.00	0.42
1:B:334:LEU:HA	1:B:334:LEU:HD23	1.80	0.42
1:B:524:PHE:HE1	1:B:554:PHE:CD2	2.37	0.42
1:B:535:VAL:HA	1:B:570:ARG:HH22	1.84	0.42
1:B:618:MET:O	1:B:690:PRO:HG3	2.18	0.42
1:B:633:PRO:HA	1:B:636:ARG:HG3	2.00	0.42
1:C:607:LYS:NZ	1:C:695:ASP:OD2	2.43	0.42
1:B:365:THR:CG2	1:B:389:ARG:HE	2.32	0.42
1:D:85:ALA:HA	1:D:163:ASN:HD21	1.84	0.42
1:D:500:PHE:N	1:D:622:ALA:O	2.38	0.42
1:F:116:MET:SD	1:F:117:ARG:HG3	2.59	0.42
1:D:491:CYS:SG	1:D:684:MET:HE2	2.59	0.42
1:F:83:LEU:HD12	1:F:84:THR:N	2.34	0.42
1:F:259:ILE:HD12	1:F:275:VAL:HG12	2.00	0.42
1:C:424:ASP:OD1	1:C:425:GLY:N	2.45	0.42
1:C:571:SER:HA	1:C:574:ILE:HG13	2.01	0.42
1:D:498:LEU:HD22	1:D:574:ILE:HD12	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:529:GLN:NE2	1:D:559:PRO:HD3	2.35	0.42
1:E:407:ASP:OD1	1:E:438:CYS:HA	2.20	0.42
1:B:490:LEU:HD11	1:B:672:LEU:HB3	2.01	0.42
1:C:461:LEU:HD11	1:C:668:PHE:HB2	2.01	0.42
1:D:693:ILE:HG22	1:D:695:ASP:H	1.84	0.42
1:A:413:LEU:HD12	1:A:413:LEU:HA	1.87	0.42
1:A:549:LEU:HD21	1:A:595:ARG:HH21	1.83	0.42
1:C:629:HIS:ND1	1:C:631:SER:HB3	2.35	0.42
1:E:534:ASP:C	1:E:570:ARG:HH22	2.28	0.42
1:C:450:LYS:HD3	1:C:666:PHE:CD2	2.54	0.42
1:D:561:PHE:HD1	1:D:566:SER:HB3	1.85	0.42
1:E:465:ILE:HD11	1:E:482:TYR:HE2	1.85	0.42
1:E:469:GLN:HB3	1:E:479:ARG:NH1	2.35	0.42
1:F:87:GLN:O	1:F:91:ILE:HG12	2.20	0.42
1:F:458:MET:HE1	1:F:671:LEU:HD21	2.01	0.42
1:A:553:VAL:HB	1:A:600:ILE:HD13	2.02	0.42
1:A:577:LEU:HD13	1:A:582:VAL:HG21	2.01	0.42
1:B:543:PHE:CE1	1:C:583:ILE:HG21	2.55	0.42
1:E:558:LEU:HA	1:E:559:PRO:HD3	1.84	0.42
1:F:158:SER:HB2	1:F:169:ILE:HD11	2.02	0.42
1:F:474:GLU:CD	1:F:474:GLU:H	2.28	0.42
1:F:503:GLY:O	1:F:605:ASN:HA	2.19	0.42
1:A:458:MET:HE1	1:A:670:TYR:HD2	1.85	0.42
1:C:482:TYR:O	1:C:486:LEU:HD23	2.19	0.42
1:D:181:ARG:NH1	1:D:194:ILE:HA	2.30	0.42
1:F:78:ASP:OD1	1:F:78:ASP:N	2.52	0.42
1:F:490:LEU:HD11	1:F:672:LEU:HB3	2.02	0.42
1:F:495:LYS:HE3	1:F:599:THR:OG1	2.19	0.42
1:D:568:LYS:HG2	1:D:609:VAL:HG13	2.01	0.42
1:F:71:VAL:HG13	1:F:168:SER:HB2	2.01	0.42
1:A:327:PHE:CZ	1:A:399:MET:HE2	2.55	0.41
1:B:602:ILE:HG22	1:B:604:THR:HG23	2.02	0.41
1:F:81:ASP:HA	1:F:84:THR:HG22	2.02	0.41
1:F:525:VAL:HB	1:F:550:LYS:NZ	2.35	0.41
1:F:554:PHE:CD1	1:F:601:ILE:HB	2.55	0.41
1:F:555:CYS:HB3	1:F:602:ILE:HG13	2.02	0.41
1:F:652:ASP:OD2	1:F:655:LEU:HB2	2.20	0.41
1:A:686:LEU:H	1:A:686:LEU:HD23	1.86	0.41
1:B:513:LYS:HA	1:B:554:PHE:HE2	1.85	0.41
1:F:680:HIS:ND1	1:F:684:MET:HG2	2.34	0.41
1:D:375:LEU:CD2	1:D:379:TYR:HB2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:570:ARG:O	1:D:570:ARG:HG3	2.20	0.41
1:E:329:ILE:HG21	1:E:383:LEU:HD21	2.01	0.41
1:E:369:LEU:O	1:E:372:ARG:HG2	2.20	0.41
1:F:98:ALA:HB2	1:F:113:ILE:HG13	2.03	0.41
1:B:525:VAL:HB	1:B:550:LYS:HE2	2.03	0.41
1:E:470:PRO:HD2	1:E:475:ASN:HD22	1.86	0.41
1:E:570:ARG:O	1:E:572:ASP:N	2.53	0.41
1:E:697:ALA:O	1:E:701:LYS:N	2.46	0.41
1:A:548:HIS:CE1	1:A:549:LEU:CD2	3.04	0.41
1:B:365:THR:HG22	1:B:389:ARG:HE	1.85	0.41
1:B:412:LYS:HE2	1:B:436:TYR:CE1	2.55	0.41
1:C:461:LEU:HD13	1:C:667:ALA:HB3	2.01	0.41
1:C:462:MET:HE3	1:C:466:ASN:OD1	2.21	0.41
1:F:629:HIS:CE1	1:F:631:SER:HB3	2.56	0.41
1:A:457:GLU:HB3	1:A:664:TYR:CD1	2.55	0.41
1:A:558:LEU:HA	1:A:559:PRO:HD3	1.85	0.41
1:B:509:LYS:HB2	1:B:509:LYS:HE2	1.92	0.41
1:B:525:VAL:HG12	1:B:553:VAL:HG12	2.03	0.41
1:B:558:LEU:HD23	1:B:558:LEU:HA	1.90	0.41
1:C:554:PHE:CE1	1:C:601:ILE:HB	2.55	0.41
1:D:636:ARG:O	1:D:639:ALA:HB3	2.19	0.41
1:F:143:THR:OG1	1:F:145:ASP:OD1	2.35	0.41
1:B:582:VAL:HB	1:B:594:ASN:HB2	2.02	0.41
1:E:498:LEU:HD21	1:E:602:ILE:HD12	2.01	0.41
1:E:559:PRO:HD2	1:E:561:PHE:CE1	2.56	0.41
1:F:64:ILE:HG12	1:F:143:THR:HG22	2.03	0.41
1:A:348:ILE:HG22	1:A:357:PHE:HD1	1.85	0.41
1:A:474:GLU:HG2	1:A:475:ASN:N	2.35	0.41
1:C:509:LYS:HB2	1:C:509:LYS:HE2	1.95	0.41
1:C:510:SER:HB3	1:C:514:ARG:NH1	2.36	0.41
1:C:618:MET:O	1:C:690:PRO:HG3	2.21	0.41
1:D:176:ARG:H	1:D:176:ARG:HG3	1.70	0.41
1:D:454:ASP:O	1:D:458:MET:HB3	2.21	0.41
1:E:348:ILE:HG22	1:E:357:PHE:HB2	2.02	0.41
1:E:428:TYR:HB3	1:E:432:ASP:HB2	2.02	0.41
1:E:500:PHE:HE2	1:E:621:ILE:HD12	1.85	0.41
1:E:514:ARG:HE	1:E:659:ILE:HD11	1.86	0.41
1:E:681:ILE:HA	1:E:682:PRO:HA	1.85	0.41
1:F:386:PRO:O	1:F:390:LYS:HG2	2.21	0.41
1:F:507:THR:HB	1:F:626:PHE:HB3	2.03	0.41
1:A:524:PHE:HE1	1:A:554:PHE:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:ARG:O	1:A:646:ASP:N	2.31	0.41
1:D:167:ARG:HH11	1:E:302:ALA:HB2	1.84	0.41
1:E:458:MET:SD	1:E:667:ALA:HB1	2.61	0.41
1:E:490:LEU:HD11	1:E:672:LEU:HB3	2.03	0.41
1:F:263:ASP:O	1:F:268:ASN:ND2	2.50	0.41
1:F:491:CYS:HB2	1:F:676:TYR:HE2	1.86	0.41
1:A:471:LEU:HG	1:A:479:ARG:NH1	2.37	0.40
1:C:450:LYS:HD3	1:C:666:PHE:HD2	1.86	0.40
1:D:83:LEU:O	1:D:86:ILE:HG22	2.21	0.40
1:D:94:SER:HA	1:D:116:MET:CE	2.51	0.40
1:D:534:ASP:C	1:D:570:ARG:HH21	2.29	0.40
1:F:504:GLU:O	1:F:509:LYS:NZ	2.54	0.40
1:A:508:GLY:H	2:A:801:ANP:PA	2.44	0.40
1:B:473:ASP:OD1	1:B:474:GLU:N	2.54	0.40
1:B:494:THR:HG21	1:B:580:PRO:HA	2.03	0.40
1:B:517:LYS:HG3	1:B:524:PHE:CD2	2.56	0.40
1:B:563:CYS:SG	1:B:564:SER:N	2.93	0.40
1:D:514:ARG:NH2	1:D:660:GLN:HB3	2.36	0.40
1:E:673:VAL:HG12	1:E:677:LYS:NZ	2.36	0.40
1:B:658:LYS:HB2	1:B:663:ARG:HD3	2.03	0.40
1:D:114:LYS:O	1:D:118:SER:OG	2.28	0.40
1:D:558:LEU:HB3	1:D:561:PHE:CE2	2.56	0.40
1:E:334:LEU:HD11	1:E:399:MET:HB2	2.02	0.40
1:F:91:ILE:O	1:F:94:SER:OG	2.33	0.40
1:F:499:THR:CG2	1:F:601:ILE:HG12	2.51	0.40
1:A:483:GLU:HA	1:A:675:TRP:CZ3	2.57	0.40
1:D:469:GLN:OE1	1:D:478:ASN:ND2	2.55	0.40
1:E:342:THR:OG1	1:E:346:ASP:OD1	2.23	0.40
1:F:88:ASP:O	1:F:92:GLU:OE1	2.39	0.40
1:F:184:GLY:N	1:F:195:HIS:O	2.29	0.40
1:F:623:VAL:HG21	1:F:692:GLU:HB3	2.02	0.40
1:C:569:ILE:HG13	1:C:610:PHE:CD1	2.57	0.40
1:D:13:VAL:HG21	1:D:52:LEU:HD12	2.04	0.40
1:D:534:ASP:O	1:D:570:ARG:NH2	2.55	0.40
1:E:235:LEU:HD13	1:E:270:THR:OG1	2.21	0.40
1:F:12:PHE:HB2	1:F:57:ARG:CD	2.51	0.40
1:F:21:SER:OG	1:F:177:LYS:NZ	2.55	0.40
1:F:291:LYS:H	1:F:291:LYS:HG2	1.61	0.40
1:F:347:HIS:O	1:F:358:ASN:HB2	2.22	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	351/785 (45%)	336 (96%)	12 (3%)	3 (1%)	14	43
1	B	351/785 (45%)	334 (95%)	16 (5%)	1 (0%)	36	66
1	C	359/785 (46%)	342 (95%)	15 (4%)	2 (1%)	21	52
1	D	581/785 (74%)	563 (97%)	15 (3%)	3 (0%)	24	56
1	E	455/785 (58%)	438 (96%)	14 (3%)	3 (1%)	18	49
1	F	666/785 (85%)	635 (95%)	29 (4%)	2 (0%)	36	66
All	All	2763/4710 (59%)	2648 (96%)	101 (4%)	14 (0%)	26	56

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	405	GLU
1	A	453	GLU
1	C	453	GLU
1	C	455	SER
1	B	453	GLU
1	D	453	GLU
1	E	453	GLU
1	F	453	GLU
1	A	455	SER
1	D	455	SER
1	F	455	SER
1	E	455	SER
1	D	571	SER
1	E	571	SER

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	323/725 (45%)	323 (100%)	0	100	100
1	B	322/725 (44%)	317 (98%)	5 (2%)	55	71
1	C	329/725 (45%)	328 (100%)	1 (0%)	86	85
1	D	537/725 (74%)	537 (100%)	0	100	100
1	E	412/725 (57%)	411 (100%)	1 (0%)	87	87
1	F	601/725 (83%)	598 (100%)	3 (0%)	81	82
All	All	2524/4350 (58%)	2514 (100%)	10 (0%)	81	83

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	514	ARG
1	B	579	GLU
1	B	581	CYS
1	B	582	VAL
1	B	593	ASN
1	C	404	VAL
1	E	290	HIS
1	F	45	ASP
1	F	276	ILE
1	F	282	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	331	GLN
1	A	347	HIS
1	A	475	ASN
1	A	615	ASN
1	A	661	ASN
1	A	662	ASN
1	B	347	HIS
1	B	661	ASN
1	C	469	GLN
1	C	475	ASN
1	C	605	ASN
1	D	25	GLN

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Mol	Chain	Res	Type
1	D	46	ASN
1	D	109	HIS
1	D	134	HIS
1	D	642	ASN
1	E	290	HIS
1	E	294	HIS
1	E	373	HIS
1	E	573	ASN
1	E	605	ASN
1	E	661	ASN
1	F	127	ASN
1	F	224	GLN
1	F	310	ASN
1	F	312	HIS
1	F	662	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ANP	A	801	-	33,33,33	0.69	1 (3%)	45,52,52	0.55	1 (2%)
2	ANP	C	801	-	33,33,33	0.70	1 (3%)	45,52,52	0.56	1 (2%)
3	AN2	B	801	-	28,29,29	1.10	2 (7%)	40,45,45	0.59	2 (5%)
3	AN2	F	801	-	28,29,29	1.13	2 (7%)	40,45,45	0.66	1 (2%)
2	ANP	D	801	-	33,33,33	0.70	1 (3%)	45,52,52	0.56	1 (2%)
3	AN2	E	801	-	28,29,29	1.12	2 (7%)	40,45,45	0.67	2 (5%)

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
2	ANP	A	801	-	-	9/18/38/38	0/3/3/3
2	ANP	C	801	-	-	5/18/38/38	0/3/3/3
3	AN2	B	801	-	-	0/13/32/32	0/3/3/3
3	AN2	F	801	-	-	2/13/32/32	0/3/3/3
2	ANP	D	801	-	-	3/18/38/38	0/3/3/3
3	AN2	E	801	-	-	3/13/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	801	AN2	PB-O1B	4.64	1.53	1.46
3	B	801	AN2	PB-O1B	4.58	1.53	1.46
3	E	801	AN2	PB-O1B	4.56	1.53	1.46
3	B	801	AN2	PB-O2B	-3.36	1.47	1.56
3	E	801	AN2	PB-O2B	-3.33	1.48	1.56
3	F	801	AN2	PB-O2B	-3.27	1.48	1.56
2	C	801	ANP	PG-O1G	2.20	1.49	1.46
2	A	801	ANP	PG-O1G	2.14	1.49	1.46
2	D	801	ANP	PG-O1G	2.10	1.49	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	ANP	O2B-PB-O1B	2.73	115.72	109.87
2	A	801	ANP	O2B-PB-O1B	2.70	115.65	109.87
2	D	801	ANP	O2B-PB-O1B	2.68	115.61	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	801	AN2	O2B-PB-O3A	2.28	112.26	104.64
3	E	801	AN2	O2B-PB-O3A	2.26	112.17	104.64
3	B	801	AN2	O2B-PB-O3A	2.23	112.10	104.64
3	B	801	AN2	O2B-PB-O1B	2.19	115.93	110.26
3	E	801	AN2	O2B-PB-O1B	2.13	115.77	110.26

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	ANP	PB-N3B-PG-O1G
2	A	801	ANP	PG-N3B-PB-O1B
2	A	801	ANP	PG-N3B-PB-O3A
2	A	801	ANP	C5'-O5'-PA-O1A
2	A	801	ANP	C5'-O5'-PA-O2A
2	A	801	ANP	C5'-O5'-PA-O3A
2	C	801	ANP	PB-N3B-PG-O1G
2	C	801	ANP	PG-N3B-PB-O1B
2	C	801	ANP	PG-N3B-PB-O3A
2	D	801	ANP	PB-N3B-PG-O1G
2	D	801	ANP	PG-N3B-PB-O1B
2	D	801	ANP	PG-N3B-PB-O3A
3	E	801	AN2	O4'-C4'-C5'-O5'
2	A	801	ANP	C3'-C4'-C5'-O5'
3	E	801	AN2	C3'-C4'-C5'-O5'
2	A	801	ANP	O4'-C4'-C5'-O5'
3	E	801	AN2	C4'-C5'-O5'-PA
2	C	801	ANP	O4'-C4'-C5'-O5'
3	F	801	AN2	O4'-C4'-C5'-O5'
2	C	801	ANP	C3'-C4'-C5'-O5'
2	A	801	ANP	PB-O3A-PA-O2A
3	F	801	AN2	C3'-C4'-C5'-O5'

There are no ring outliers.

5 monomers are involved in 10 short contacts:

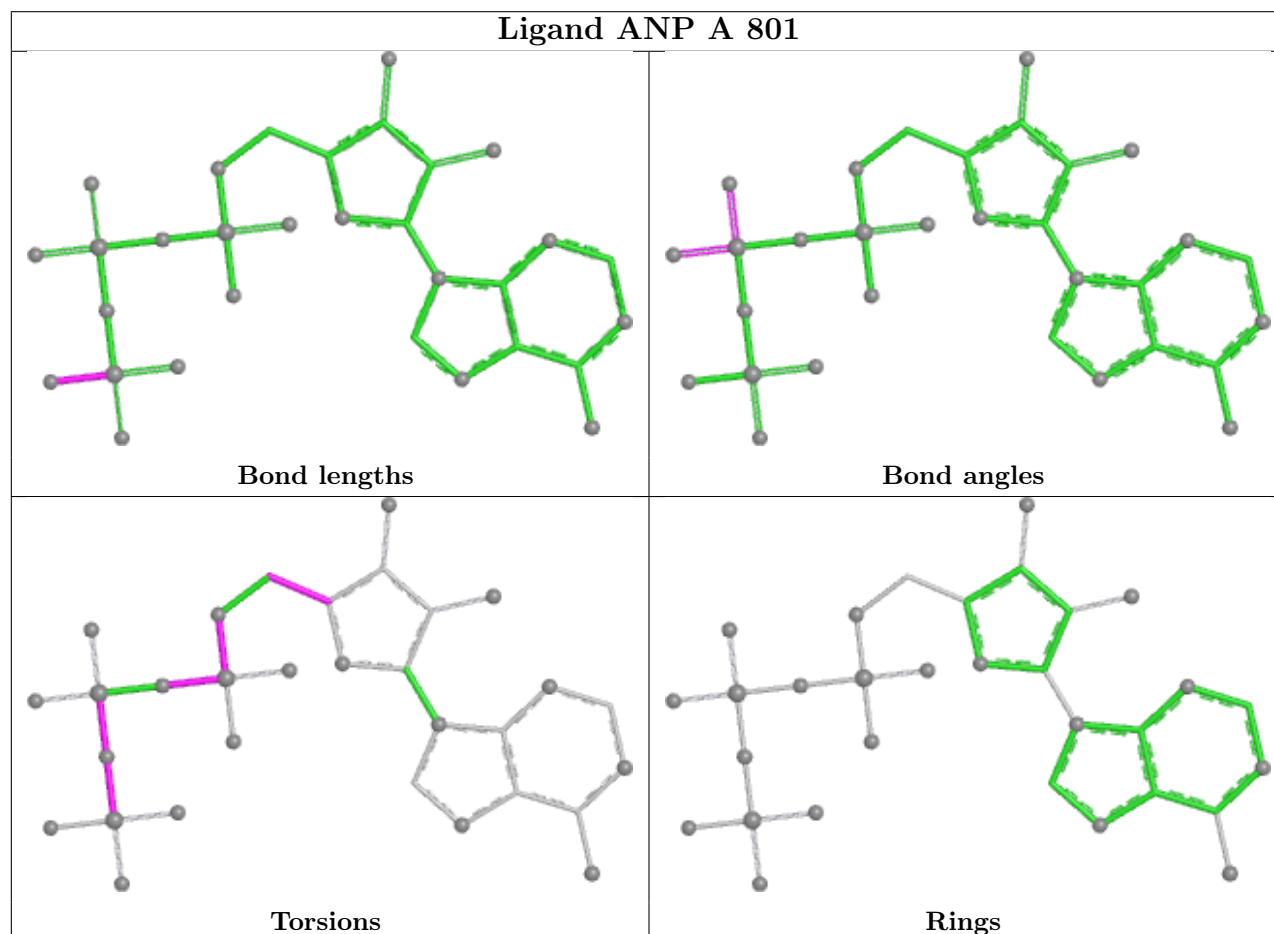
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	ANP	4	0
2	C	801	ANP	1	0
3	B	801	AN2	3	0
3	F	801	AN2	1	0

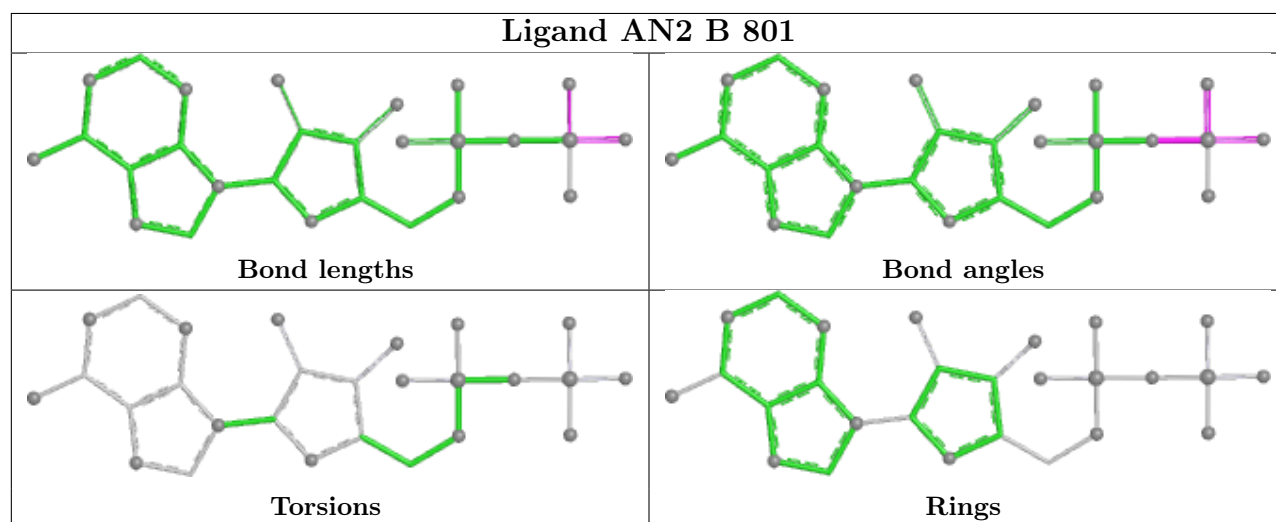
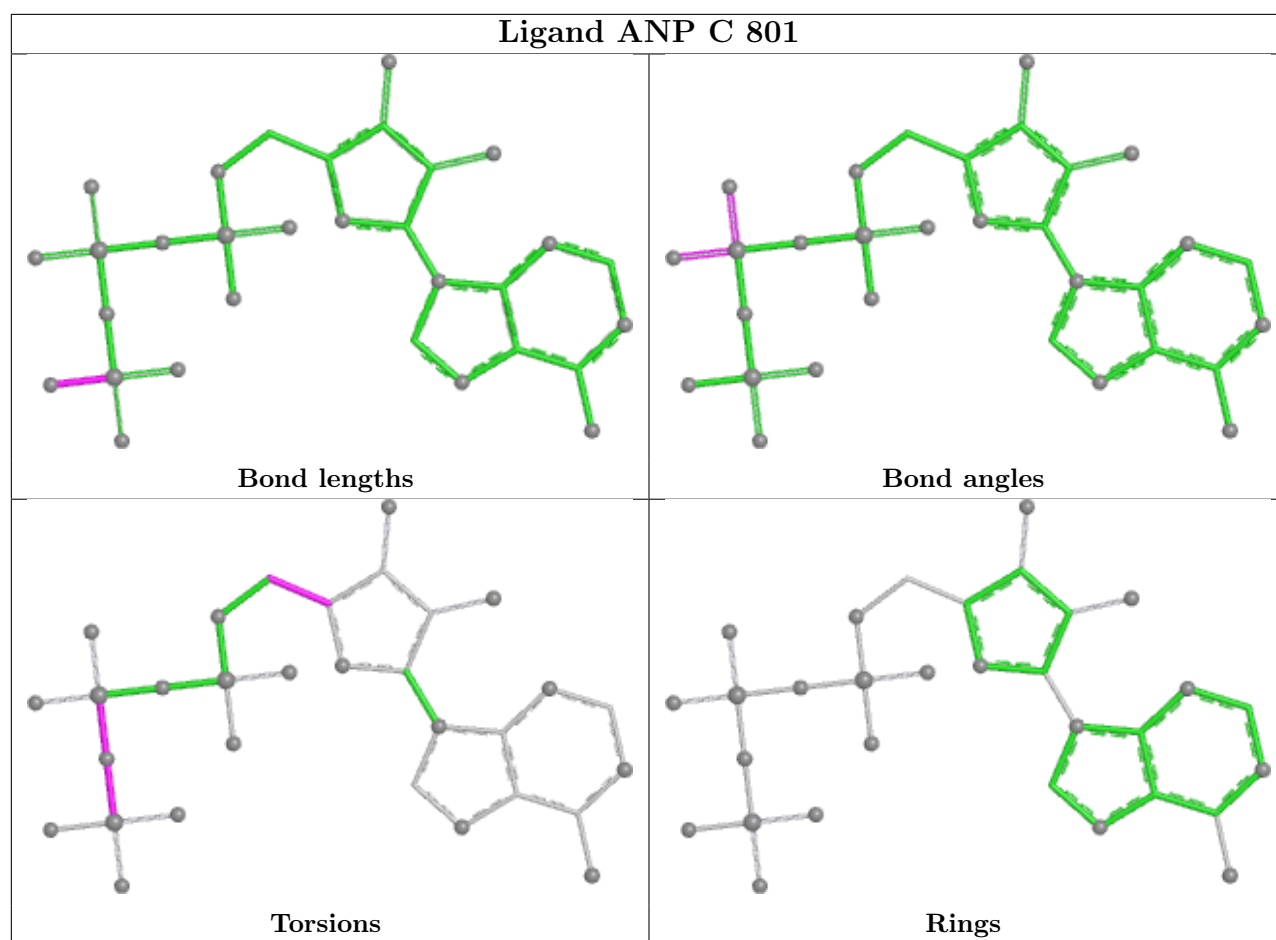
Continued on next page...

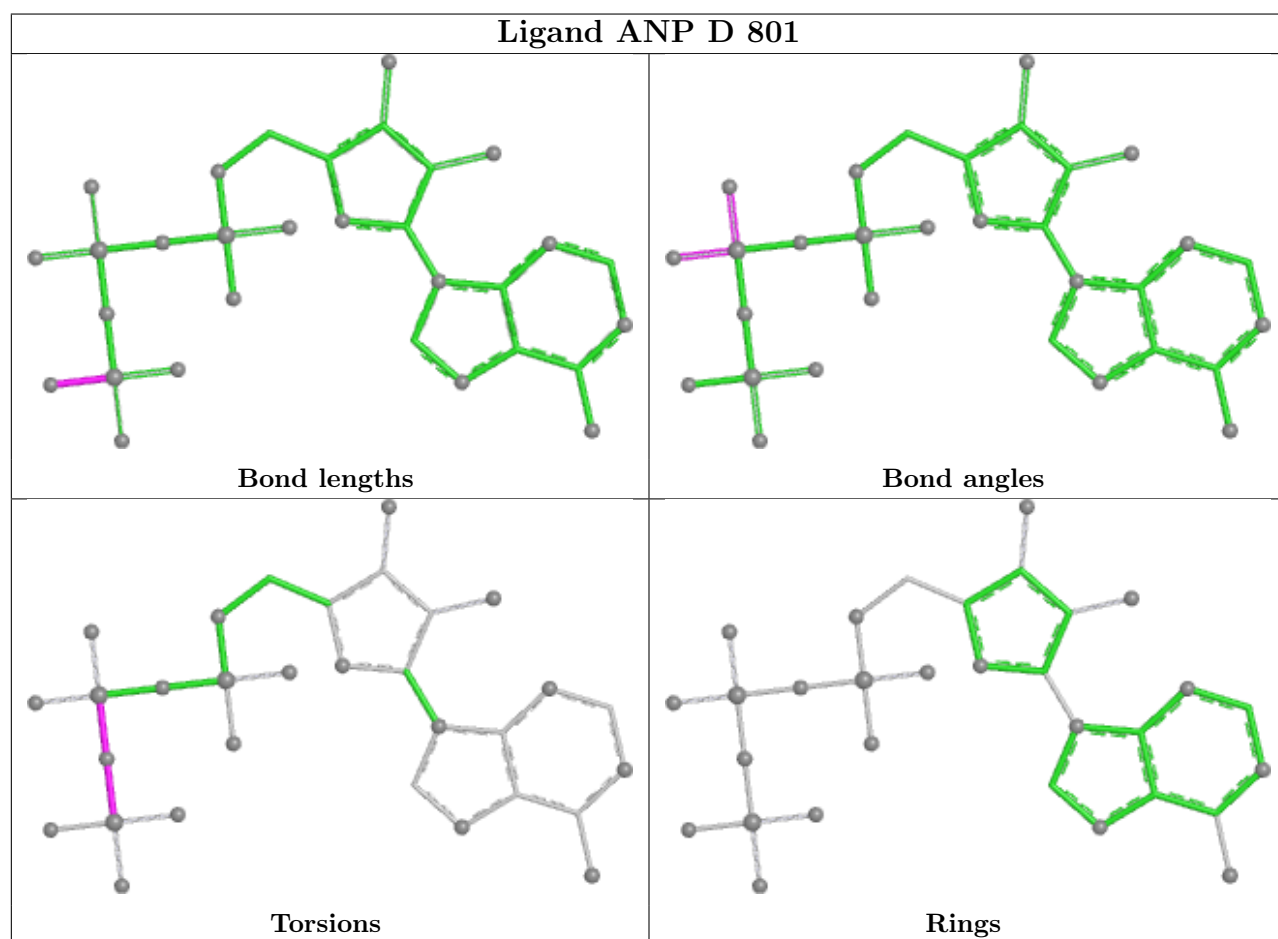
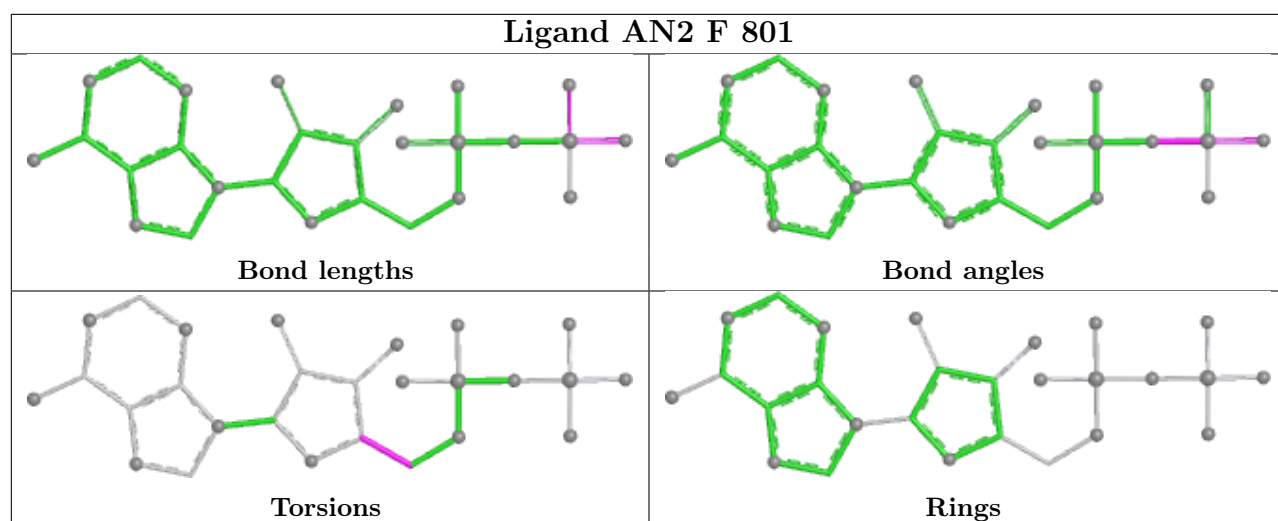
Continued from previous page...

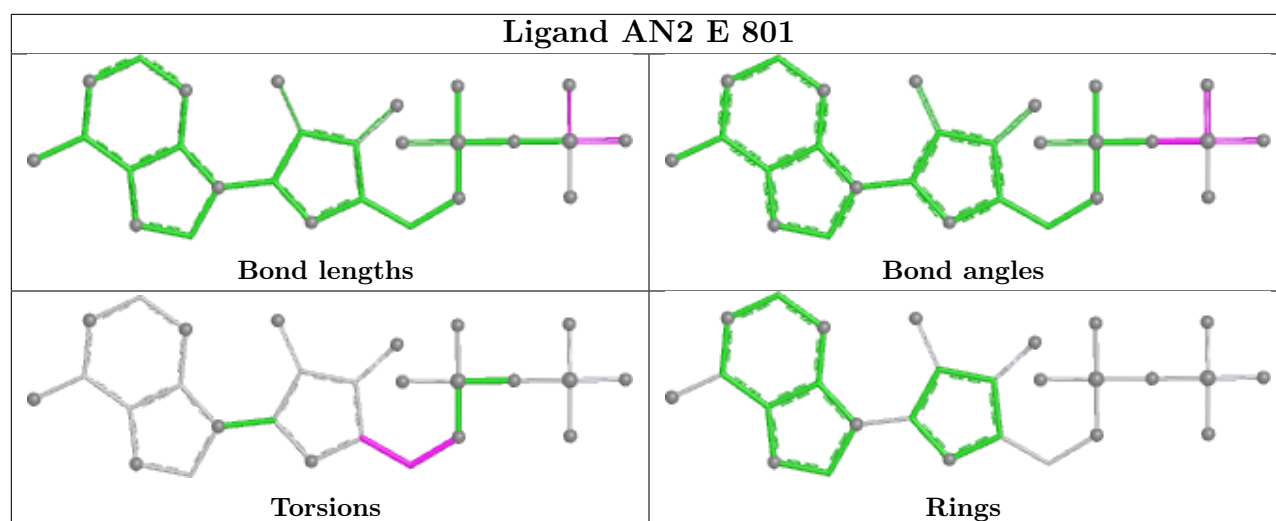
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	801	AN2	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

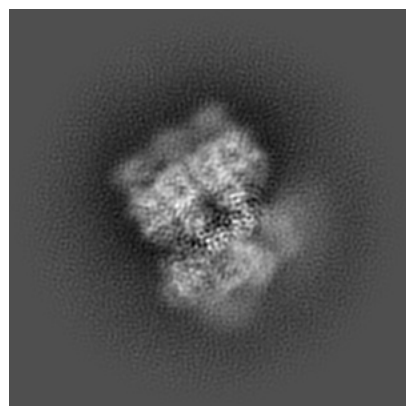
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38394. These allow visual inspection of the internal detail of the map and identification of artifacts.

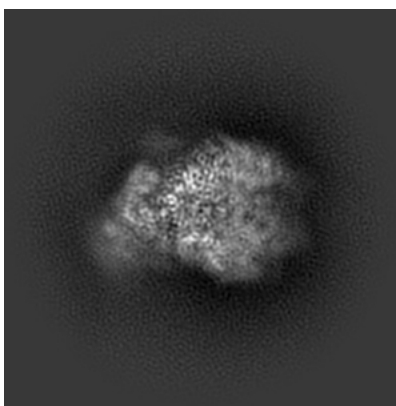
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

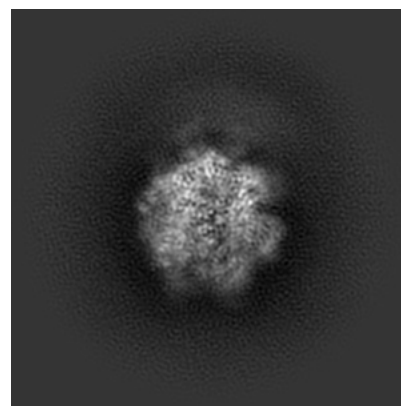
6.1.1 Primary map



X

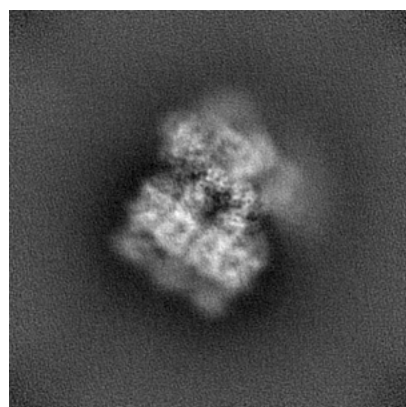


Y

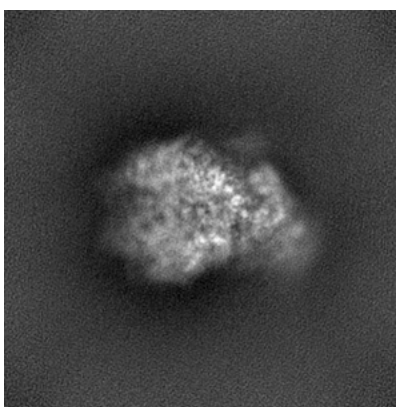


Z

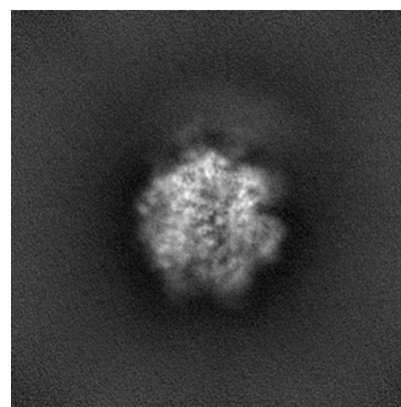
6.1.2 Raw map



X



Y

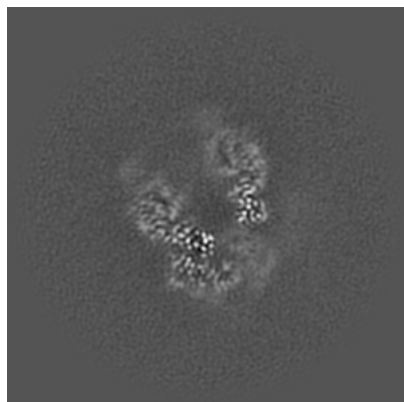


Z

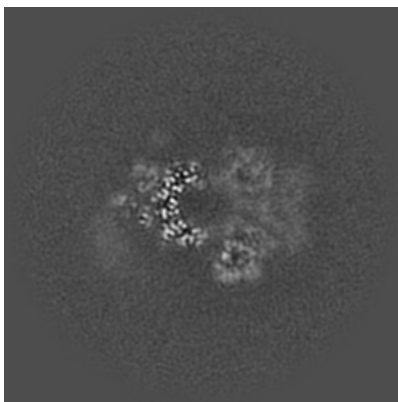
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

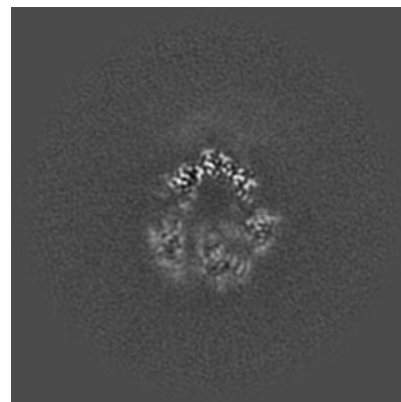
6.2.1 Primary map



X Index: 140

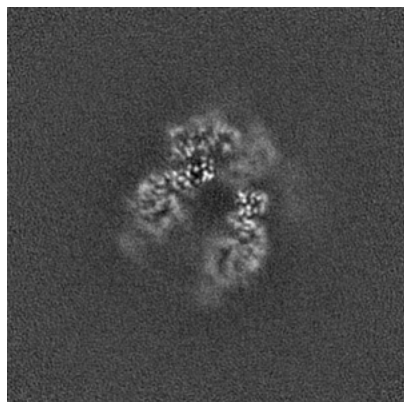


Y Index: 140

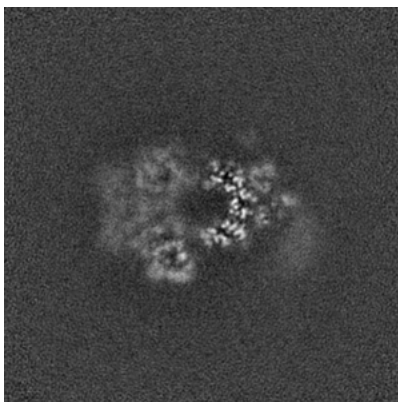


Z Index: 140

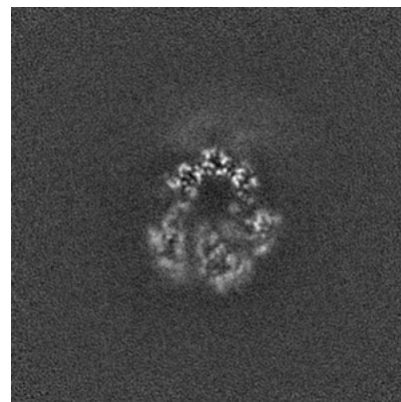
6.2.2 Raw map



X Index: 140



Y Index: 140

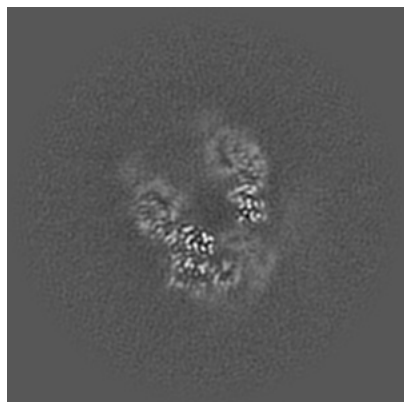


Z Index: 140

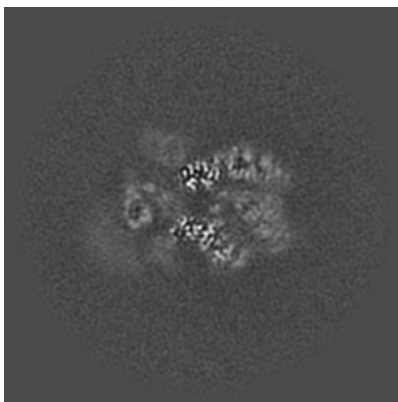
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

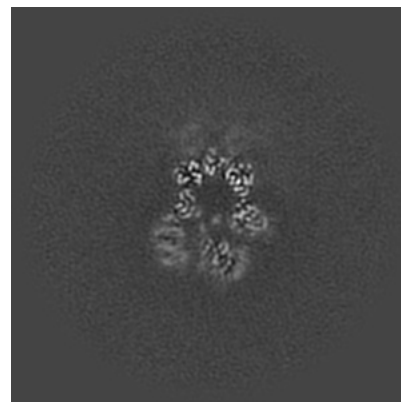
6.3.1 Primary map



X Index: 139

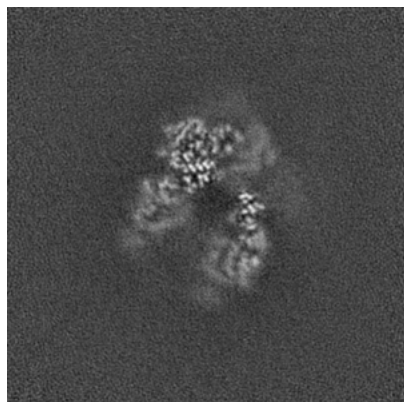


Y Index: 156

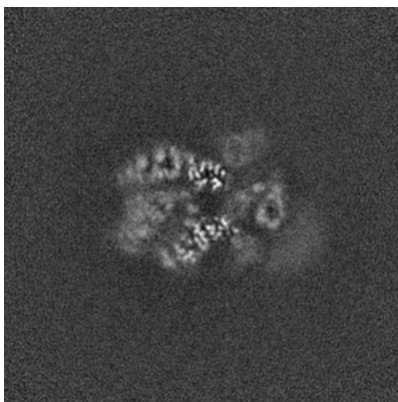


Z Index: 131

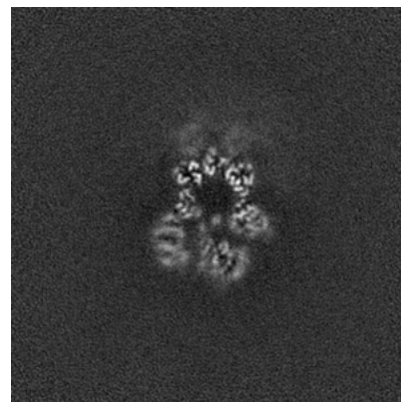
6.3.2 Raw map



X Index: 136



Y Index: 156

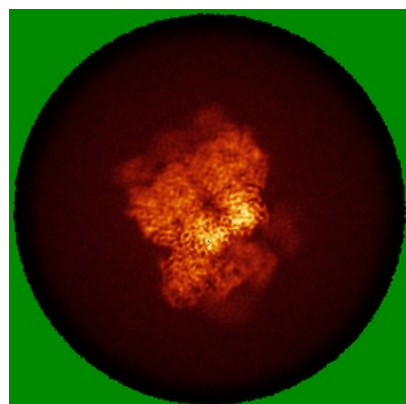


Z Index: 148

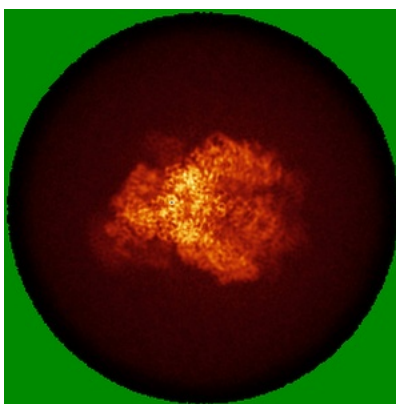
The images above show the largest variance slices of the map in three orthogonal directions.

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

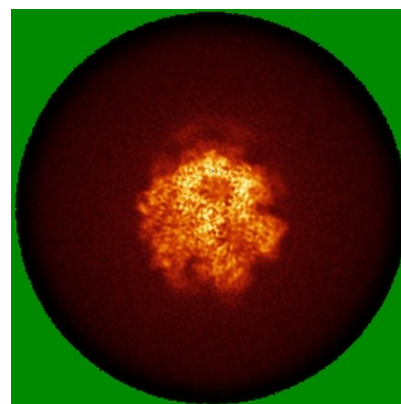
6.4.1 Primary map



X

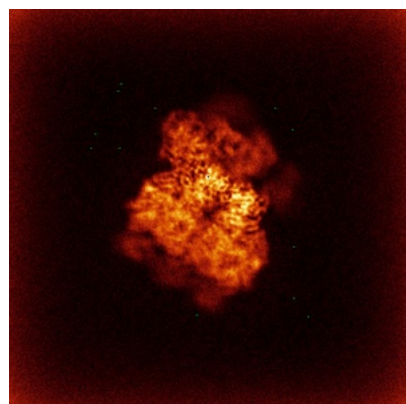


Y

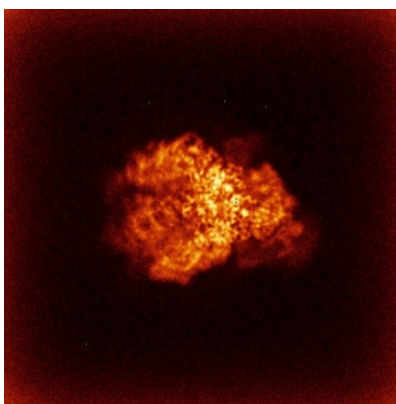


Z

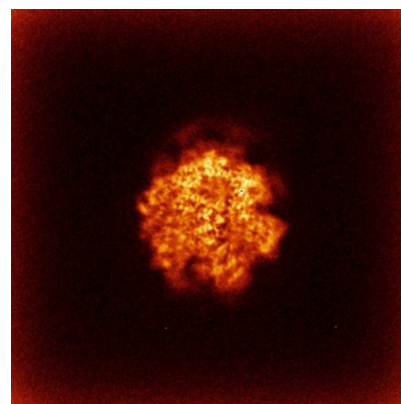
6.4.2 Raw map



X



Y



Z

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

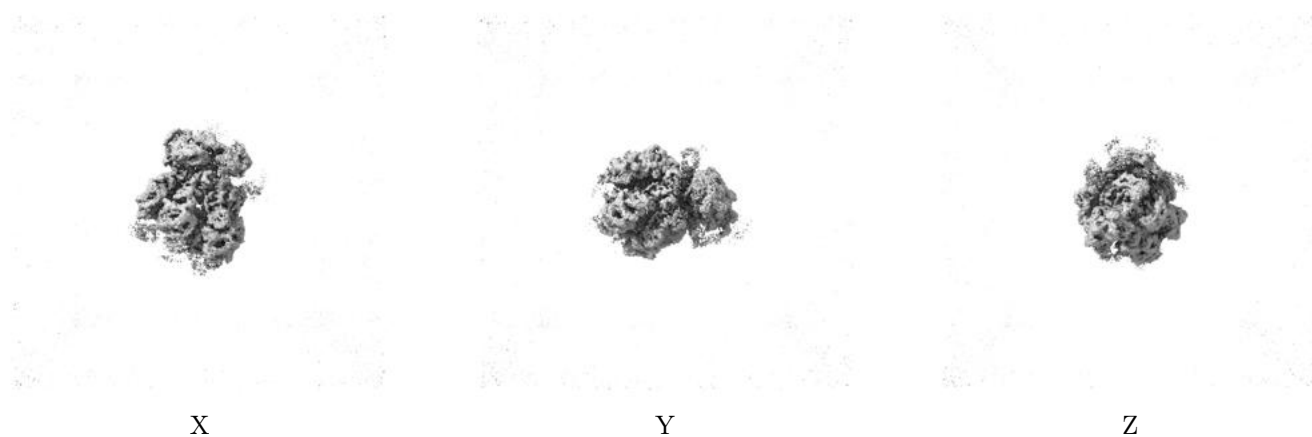
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.336. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

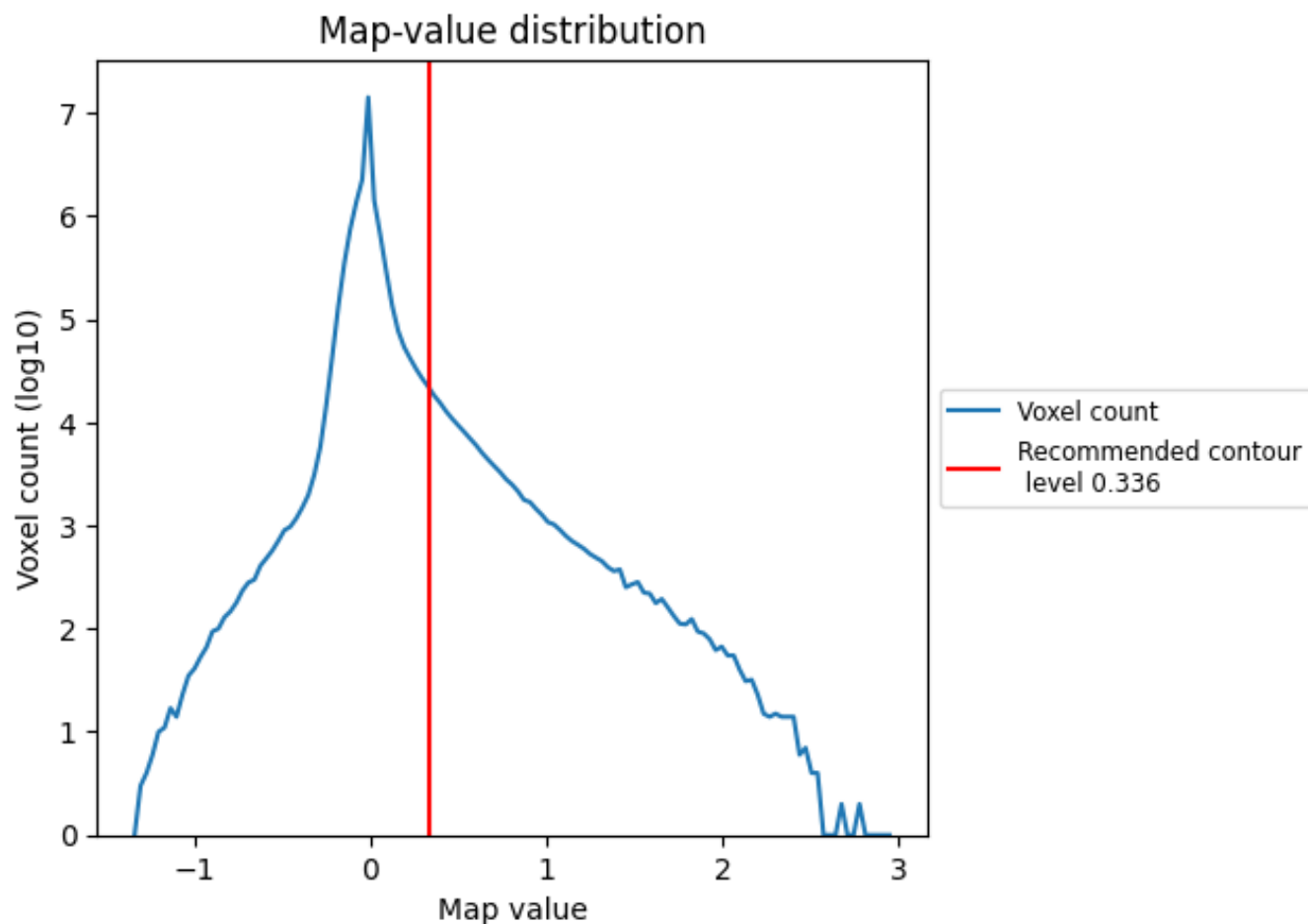
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

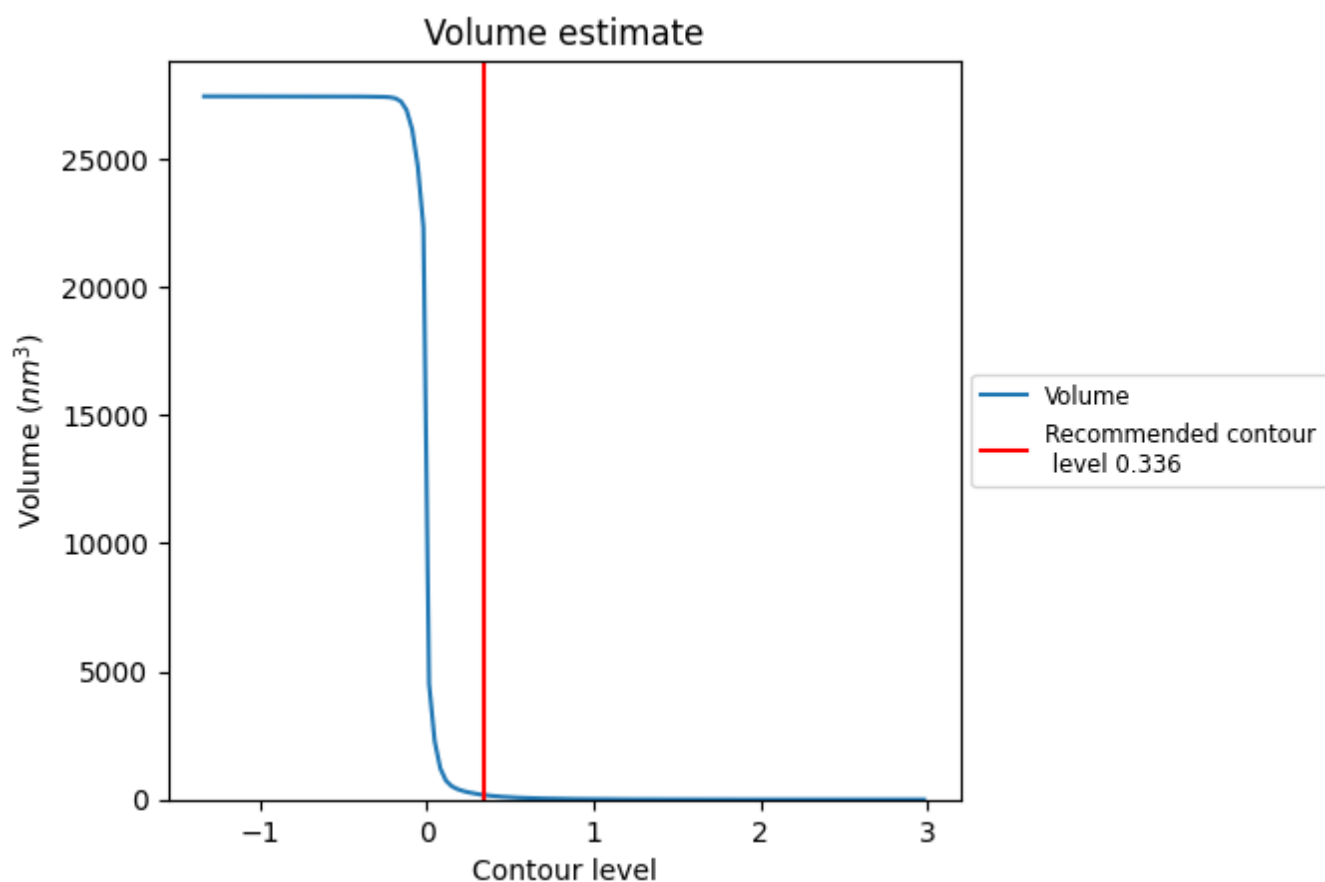
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

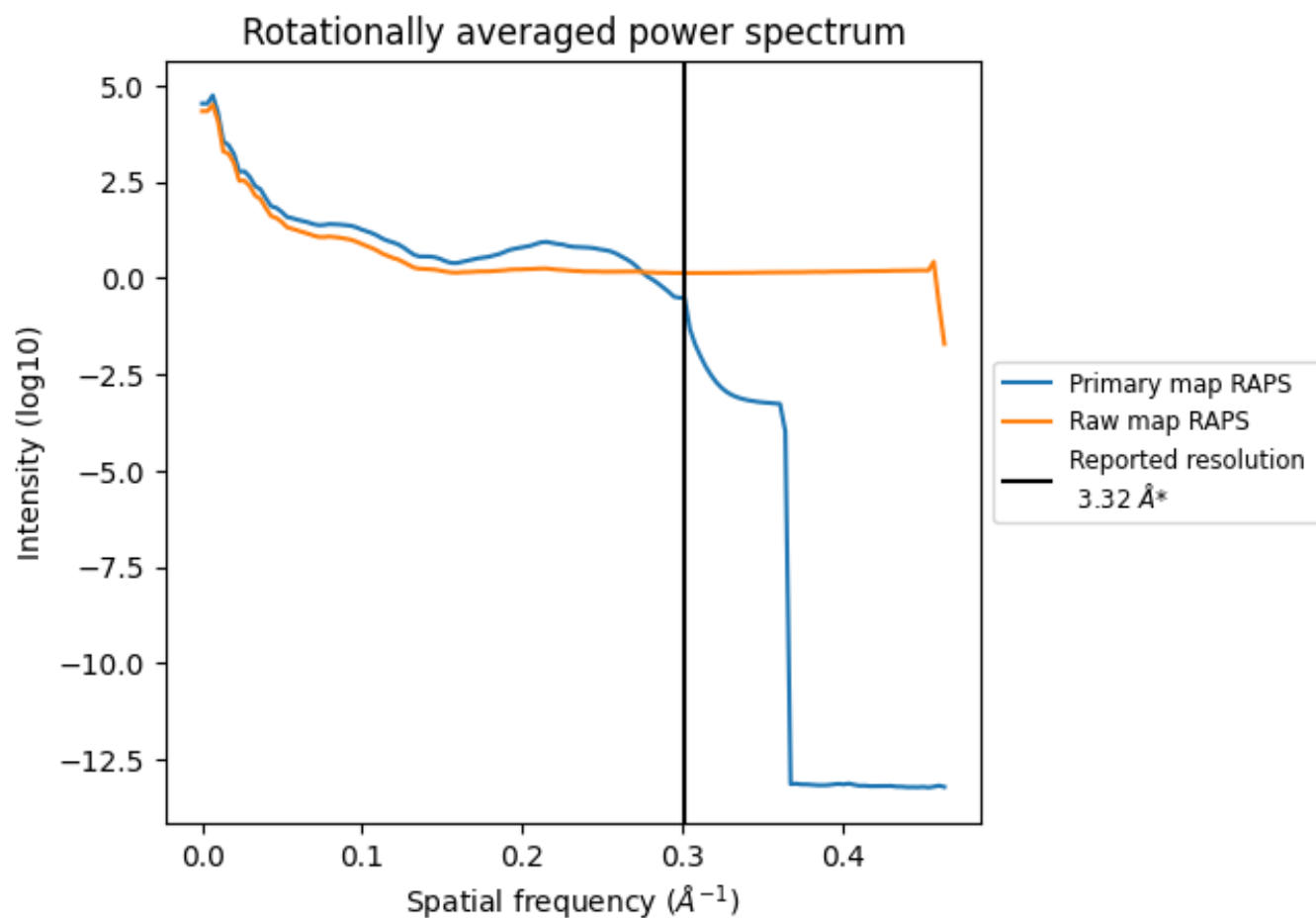
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 184 nm³; this corresponds to an approximate mass of 166 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 ⓘ

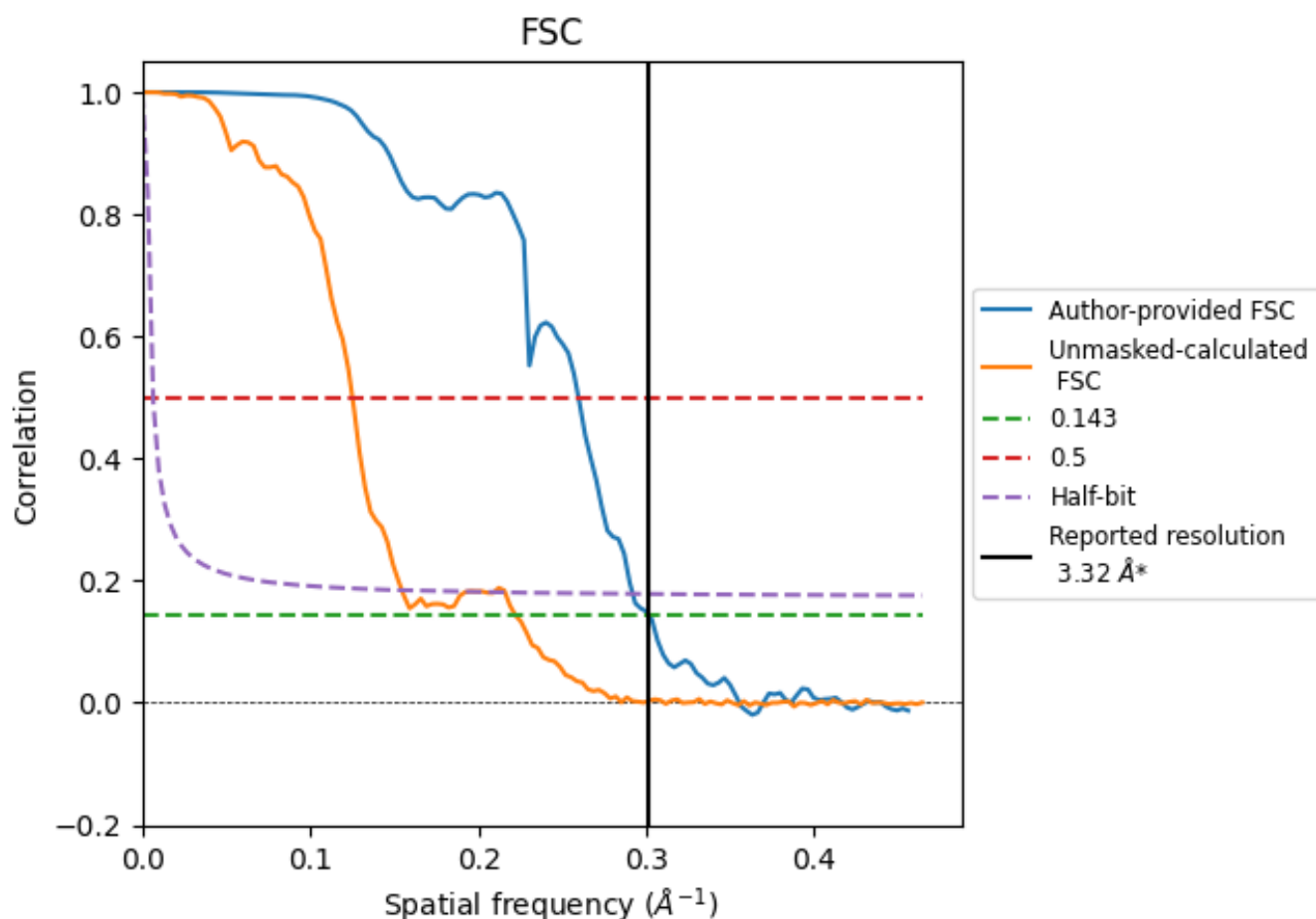


*Reported resolution corresponds to spatial frequency of 0.301 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.301 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

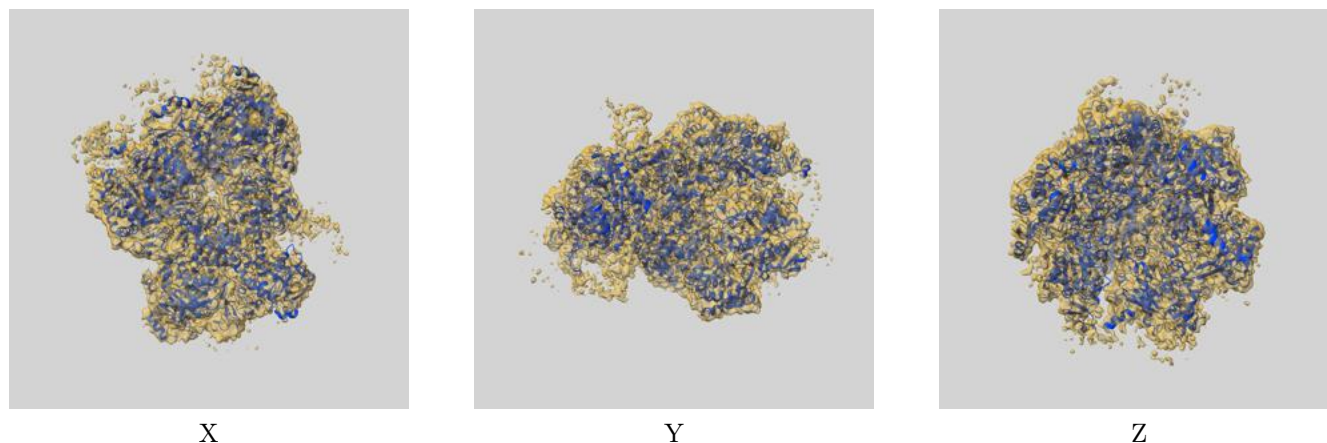
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.32	-	-
Author-provided FSC curve	3.31	3.85	3.43
Unmasked-calculated*	4.50	8.00	6.47

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.50 differs from the reported value 3.32 by more than 10 %

9 Map-model fit [i](#)

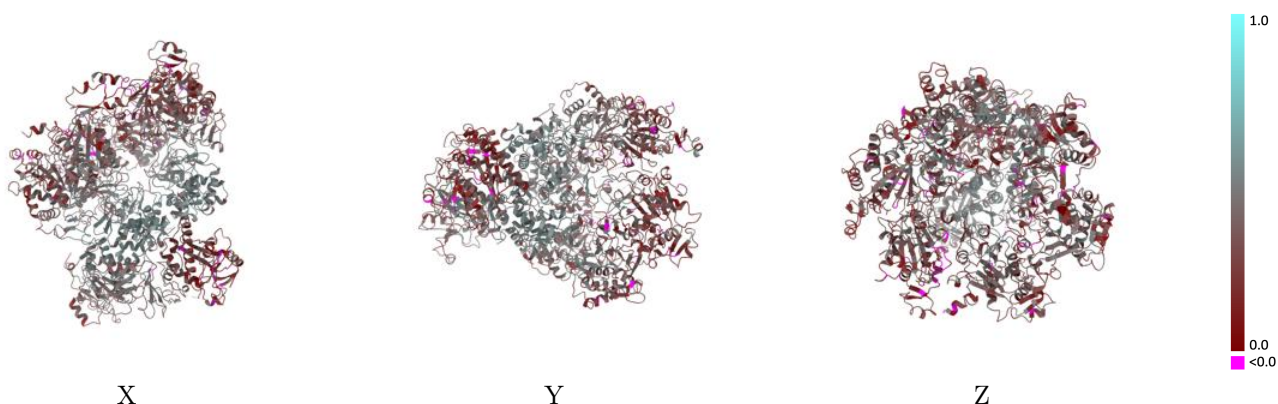
This section contains information regarding the fit between EMDB map EMD-38394 and PDB model 8XJ6. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



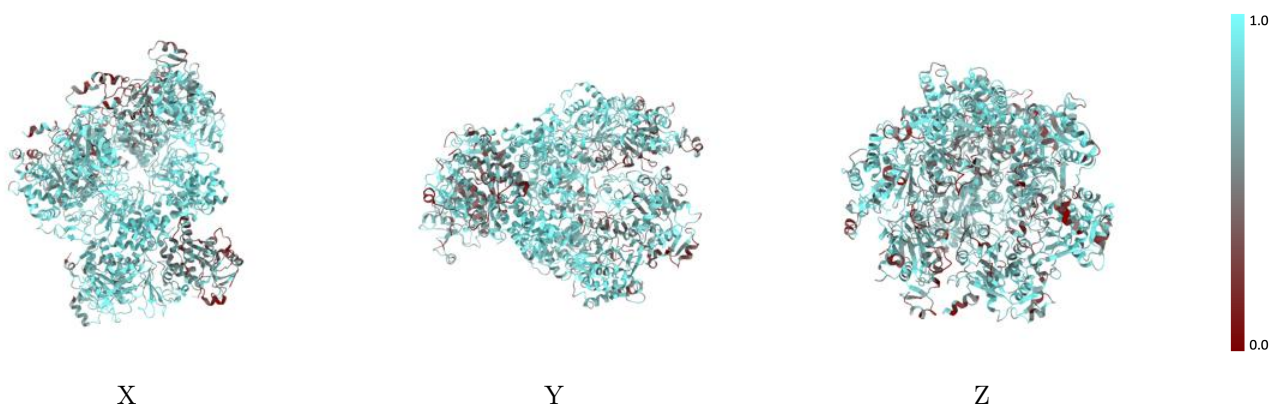
The images above show the 3D surface view of the map at the recommended contour level 0.336 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



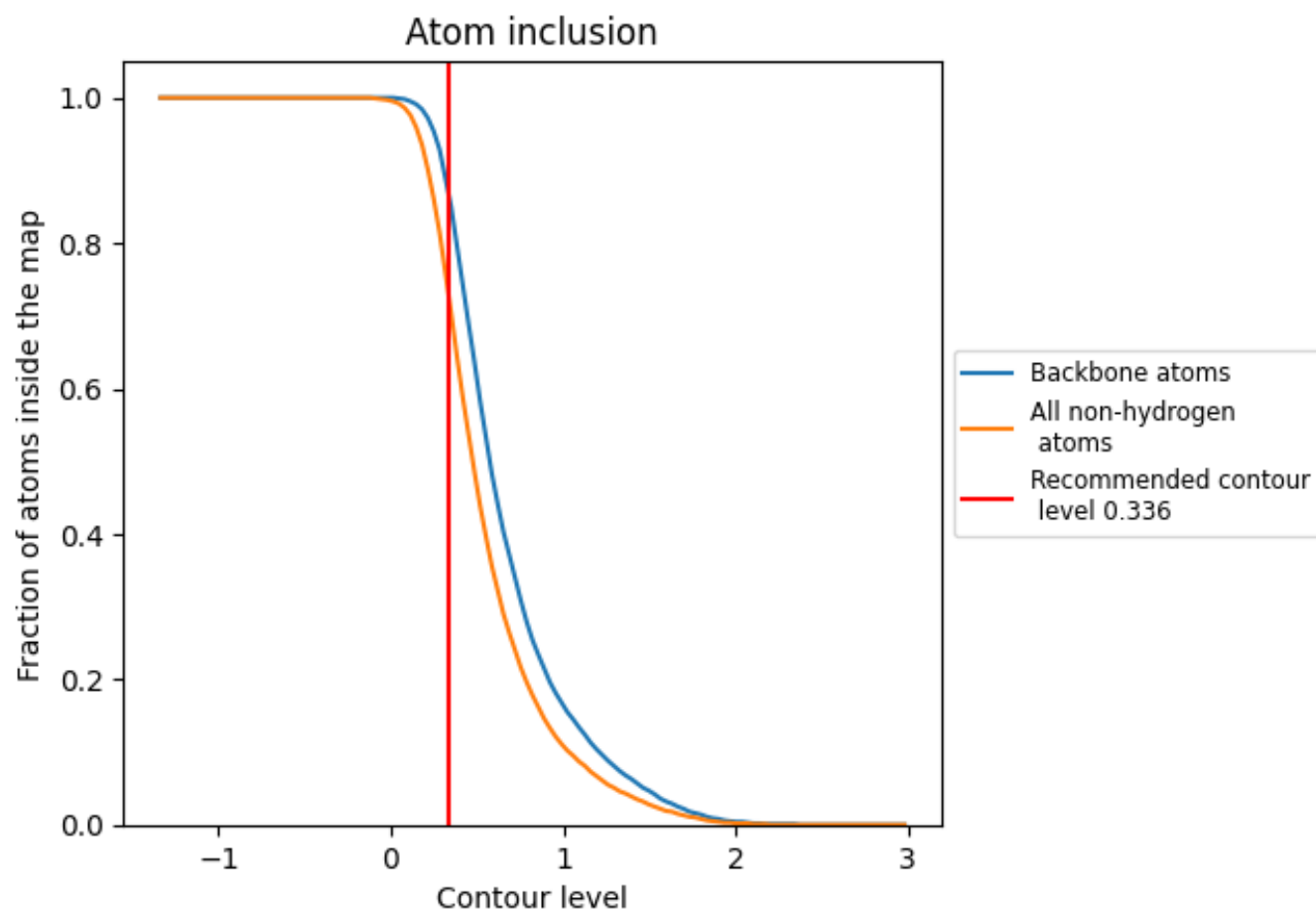
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.336).

9.4 Atom inclusion ⓘ



At the recommended contour level, 87% of all backbone atoms, 73% 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 (0.336) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7270	0.3620
A	0.7200	0.3540
B	0.7200	0.3420
C	0.7500	0.3680
D	0.7350	0.3720
E	0.7760	0.3970
F	0.6800	0.3380

1.0

0.0

<0.0