



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 07:53 AM UTC

PDB ID : 9DH3 / pdb_00009dh3
EMDB ID : EMD-46855
Title : Cryo-EM structure of NLRP3 complex with Compound C
Authors : Matico, R.; Grauwen, K.; Van Gool, M.; Muratore, E.M.; Yu, X.; Abdiaj, I.; Adhikary, S.; Adriaensen, I.; Aranzazu, G.M.; Alcazar, J.; Bassi, M.; Brisse, E.; Canellas, S.; Chaudhuri, S.; Chauhan, D.; Delgado, F.; Dieguez-Vazquez, A.; Du Jardin, M.; Eastham, V.; Finley, M.; Jacobs, T.; Keustermans, K.; Kuhn, R.; Llaveria, J.; Leenaerts, J.; Linares, M.L.; Martin, M.L.; Martinez, C.; Miller, R.; Munoz, F.M.; Nooyens, A.; Perez, L.B.; Perrier, M.; Pietrak, B.; Serre, J.; Sharma, S.; Somers, M.; Suarez, J.; Tresadern, G.; Trabanco, A.A.; Van den Bulck, D.; Van Hauwermeiren, F.; Varghese, T.; Vega, J.A.; Youssef, S.A.; Edwards, M.J.; Oehlich, D.; Van Opdenbosch, N.
Deposited on : 2024-09-03
Resolution : 3.76 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)

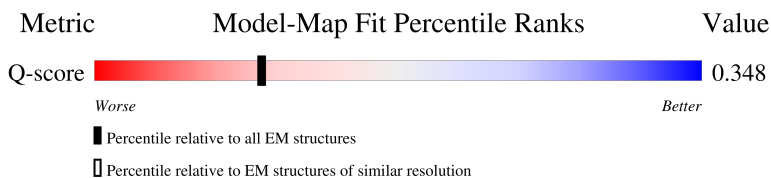
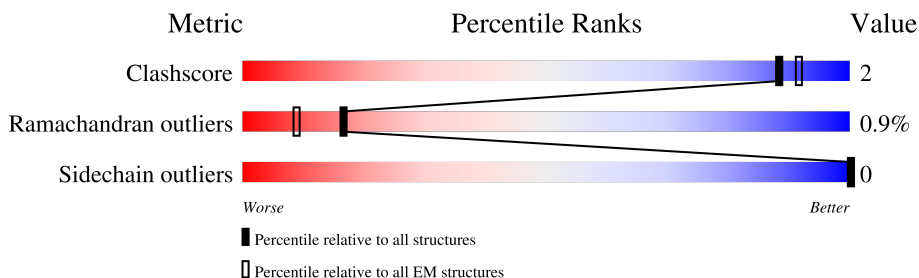
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.76 Å.

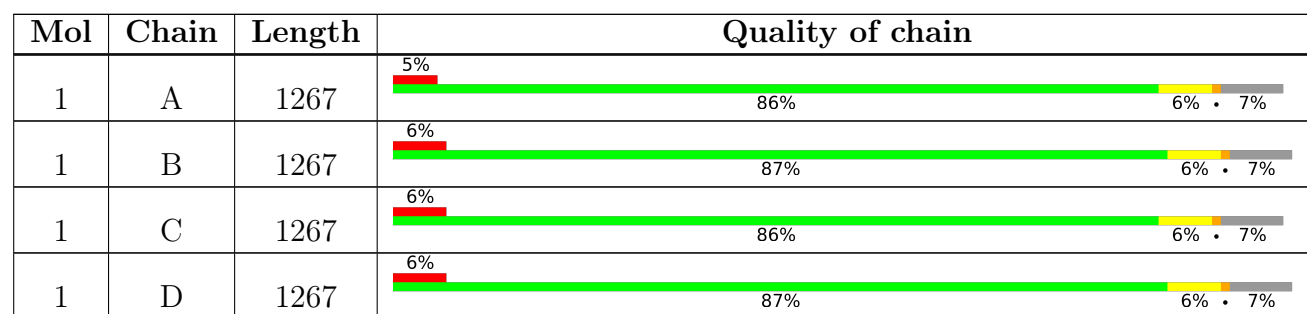
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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	10214 (3.26 - 4.26)

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.

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



2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 37752 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.

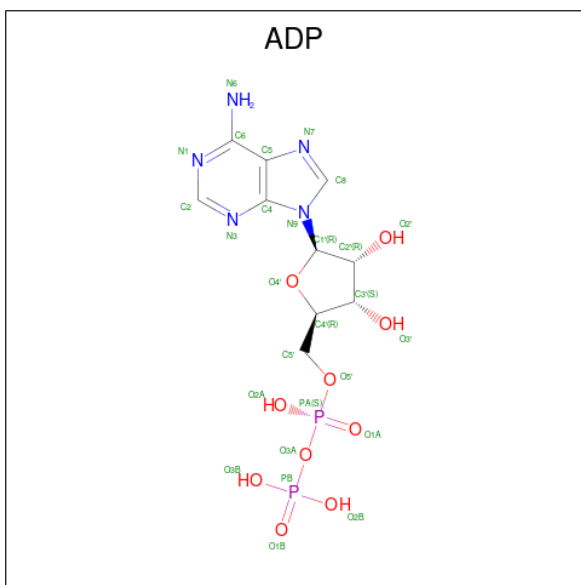
- Molecule 1 is a protein called Maltose/maltodextrin-binding periplasmic protein,NACHT, LRR and PYD domains-containing protein 3 chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1181	Total	C	N	O	S	0	0
			9344	5979	1561	1742	62		
1	B	1181	Total	C	N	O	S	0	0
			9344	5979	1561	1742	62		
1	C	1181	Total	C	N	O	S	0	0
			9344	5979	1561	1742	62		
1	D	1181	Total	C	N	O	S	0	0
			9344	5979	1561	1742	62		

There are 4 discrepancies between the modelled and reference sequences:

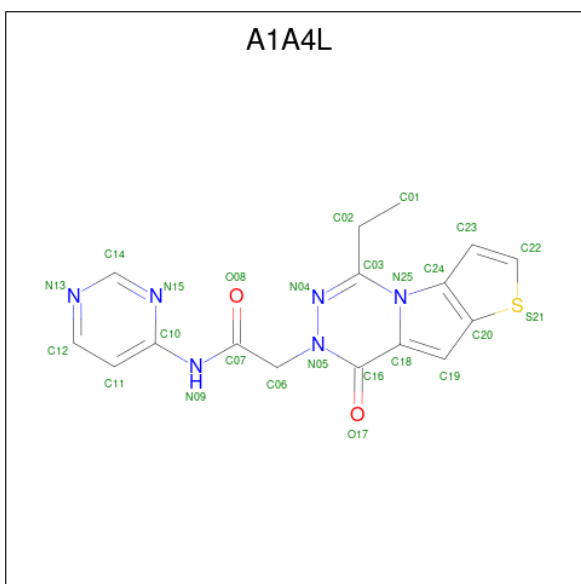
Chain	Residue	Modelled	Actual	Comment	Reference
A	81	VAL	ALA	conflict	UNP P0AEX9
B	81	VAL	ALA	conflict	UNP P0AEX9
C	81	VAL	ALA	conflict	UNP P0AEX9
D	81	VAL	ALA	conflict	UNP P0AEX9

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



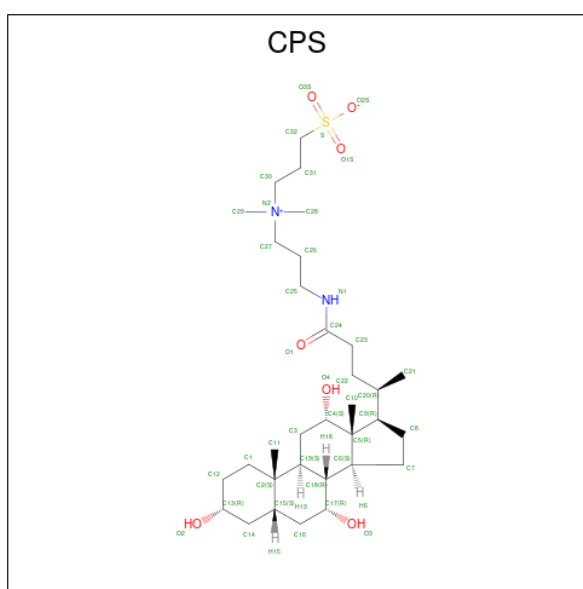
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 3 is 2-[(4S)-5-ethyl-8-oxothieno[2',3':4,5]pyrrolo[1,2-d][1,2,4]triazin-7(8H)-yl]-N-(p-ymidin-4-yl)acetamide (CCD ID: A1A4L) (formula: C₁₆H₁₄N₆O₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	S	0
			25	16	6	2	1	
3	B	1	Total	C	N	O	S	0
			25	16	6	2	1	
3	C	1	Total	C	N	O	S	0
			25	16	6	2	1	
3	D	1	Total	C	N	O	S	0
			25	16	6	2	1	

- Molecule 4 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFO NATE (CCD ID: CPS) (formula: $C_{32}H_{58}N_2O_7S$).

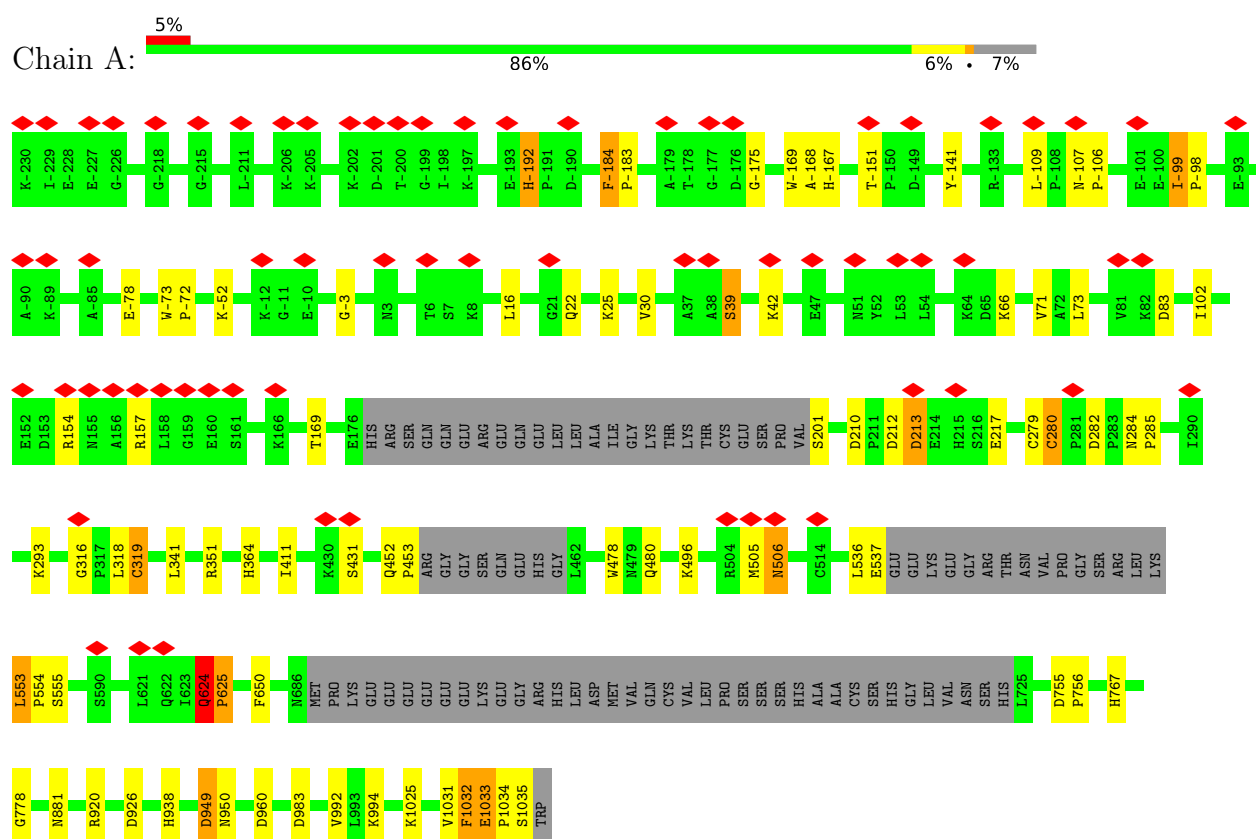


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	S	0
			42	32	2	7	1	
4	B	1	Total	C	N	O	S	0
			42	32	2	7	1	
4	C	1	Total	C	N	O	S	0
			42	32	2	7	1	
4	D	1	Total	C	N	O	S	0
			42	32	2	7	1	

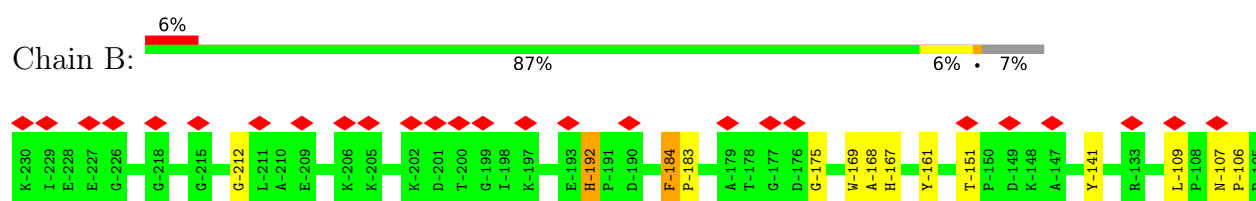
3 Residue-property plots

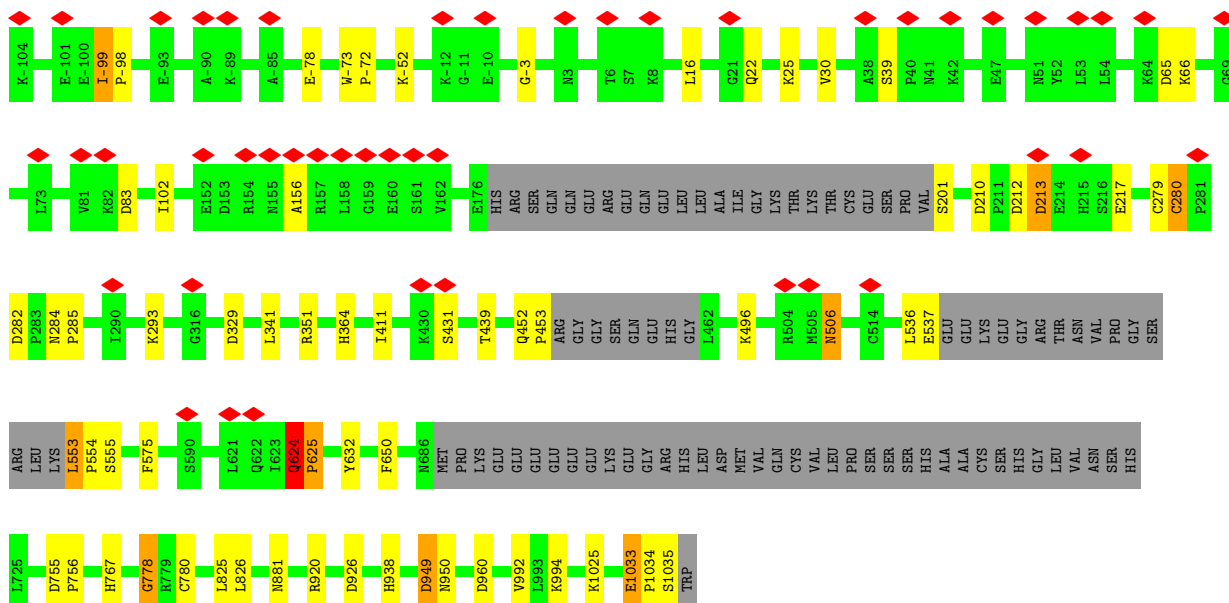
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Maltose/maltodextrin-binding periplasmic protein,NACHT, LRR and PYD domains-containing protein 3 chimera

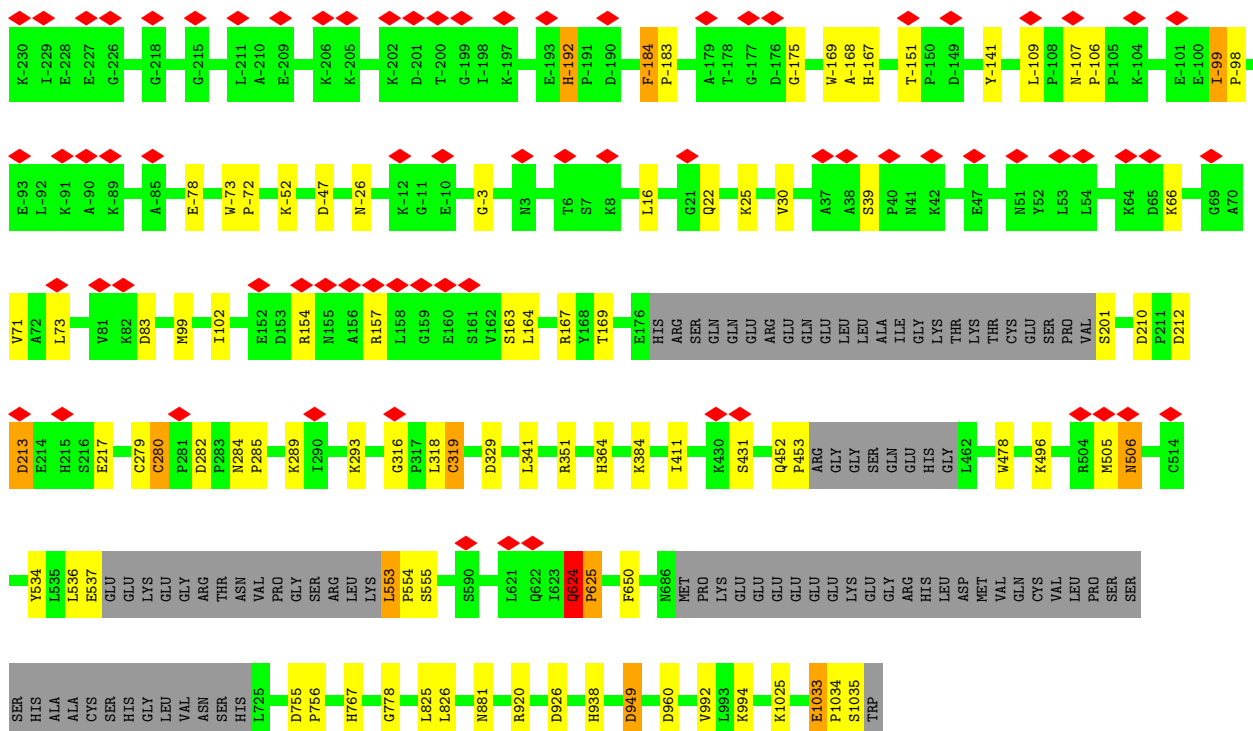
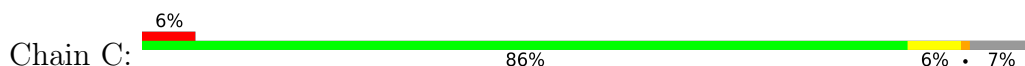


- Molecule 1: Maltose/maltodextrin-binding periplasmic protein,NACHT, LRR and PYD domains-containing protein 3 chimera

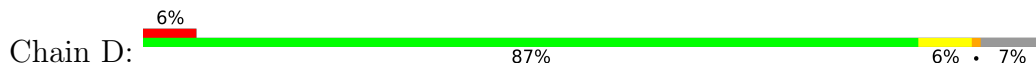


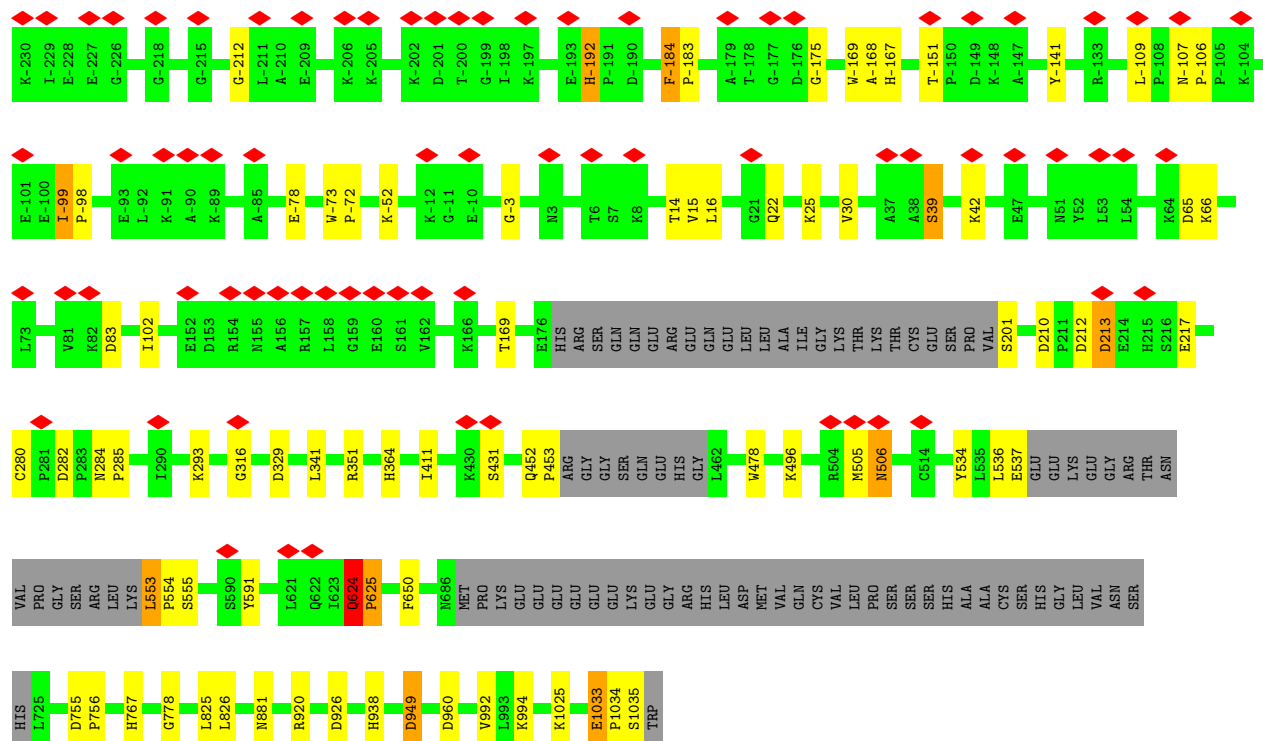


- Molecule 1: Maltose/maltodextrin-binding periplasmic protein,NACHT, LRR and PYD domains-containing protein 3 chimera



- Molecule 1: Maltose/maltodextrin-binding periplasmic protein,NACHT, LRR and PYD domains-containing protein 3 chimera





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	94472	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 ($e^-/\text{\AA}^2$)	44.57	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.112	Depositor
Minimum map value	-0.059	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	312.0, 312.0, 312.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1A4L, ADP, CPS

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	0.65	0/9535	0.91	76/12887 (0.6%)
1	B	0.66	0/9535	0.92	75/12887 (0.6%)
1	C	0.65	0/9535	0.92	80/12887 (0.6%)
1	D	0.65	0/9535	0.91	76/12887 (0.6%)
All	All	0.65	0/38140	0.92	307/51548 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (307) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	-107	ASN	CA-C-N	9.47	126.57	119.66
1	A	-107	ASN	C-N-CA	9.47	126.57	119.66
1	B	-107	ASN	CA-C-N	9.41	126.53	119.66
1	B	-107	ASN	C-N-CA	9.41	126.53	119.66
1	D	-107	ASN	CA-C-N	9.38	126.51	119.66
1	D	-107	ASN	C-N-CA	9.38	126.51	119.66
1	C	-107	ASN	CA-C-N	9.37	126.50	119.66
1	C	-107	ASN	C-N-CA	9.37	126.50	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	-175	GLY	CA-C-N	7.78	127.94	120.31
1	C	-175	GLY	C-N-CA	7.78	127.94	120.31
1	D	217	GLU	CA-C-N	7.72	127.67	120.03
1	D	217	GLU	C-N-CA	7.72	127.67	120.03
1	C	-141	TYR	CA-C-N	7.65	127.83	119.87
1	C	-141	TYR	C-N-CA	7.65	127.83	119.87
1	B	-175	GLY	CA-C-N	7.64	128.09	120.52
1	B	-175	GLY	C-N-CA	7.64	128.09	120.52
1	A	-175	GLY	CA-C-N	7.64	127.80	120.31
1	A	-175	GLY	C-N-CA	7.64	127.80	120.31
1	D	83	ASP	CA-C-N	7.58	127.30	119.56
1	D	83	ASP	C-N-CA	7.58	127.30	119.56
1	B	83	ASP	CA-C-N	7.55	127.26	119.56
1	B	83	ASP	C-N-CA	7.55	127.26	119.56
1	B	575	PHE	CA-CB-CG	-7.50	106.30	113.80
1	B	-141	TYR	CA-C-N	7.48	127.65	119.87
1	B	-141	TYR	C-N-CA	7.48	127.65	119.87
1	A	-141	TYR	CA-C-N	7.46	127.63	119.87
1	A	-141	TYR	C-N-CA	7.46	127.63	119.87
1	B	217	GLU	CA-C-N	7.45	127.41	120.03
1	B	217	GLU	C-N-CA	7.45	127.41	120.03
1	D	1025	LYS	CA-C-N	7.45	127.09	119.56
1	D	1025	LYS	C-N-CA	7.45	127.09	119.56
1	D	-175	GLY	CA-C-N	7.42	127.58	120.31
1	D	-175	GLY	C-N-CA	7.42	127.58	120.31
1	C	1025	LYS	CA-C-N	7.40	127.04	119.56
1	C	1025	LYS	C-N-CA	7.40	127.04	119.56
1	D	-3	GLY	CA-C-N	7.38	127.09	119.56
1	D	-3	GLY	C-N-CA	7.38	127.09	119.56
1	B	1025	LYS	CA-C-N	7.38	127.02	119.56
1	B	1025	LYS	C-N-CA	7.38	127.02	119.56
1	A	-3	GLY	CA-C-N	7.32	127.02	119.56
1	A	-3	GLY	C-N-CA	7.32	127.02	119.56
1	B	-3	GLY	CA-C-N	7.29	126.99	119.56
1	B	-3	GLY	C-N-CA	7.29	126.99	119.56
1	C	-3	GLY	CA-C-N	7.29	126.99	119.56
1	C	-3	GLY	C-N-CA	7.29	126.99	119.56
1	D	-141	TYR	CA-C-N	7.11	127.27	119.87
1	D	-141	TYR	C-N-CA	7.11	127.27	119.87
1	A	282	ASP	CA-C-N	7.10	127.25	119.87
1	A	282	ASP	C-N-CA	7.10	127.25	119.87
1	A	280	CYS	CA-C-N	7.09	126.80	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CYS	C-N-CA	7.09	126.80	119.56
1	A	1025	LYS	CA-C-N	7.08	126.71	119.56
1	A	1025	LYS	C-N-CA	7.08	126.71	119.56
1	A	217	GLU	CA-C-N	7.06	127.23	120.31
1	A	217	GLU	C-N-CA	7.06	127.23	120.31
1	C	217	GLU	CA-C-N	7.06	127.23	120.31
1	C	217	GLU	C-N-CA	7.06	127.23	120.31
1	B	280	CYS	CA-C-N	7.02	126.72	119.56
1	B	280	CYS	C-N-CA	7.02	126.72	119.56
1	C	280	CYS	CA-C-N	7.02	126.72	119.56
1	C	280	CYS	C-N-CA	7.02	126.72	119.56
1	B	282	ASP	CA-C-N	6.93	127.08	119.87
1	B	282	ASP	C-N-CA	6.93	127.08	119.87
1	C	553	LEU	CA-C-N	6.90	126.42	119.24
1	C	553	LEU	C-N-CA	6.90	126.42	119.24
1	C	364	HIS	CA-C-N	6.84	127.01	120.31
1	C	364	HIS	C-N-CA	6.84	127.01	120.31
1	C	282	ASP	CA-C-N	6.83	126.97	119.87
1	C	282	ASP	C-N-CA	6.83	126.97	119.87
1	A	-78	GLU	CA-C-N	6.83	127.39	119.47
1	A	-78	GLU	C-N-CA	6.83	127.39	119.47
1	C	102	ILE	CA-C-N	6.82	126.52	119.56
1	C	102	ILE	C-N-CA	6.82	126.52	119.56
1	B	102	ILE	CA-C-N	6.79	126.48	119.56
1	B	102	ILE	C-N-CA	6.79	126.48	119.56
1	D	282	ASP	CA-C-N	6.78	126.92	119.87
1	D	282	ASP	C-N-CA	6.78	126.92	119.87
1	B	-106	PRO	CA-C-N	6.77	126.69	119.85
1	B	-106	PRO	C-N-CA	6.77	126.69	119.85
1	A	102	ILE	CA-C-N	6.76	126.45	119.56
1	A	102	ILE	C-N-CA	6.76	126.45	119.56
1	C	-106	PRO	CA-C-N	6.75	126.67	119.85
1	C	-106	PRO	C-N-CA	6.75	126.67	119.85
1	D	102	ILE	CA-C-N	6.75	126.44	119.56
1	D	102	ILE	C-N-CA	6.75	126.44	119.56
1	D	280	CYS	CA-C-N	6.71	126.41	119.56
1	D	280	CYS	C-N-CA	6.71	126.41	119.56
1	A	-106	PRO	CA-C-N	6.71	126.62	119.85
1	A	-106	PRO	C-N-CA	6.71	126.62	119.85
1	B	-109	LEU	CA-C-N	6.70	126.33	119.56
1	B	-109	LEU	C-N-CA	6.70	126.33	119.56
1	C	39	SER	CA-C-N	6.68	127.26	120.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	39	SER	C-N-CA	6.68	127.26	120.04
1	D	-106	PRO	CA-C-N	6.67	126.59	119.85
1	D	-106	PRO	C-N-CA	6.67	126.59	119.85
1	A	-109	LEU	CA-C-N	6.64	126.27	119.56
1	A	-109	LEU	C-N-CA	6.64	126.27	119.56
1	C	1033	GLU	CA-C-N	6.64	126.33	119.56
1	C	1033	GLU	C-N-CA	6.64	126.33	119.56
1	B	1033	GLU	CA-C-N	6.60	126.29	119.56
1	B	1033	GLU	C-N-CA	6.60	126.29	119.56
1	D	1033	GLU	CA-C-N	6.59	126.29	119.56
1	D	1033	GLU	C-N-CA	6.59	126.29	119.56
1	C	316	GLY	CA-C-N	6.58	126.50	119.85
1	C	316	GLY	C-N-CA	6.58	126.50	119.85
1	B	411	ILE	CA-C-N	6.57	126.81	119.32
1	B	411	ILE	C-N-CA	6.57	126.81	119.32
1	A	364	HIS	CA-C-N	6.56	126.74	120.31
1	A	364	HIS	C-N-CA	6.56	126.74	120.31
1	C	293	LYS	CA-C-N	6.54	126.50	120.03
1	C	293	LYS	C-N-CA	6.54	126.50	120.03
1	D	293	LYS	CA-C-N	6.50	126.46	120.03
1	D	293	LYS	C-N-CA	6.50	126.46	120.03
1	C	16	LEU	CA-C-N	6.47	126.84	119.92
1	C	16	LEU	C-N-CA	6.47	126.84	119.92
1	D	201	SER	CA-C-N	6.46	126.43	120.03
1	D	201	SER	C-N-CA	6.46	126.43	120.03
1	A	25	LYS	CA-C-N	6.46	126.37	119.85
1	A	25	LYS	C-N-CA	6.46	126.37	119.85
1	A	316	GLY	CA-C-N	6.45	126.37	119.85
1	A	316	GLY	C-N-CA	6.45	126.37	119.85
1	B	39	SER	CA-C-N	6.45	127.01	120.04
1	B	39	SER	C-N-CA	6.45	127.01	120.04
1	A	293	LYS	CA-C-N	6.45	126.42	120.03
1	A	293	LYS	C-N-CA	6.45	126.42	120.03
1	D	25	LYS	CA-C-N	6.45	126.36	119.85
1	D	25	LYS	C-N-CA	6.45	126.36	119.85
1	B	16	LEU	CA-C-N	6.43	126.81	119.92
1	B	16	LEU	C-N-CA	6.43	126.81	119.92
1	D	364	HIS	CA-C-N	6.43	126.61	120.31
1	D	364	HIS	C-N-CA	6.43	126.61	120.31
1	C	25	LYS	CA-C-N	6.42	126.33	119.85
1	C	25	LYS	C-N-CA	6.42	126.33	119.85
1	C	201	SER	CA-C-N	6.40	126.37	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	201	SER	C-N-CA	6.40	126.37	120.03
1	B	201	SER	CA-C-N	6.40	126.37	120.03
1	B	201	SER	C-N-CA	6.40	126.37	120.03
1	A	411	ILE	CA-C-N	6.40	126.61	119.32
1	A	411	ILE	C-N-CA	6.40	126.61	119.32
1	A	201	SER	CA-C-N	6.39	126.36	120.03
1	A	201	SER	C-N-CA	6.39	126.36	120.03
1	C	-78	GLU	CA-C-N	6.39	127.83	119.84
1	C	-78	GLU	C-N-CA	6.39	127.83	119.84
1	B	-184	PHE	CA-C-N	6.37	126.06	119.56
1	B	-184	PHE	C-N-CA	6.37	126.06	119.56
1	D	-192	HIS	CA-C-N	6.37	126.28	119.85
1	D	-192	HIS	C-N-CA	6.37	126.28	119.85
1	D	39	SER	CA-C-N	6.35	126.47	119.87
1	D	39	SER	C-N-CA	6.35	126.47	119.87
1	B	25	LYS	CA-C-N	6.34	126.26	119.85
1	B	25	LYS	C-N-CA	6.34	126.26	119.85
1	C	411	ILE	CA-C-N	6.33	126.53	119.32
1	C	411	ILE	C-N-CA	6.33	126.53	119.32
1	A	16	LEU	CA-C-N	6.31	126.67	119.92
1	A	16	LEU	C-N-CA	6.31	126.67	119.92
1	B	22	GLN	CA-C-N	6.30	126.27	120.03
1	B	22	GLN	C-N-CA	6.30	126.27	120.03
1	D	22	GLN	CA-C-N	6.29	126.26	120.03
1	D	22	GLN	C-N-CA	6.29	126.26	120.03
1	B	-78	GLU	CA-C-N	6.29	127.70	119.84
1	B	-78	GLU	C-N-CA	6.29	127.70	119.84
1	D	-78	GLU	CA-C-N	6.29	127.70	119.84
1	D	-78	GLU	C-N-CA	6.29	127.70	119.84
1	A	39	SER	CA-C-N	6.28	126.40	119.87
1	A	39	SER	C-N-CA	6.28	126.40	119.87
1	C	-151	THR	CA-C-N	6.27	126.03	119.76
1	C	-151	THR	C-N-CA	6.27	126.03	119.76
1	A	-184	PHE	CA-C-N	6.26	125.94	119.56
1	A	-184	PHE	C-N-CA	6.26	125.94	119.56
1	A	938	HIS	CA-C-N	6.24	125.92	119.56
1	A	938	HIS	C-N-CA	6.24	125.92	119.56
1	C	-109	LEU	CA-C-N	6.23	126.35	119.87
1	C	-109	LEU	C-N-CA	6.23	126.35	119.87
1	D	-109	LEU	CA-C-N	6.23	126.35	119.87
1	D	-109	LEU	C-N-CA	6.23	126.35	119.87
1	A	1033	GLU	CA-C-N	6.23	125.85	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1033	GLU	C-N-CA	6.23	125.85	119.56
1	C	22	GLN	CA-C-N	6.23	126.19	120.03
1	C	22	GLN	C-N-CA	6.23	126.19	120.03
1	B	293	LYS	CA-C-N	6.21	126.18	120.03
1	B	293	LYS	C-N-CA	6.21	126.18	120.03
1	B	364	HIS	CA-C-N	6.17	126.35	120.31
1	B	364	HIS	C-N-CA	6.17	126.35	120.31
1	C	-184	PHE	CA-C-N	6.13	125.81	119.56
1	C	-184	PHE	C-N-CA	6.13	125.81	119.56
1	A	22	GLN	CA-C-N	6.13	126.10	120.03
1	A	22	GLN	C-N-CA	6.13	126.10	120.03
1	D	16	LEU	CA-C-N	6.12	126.47	119.92
1	D	16	LEU	C-N-CA	6.12	126.47	119.92
1	C	938	HIS	CA-C-N	6.12	125.80	119.56
1	C	938	HIS	C-N-CA	6.12	125.80	119.56
1	B	-151	THR	CA-C-N	6.10	126.01	119.85
1	B	-151	THR	C-N-CA	6.10	126.01	119.85
1	D	-184	PHE	CA-C-N	6.09	125.77	119.56
1	D	-184	PHE	C-N-CA	6.09	125.77	119.56
1	B	650	PHE	CA-C-N	6.07	125.75	119.56
1	B	650	PHE	C-N-CA	6.07	125.75	119.56
1	C	83	ASP	CA-C-N	6.07	127.43	119.84
1	C	83	ASP	C-N-CA	6.07	127.43	119.84
1	D	-151	THR	CA-C-N	6.07	125.97	119.85
1	D	-151	THR	C-N-CA	6.07	125.97	119.85
1	B	284	ASN	CA-C-N	6.06	126.62	120.38
1	B	284	ASN	C-N-CA	6.06	126.62	120.38
1	B	938	HIS	CA-C-N	6.06	125.74	119.56
1	B	938	HIS	C-N-CA	6.06	125.74	119.56
1	A	553	LEU	CA-C-N	6.05	125.94	119.28
1	A	553	LEU	C-N-CA	6.05	125.94	119.28
1	A	210	ASP	CA-C-N	6.04	126.05	119.89
1	A	210	ASP	C-N-CA	6.04	126.05	119.89
1	D	938	HIS	CA-C-N	6.01	125.69	119.56
1	D	938	HIS	C-N-CA	6.01	125.69	119.56
1	A	650	PHE	CA-C-N	5.97	125.65	119.56
1	A	650	PHE	C-N-CA	5.97	125.65	119.56
1	D	650	PHE	CA-C-N	5.95	125.63	119.56
1	D	650	PHE	C-N-CA	5.95	125.63	119.56
1	C	210	ASP	CA-C-N	5.93	125.94	119.89
1	C	210	ASP	C-N-CA	5.93	125.94	119.89
1	C	650	PHE	CA-C-N	5.93	125.61	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	650	PHE	C-N-CA	5.93	125.61	119.56
1	A	83	ASP	CA-C-N	5.91	127.23	119.84
1	A	83	ASP	C-N-CA	5.91	127.23	119.84
1	A	284	ASN	CA-C-N	5.91	126.47	120.38
1	A	284	ASN	C-N-CA	5.91	126.47	120.38
1	D	351	ARG	CA-C-N	5.91	126.06	119.32
1	D	351	ARG	C-N-CA	5.91	126.06	119.32
1	C	284	ASN	CA-C-N	5.83	126.39	120.38
1	C	284	ASN	C-N-CA	5.83	126.39	120.38
1	B	351	ARG	CA-C-N	5.82	125.95	119.32
1	B	351	ARG	C-N-CA	5.82	125.95	119.32
1	A	767	HIS	CA-C-N	5.82	126.22	119.47
1	A	767	HIS	C-N-CA	5.82	126.22	119.47
1	C	351	ARG	CA-C-N	5.82	125.68	119.28
1	C	351	ARG	C-N-CA	5.82	125.68	119.28
1	A	-151	THR	CA-C-N	5.81	125.72	119.85
1	A	-151	THR	C-N-CA	5.81	125.72	119.85
1	B	767	HIS	CA-C-N	5.76	126.15	119.47
1	B	767	HIS	C-N-CA	5.76	126.15	119.47
1	C	767	HIS	CA-C-N	5.73	126.12	119.47
1	C	767	HIS	C-N-CA	5.73	126.12	119.47
1	D	284	ASN	CA-C-N	5.69	126.25	120.38
1	D	284	ASN	C-N-CA	5.69	126.25	120.38
1	D	767	HIS	CA-C-N	5.69	126.07	119.47
1	D	767	HIS	C-N-CA	5.69	126.07	119.47
1	B	-192	HIS	CA-C-N	5.65	125.56	119.85
1	B	-192	HIS	C-N-CA	5.65	125.56	119.85
1	A	-99	ILE	CA-C-N	5.64	125.11	119.24
1	A	-99	ILE	C-N-CA	5.64	125.11	119.24
1	A	66	LYS	CA-C-N	5.54	125.86	119.93
1	A	66	LYS	C-N-CA	5.54	125.86	119.93
1	A	-192	HIS	CA-C-N	5.53	125.44	119.85
1	A	-192	HIS	C-N-CA	5.53	125.44	119.85
1	C	-99	ILE	CA-C-N	5.52	124.98	119.24
1	C	-99	ILE	C-N-CA	5.52	124.98	119.24
1	D	411	ILE	CA-C-N	5.51	125.60	119.32
1	D	411	ILE	C-N-CA	5.51	125.60	119.32
1	C	341	LEU	CA-C-N	5.50	125.45	119.78
1	C	341	LEU	C-N-CA	5.50	125.45	119.78
1	D	-99	ILE	CA-C-N	5.50	124.96	119.24
1	D	-99	ILE	C-N-CA	5.50	124.96	119.24
1	B	210	ASP	CA-C-N	5.49	125.49	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	ASP	C-N-CA	5.49	125.49	119.89
1	D	210	ASP	CA-C-N	5.49	125.43	119.78
1	D	210	ASP	C-N-CA	5.49	125.43	119.78
1	B	-99	ILE	CA-C-N	5.48	124.94	119.24
1	B	-99	ILE	C-N-CA	5.48	124.94	119.24
1	B	285	PRO	CA-C-N	5.47	126.68	119.84
1	B	285	PRO	C-N-CA	5.47	126.68	119.84
1	C	-192	HIS	CA-C-N	5.45	125.36	119.85
1	C	-192	HIS	C-N-CA	5.45	125.36	119.85
1	A	285	PRO	CA-C-N	5.45	126.65	119.84
1	A	285	PRO	C-N-CA	5.45	126.65	119.84
1	D	66	LYS	CA-C-N	5.42	125.73	119.93
1	D	66	LYS	C-N-CA	5.42	125.73	119.93
1	B	553	LEU	CA-C-N	5.41	126.61	119.84
1	B	553	LEU	C-N-CA	5.41	126.61	119.84
1	C	66	LYS	CA-C-N	5.41	125.72	119.93
1	C	66	LYS	C-N-CA	5.41	125.72	119.93
1	A	351	ARG	CA-C-N	5.37	125.18	119.28
1	A	351	ARG	C-N-CA	5.37	125.18	119.28
1	D	341	LEU	CA-C-N	5.35	125.29	119.78
1	D	341	LEU	C-N-CA	5.35	125.29	119.78
1	D	553	LEU	CA-C-N	5.33	126.50	119.84
1	D	553	LEU	C-N-CA	5.33	126.50	119.84
1	C	289	LYS	CA-C-O	5.30	121.01	117.94
1	C	289	LYS	CB-CA-C	-5.29	109.45	117.07
1	A	881	ASN	CA-C-N	5.27	126.43	119.84
1	A	881	ASN	C-N-CA	5.27	126.43	119.84
1	B	881	ASN	CA-C-N	5.25	126.40	119.84
1	B	881	ASN	C-N-CA	5.25	126.40	119.84
1	A	341	LEU	CA-C-N	5.22	125.16	119.78
1	A	341	LEU	C-N-CA	5.22	125.16	119.78
1	C	881	ASN	CA-C-N	5.22	126.37	119.84
1	C	881	ASN	C-N-CA	5.22	126.37	119.84
1	D	285	PRO	CA-C-N	5.22	126.37	119.84
1	D	285	PRO	C-N-CA	5.22	126.37	119.84
1	B	341	LEU	CA-C-N	5.20	125.14	119.78
1	B	341	LEU	C-N-CA	5.20	125.14	119.78
1	C	285	PRO	CA-C-N	5.16	126.29	119.84
1	C	285	PRO	C-N-CA	5.16	126.29	119.84
1	D	881	ASN	CA-C-N	5.10	126.22	119.84
1	D	881	ASN	C-N-CA	5.10	126.22	119.84
1	D	316	GLY	CA-C-N	5.06	126.17	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	316	GLY	C-N-CA	5.06	126.17	119.84
1	B	66	LYS	CA-C-N	5.06	125.34	119.93
1	B	66	LYS	C-N-CA	5.06	125.34	119.93
1	C	99	MET	CA-C-N	5.06	125.06	119.90
1	C	99	MET	C-N-CA	5.06	125.06	119.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	624	GLN	Peptide
1	B	624	GLN	Peptide
1	C	624	GLN	Peptide
1	D	624	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9344	0	9380	37	0
1	B	9344	0	9380	36	0
1	C	9344	0	9380	38	0
1	D	9344	0	9380	33	0
2	A	27	0	12	1	0
2	B	27	0	12	0	0
2	C	27	0	12	1	0
2	D	27	0	12	1	0
3	A	25	0	0	0	0
3	B	25	0	0	1	0
3	C	25	0	0	0	0
3	D	25	0	0	0	0
4	A	42	0	58	0	0
4	B	42	0	58	0	0
4	C	42	0	58	1	0
4	D	42	0	58	0	0
All	All	37752	0	37800	141	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 2.

All (141) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:624:GLN:HB2	1:C:625:PRO:HD3	1.81	0.63
1:D:624:GLN:HB2	1:D:625:PRO:HD3	1.81	0.62
1:B:624:GLN:HB2	1:B:625:PRO:HD3	1.80	0.62
1:A:624:GLN:HB2	1:A:625:PRO:HD3	1.85	0.58
1:C:553:LEU:N	1:C:554:PRO:CD	2.67	0.58
1:A:553:LEU:N	1:A:554:PRO:CD	2.69	0.56
1:B:279:CYS:SG	1:B:280:CYS:N	2.80	0.55
1:C:-192:HIS:O	1:C:-192:HIS:ND1	2.41	0.54
1:A:39:SER:O	1:A:42:LYS:NZ	2.39	0.54
1:B:156:ALA:O	1:B:506:ASN:ND2	2.42	0.53
1:D:-192:HIS:O	1:D:-192:HIS:ND1	2.41	0.53
1:C:452:GLN:N	1:C:453:PRO:CD	2.73	0.52
1:B:-184:PHE:N	1:B:-183:PRO:CD	2.72	0.52
1:B:553:LEU:N	1:B:554:PRO:CD	2.73	0.52
1:A:452:GLN:N	1:A:453:PRO:CD	2.73	0.52
1:A:983:ASP:OD1	1:A:983:ASP:N	2.43	0.52
1:C:212:ASP:O	1:C:213:ASP:C	2.53	0.52
1:D:452:GLN:N	1:D:453:PRO:CD	2.72	0.52
1:B:-192:HIS:O	1:B:-192:HIS:ND1	2.43	0.52
1:B:452:GLN:N	1:B:453:PRO:CD	2.73	0.52
1:C:279:CYS:SG	1:C:280:CYS:N	2.84	0.51
1:D:624:GLN:HB2	1:D:625:PRO:CD	2.40	0.51
1:A:-184:PHE:N	1:A:-183:PRO:CD	2.73	0.51
1:C:-184:PHE:N	1:C:-183:PRO:CD	2.74	0.51
1:A:-192:HIS:ND1	1:A:-192:HIS:O	2.42	0.51
1:A:318:LEU:O	1:A:319:CYS:C	2.53	0.51
1:B:1034:PRO:O	1:B:1035:SER:CB	2.59	0.51
1:A:624:GLN:HB2	1:A:625:PRO:CD	2.40	0.50
1:D:553:LEU:N	1:D:554:PRO:CD	2.74	0.50
1:B:624:GLN:HB2	1:B:625:PRO:CD	2.41	0.50
1:B:212:ASP:O	1:B:213:ASP:C	2.54	0.50
1:D:1034:PRO:O	1:D:1035:SER:CB	2.60	0.50
1:A:212:ASP:O	1:A:213:ASP:C	2.55	0.49
1:D:-167:HIS:CD2	1:D:30:VAL:H	2.30	0.49
1:B:-167:HIS:CD2	1:B:30:VAL:H	2.30	0.49
1:D:212:ASP:O	1:D:213:ASP:C	2.55	0.49
1:A:-167:HIS:CD2	1:A:30:VAL:H	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:CYS:SG	1:A:280:CYS:N	2.85	0.49
1:C:-167:HIS:CD2	1:C:30:VAL:H	2.30	0.49
1:C:318:LEU:O	1:C:319:CYS:C	2.55	0.49
1:D:-184:PHE:N	1:D:-183:PRO:CD	2.75	0.49
1:C:624:GLN:HB2	1:C:625:PRO:CD	2.42	0.49
1:D:536:LEU:O	1:D:537:GLU:CB	2.61	0.49
1:C:-73:TRP:N	1:C:-72:PRO:CD	2.76	0.48
1:B:960:ASP:OD1	1:D:-52:LYS:NZ	2.47	0.48
1:C:1034:PRO:O	1:C:1035:SER:CB	2.61	0.48
1:B:536:LEU:O	1:B:537:GLU:CB	2.62	0.48
1:C:505:MET:O	1:C:506:ASN:C	2.57	0.48
1:B:-73:TRP:N	1:B:-72:PRO:CD	2.77	0.47
1:C:926:ASP:N	1:C:926:ASP:OD1	2.48	0.47
1:A:-73:TRP:N	1:A:-72:PRO:CD	2.78	0.47
1:A:949:ASP:O	1:A:950:ASN:C	2.57	0.47
1:D:-73:TRP:N	1:D:-72:PRO:CD	2.77	0.47
1:A:505:MET:O	1:A:506:ASN:C	2.58	0.47
1:A:536:LEU:O	1:A:537:GLU:CB	2.62	0.47
1:D:505:MET:O	1:D:506:ASN:C	2.57	0.47
1:A:1031:VAL:O	1:A:1032:PHE:HB2	2.15	0.46
1:D:926:ASP:N	1:D:926:ASP:OD1	2.48	0.46
1:C:536:LEU:O	1:C:537:GLU:CB	2.64	0.46
1:A:169:THR:H	2:A:1101:ADP:HN62	1.65	0.45
1:C:-192:HIS:O	1:C:-192:HIS:CG	2.70	0.45
1:B:926:ASP:N	1:B:926:ASP:OD1	2.49	0.45
1:B:-52:LYS:NZ	1:D:960:ASP:OD1	2.50	0.45
1:A:1033:GLU:HB3	1:A:1034:PRO:CD	2.47	0.45
1:A:-52:LYS:NZ	1:C:960:ASP:OD1	2.49	0.44
1:B:992:VAL:C	1:B:994:LYS:H	2.26	0.44
1:A:755:ASP:HB2	1:A:756:PRO:HD3	2.00	0.44
1:A:926:ASP:OD1	1:A:926:ASP:N	2.47	0.44
1:B:-212:GLY:N	1:B:65:ASP:OD2	2.50	0.44
1:A:-99:ILE:N	1:A:-98:PRO:CD	2.80	0.44
1:A:960:ASP:OD1	1:C:-52:LYS:NZ	2.49	0.44
1:D:39:SER:O	1:D:42:LYS:NZ	2.41	0.44
1:B:755:ASP:HB2	1:B:756:PRO:HD3	2.00	0.44
1:D:-192:HIS:O	1:D:-192:HIS:CG	2.71	0.44
1:A:624:GLN:CB	1:A:625:PRO:CD	2.96	0.43
1:A:992:VAL:C	1:A:994:LYS:H	2.26	0.43
1:D:478:TRP:HE1	1:D:534:TYR:HH	1.62	0.43
1:D:992:VAL:C	1:D:994:LYS:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:-212:GLY:N	1:D:65:ASP:OD2	2.51	0.43
1:B:439:THR:OG1	1:B:632:TYR:OH	2.34	0.43
1:D:169:THR:H	2:D:1101:ADP:HN62	1.67	0.43
1:D:755:ASP:HB2	1:D:756:PRO:HD3	2.01	0.43
1:C:169:THR:H	2:C:1101:ADP:HN62	1.67	0.43
1:D:329:ASP:OD1	1:D:329:ASP:N	2.51	0.43
1:A:920:ARG:HB2	1:A:949:ASP:HB3	1.99	0.43
1:A:1033:GLU:HB3	1:A:1034:PRO:HD2	2.00	0.42
1:A:1034:PRO:O	1:A:1035:SER:HB2	2.19	0.42
1:B:439:THR:HG1	1:B:632:TYR:HH	1.67	0.42
1:C:-169:TRP:CG	1:C:-168:ALA:H	2.37	0.42
1:A:478:TRP:O	1:A:480:GLN:NE2	2.52	0.42
1:B:624:GLN:CB	1:B:625:PRO:CD	2.98	0.42
1:B:-169:TRP:CG	1:B:-168:ALA:H	2.37	0.42
1:C:329:ASP:OD1	1:C:329:ASP:N	2.50	0.42
1:B:-192:HIS:O	1:B:-192:HIS:CG	2.73	0.42
1:C:755:ASP:HB2	1:C:756:PRO:HD3	2.01	0.42
1:C:992:VAL:C	1:C:994:LYS:H	2.27	0.42
1:D:-99:ILE:N	1:D:-98:PRO:CD	2.82	0.42
1:D:624:GLN:CB	1:D:625:PRO:CD	2.98	0.42
1:A:-192:HIS:O	1:A:-192:HIS:CG	2.73	0.42
1:A:71:VAL:HG12	1:A:73:LEU:H	1.85	0.42
1:C:-26:ASN:C	1:C:-26:ASN:OD1	2.62	0.42
1:C:167:ARG:NH1	1:C:384:LYS:O	2.53	0.42
1:C:624:GLN:CB	1:C:625:PRO:CD	2.97	0.42
1:A:-169:TRP:CG	1:A:-168:ALA:H	2.38	0.42
1:A:154:ARG:O	1:A:157:ARG:NH1	2.50	0.42
1:B:-99:ILE:N	1:B:-98:PRO:CD	2.82	0.42
1:B:329:ASP:N	1:B:329:ASP:OD1	2.52	0.42
1:C:-99:ILE:N	1:C:-98:PRO:CD	2.82	0.42
1:C:71:VAL:HG12	1:C:73:LEU:H	1.85	0.41
1:C:163:SER:O	1:C:164:LEU:HB2	2.18	0.41
1:A:553:LEU:N	1:A:554:PRO:HD3	2.34	0.41
1:A:1034:PRO:O	1:A:1035:SER:CB	2.68	0.41
1:C:1033:GLU:HB2	1:C:1034:PRO:CD	2.50	0.41
1:B:536:LEU:O	1:B:537:GLU:HB3	2.21	0.41
1:C:-169:TRP:CG	1:C:-168:ALA:N	2.88	0.41
1:D:1033:GLU:HB2	1:D:1034:PRO:CD	2.50	0.41
1:B:-169:TRP:CD1	1:B:-168:ALA:H	2.39	0.41
1:C:920:ARG:HB2	1:C:949:ASP:HB3	2.03	0.41
1:D:536:LEU:O	1:D:537:GLU:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:920:ARG:HB2	1:D:949:ASP:HB3	2.01	0.41
1:C:154:ARG:O	1:C:157:ARG:NH1	2.50	0.41
1:D:1034:PRO:O	1:D:1035:SER:HB2	2.20	0.41
1:B:-169:TRP:CG	1:B:-168:ALA:N	2.89	0.41
1:B:949:ASP:O	1:B:950:ASN:C	2.62	0.41
1:B:1033:GLU:HB2	1:B:1034:PRO:CD	2.51	0.41
1:B:1034:PRO:O	1:B:1035:SER:HB2	2.21	0.41
1:B:920:ARG:HB2	1:B:949:ASP:HB3	2.02	0.41
3:B:1102:A1A4L:O17	3:B:1102:A1A4L:C07	2.68	0.41
1:C:478:TRP:HE1	1:C:534:TYR:HH	1.64	0.41
1:C:825:LEU:O	1:C:826:LEU:HB2	2.21	0.41
1:D:-169:TRP:CD1	1:D:-168:ALA:H	2.39	0.41
1:D:-169:TRP:CG	1:D:-168:ALA:H	2.38	0.41
1:A:-169:TRP:CG	1:A:-168:ALA:N	2.89	0.41
1:B:-183:PRO:HG3	1:B:-161:TYR:CE2	2.56	0.41
1:B:778:GLY:O	1:B:780:CYS:N	2.53	0.40
1:C:1034:PRO:O	1:C:1035:SER:HB2	2.20	0.40
1:B:825:LEU:O	1:B:826:LEU:HB2	2.21	0.40
1:C:536:LEU:O	1:C:537:GLU:HB3	2.21	0.40
1:D:14:THR:OG1	1:D:15:VAL:N	2.55	0.40
1:D:825:LEU:O	1:D:826:LEU:HB2	2.21	0.40
1:C:-47:ASP:OD2	4:C:1103:CPS:C32	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1171/1267 (92%)	1116 (95%)	44 (4%)	11 (1%)	14	43
1	B	1171/1267 (92%)	1116 (95%)	46 (4%)	9 (1%)	16	47
1	C	1171/1267 (92%)	1116 (95%)	45 (4%)	10 (1%)	14	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	1171/1267 (92%)	1115 (95%)	46 (4%)	10 (1%)	14	43
All	All	4684/5068 (92%)	4463 (95%)	181 (4%)	40 (1%)	16	43

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	506	ASN
1	C	506	ASN
1	D	506	ASN
1	A	555	SER
1	A	625	PRO
1	A	1032	PHE
1	B	506	ASN
1	D	496	LYS
1	D	625	PRO
1	A	319	CYS
1	A	431	SER
1	A	496	LYS
1	B	431	SER
1	B	496	LYS
1	B	555	SER
1	B	625	PRO
1	C	319	CYS
1	C	431	SER
1	C	496	LYS
1	C	555	SER
1	C	625	PRO
1	D	431	SER
1	D	555	SER
1	A	949	ASP
1	B	213	ASP
1	C	213	ASP
1	C	949	ASP
1	D	213	ASP
1	D	624	GLN
1	D	949	ASP
1	A	213	ASP
1	A	624	GLN
1	B	624	GLN
1	B	949	ASP
1	C	624	GLN
1	C	778	GLY

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Mol	Chain	Res	Type
1	B	778	GLY
1	D	591	TYR
1	A	778	GLY
1	D	778	GLY

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	1033/1108 (93%)	1033 (100%)	0	100	100
1	B	1033/1108 (93%)	1033 (100%)	0	100	100
1	C	1033/1108 (93%)	1033 (100%)	0	100	100
1	D	1033/1108 (93%)	1033 (100%)	0	100	100
All	All	4132/4432 (93%)	4132 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	134	GLN
1	A	314	HIS
1	A	359	GLN
1	A	452	GLN
1	A	638	GLN
1	A	663	HIS
1	A	771	ASN
1	A	824	HIS
1	A	979	ASN
1	B	134	GLN
1	B	215	HIS
1	B	359	GLN
1	B	360	HIS

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Mol	Chain	Res	Type
1	B	452	GLN
1	B	638	GLN
1	B	656	ASN
1	B	686	ASN
1	B	824	HIS
1	B	956	HIS
1	B	979	ASN
1	C	22	GLN
1	C	288	HIS
1	C	452	GLN
1	C	663	HIS
1	C	751	ASN
1	C	824	HIS
1	C	956	HIS
1	D	134	GLN
1	D	314	HIS
1	D	359	GLN
1	D	452	GLN
1	D	638	GLN
1	D	956	HIS

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](#)

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
2	ADP	A	1101	-	28,29,29	0.62	0	43,45,45	0.72	0
3	A1A4L	C	1102	-	27,28,28	1.98	7 (25%)	32,40,40	5.78	18 (56%)
3	A1A4L	D	1102	-	27,28,28	1.99	6 (22%)	32,40,40	3.09	19 (59%)
3	A1A4L	B	1102	-	27,28,28	1.71	5 (18%)	32,40,40	2.81	18 (56%)
4	CPS	C	1103	-	45,45,45	1.01	1 (2%)	70,70,70	1.49	8 (11%)
3	A1A4L	A	1102	-	27,28,28	1.67	5 (18%)	32,40,40	3.06	16 (50%)
2	ADP	C	1101	-	28,29,29	0.73	0	43,45,45	0.77	0
2	ADP	B	1101	-	28,29,29	0.70	0	43,45,45	0.81	0
4	CPS	D	1103	-	45,45,45	0.99	0	70,70,70	1.24	7 (10%)
4	CPS	B	1103	-	45,45,45	1.05	0	70,70,70	1.36	9 (12%)
4	CPS	A	1103	-	45,45,45	1.01	0	70,70,70	1.29	7 (10%)
2	ADP	D	1101	-	28,29,29	0.78	0	43,45,45	0.75	0

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	ADP	A	1101	-	-	3/16/32/32	0/3/3/3
3	A1A4L	C	1102	-	-	2/10/10/10	0/3/4/4
3	A1A4L	D	1102	-	-	4/10/10/10	0/3/4/4
3	A1A4L	B	1102	-	-	6/10/10/10	0/3/4/4
4	CPS	C	1103	-	-	8/25/90/90	0/4/4/4
3	A1A4L	A	1102	-	-	3/10/10/10	0/3/4/4
2	ADP	C	1101	-	-	5/16/32/32	0/3/3/3
2	ADP	B	1101	-	-	3/16/32/32	0/3/3/3
4	CPS	D	1103	-	-	9/25/90/90	0/4/4/4
4	CPS	B	1103	-	-	9/25/90/90	0/4/4/4
4	CPS	A	1103	-	-	10/25/90/90	0/4/4/4
2	ADP	D	1101	-	-	4/16/32/32	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1102	A1A4L	C07-N09	5.66	1.47	1.35
3	D	1102	A1A4L	C03-N04	5.12	1.32	1.28
3	C	1102	A1A4L	C18-N25	-4.82	1.29	1.40
3	A	1102	A1A4L	C07-N09	4.68	1.45	1.35
3	C	1102	A1A4L	C07-N09	4.35	1.45	1.35
3	C	1102	A1A4L	O17-C16	-4.09	1.14	1.23
3	B	1102	A1A4L	C18-N25	-4.00	1.31	1.40
3	B	1102	A1A4L	C07-N09	3.70	1.43	1.35
3	B	1102	A1A4L	C03-N04	3.55	1.30	1.28
3	D	1102	A1A4L	O17-C16	-3.25	1.16	1.23
3	A	1102	A1A4L	C03-N04	3.12	1.30	1.28
3	C	1102	A1A4L	C02-C03	2.87	1.55	1.49
3	B	1102	A1A4L	O17-C16	-2.86	1.17	1.23
3	D	1102	A1A4L	C10-N09	2.81	1.46	1.40
3	C	1102	A1A4L	C23-C24	2.74	1.49	1.44
3	D	1102	A1A4L	O08-C07	-2.69	1.17	1.23
3	A	1102	A1A4L	C18-N25	-2.56	1.34	1.40
3	A	1102	A1A4L	C18-C16	-2.45	1.42	1.47
3	D	1102	A1A4L	C18-N25	-2.45	1.34	1.40
3	C	1102	A1A4L	C10-N09	2.41	1.45	1.40
3	B	1102	A1A4L	O08-C07	-2.38	1.18	1.23
3	C	1102	A1A4L	O08-C07	-2.13	1.19	1.23
3	A	1102	A1A4L	C10-N09	2.11	1.45	1.40
4	C	1103	CPS	C2-C15	2.04	1.58	1.55

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1102	A1A4L	C19-C20-C24	-18.95	94.49	108.13
3	C	1102	A1A4L	C22-S21-C20	13.20	116.04	92.33
3	C	1102	A1A4L	C19-C20-S21	10.76	179.87	135.34
3	C	1102	A1A4L	C23-C24-N25	-9.27	125.95	136.00
3	A	1102	A1A4L	C16-N05-N04	-8.76	117.21	126.24
3	C	1102	A1A4L	C16-N05-N04	-8.09	117.91	126.24
3	D	1102	A1A4L	C16-N05-N04	-7.74	118.27	126.24
3	C	1102	A1A4L	C23-C24-C20	7.72	122.64	114.01
3	B	1102	A1A4L	C16-N05-N04	-7.10	118.92	126.24
3	A	1102	A1A4L	C03-N04-N05	6.58	124.06	114.06
3	C	1102	A1A4L	C23-C22-S21	-6.48	101.26	112.86
4	C	1103	CPS	C5-C9-C20	6.17	126.96	119.48
3	B	1102	A1A4L	C03-N04-N05	6.17	123.44	114.06
3	D	1102	A1A4L	C03-N04-N05	5.90	123.04	114.06
3	C	1102	A1A4L	C03-N04-N05	5.78	122.86	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1103	CPS	C5-C9-C20	5.60	126.27	119.48
4	B	1103	CPS	C5-C9-C20	5.57	126.23	119.48
3	D	1102	A1A4L	C07-C06-N05	5.19	121.58	111.89
4	D	1103	CPS	C5-C9-C20	5.03	125.58	119.48
3	D	1102	A1A4L	C01-C02-C03	-4.96	101.46	113.52
3	A	1102	A1A4L	C22-C23-C24	4.78	115.78	110.81
3	D	1102	A1A4L	C22-C23-C24	4.78	115.78	110.81
3	A	1102	A1A4L	C23-C22-S21	-4.69	104.47	112.86
3	A	1102	A1A4L	C22-S21-C20	4.63	100.64	92.33
4	C	1103	CPS	C9-C5-C6	-4.28	95.82	100.11
3	C	1102	A1A4L	C10-N09-C07	-4.28	120.37	128.22
3	B	1102	A1A4L	C22-S21-C20	4.22	99.92	92.33
3	D	1102	A1A4L	C23-C22-S21	-4.22	105.30	112.86
4	C	1103	CPS	C27-C26-C25	4.06	118.90	110.95
3	B	1102	A1A4L	C19-C20-C24	-4.06	105.21	108.13
3	C	1102	A1A4L	C02-C03-N04	-4.00	111.73	119.43
3	B	1102	A1A4L	C23-C22-S21	-3.87	105.92	112.86
3	C	1102	A1A4L	C22-C23-C24	3.72	114.68	110.81
4	B	1103	CPS	C9-C5-C6	-3.72	96.38	100.11
3	A	1102	A1A4L	C06-N05-N04	3.64	118.95	114.27
4	A	1103	CPS	C9-C5-C6	-3.62	96.48	100.11
3	C	1102	A1A4L	C06-N05-N04	3.55	118.84	114.27
3	B	1102	A1A4L	C10-N09-C07	-3.52	121.76	128.22
4	C	1103	CPS	C26-C27-N2	3.43	122.32	115.35
3	B	1102	A1A4L	C22-C23-C24	3.40	114.35	110.81
4	D	1103	CPS	C9-C5-C6	-3.39	96.71	100.11
3	D	1102	A1A4L	N13-C14-N15	-3.39	121.58	127.33
3	A	1102	A1A4L	C19-C20-C24	-3.38	105.69	108.13
3	A	1102	A1A4L	N13-C14-N15	-3.36	121.62	127.33
3	C	1102	A1A4L	N13-C14-N15	-3.32	121.68	127.33
3	D	1102	A1A4L	N09-C10-N15	3.30	124.77	114.87
3	D	1102	A1A4L	C06-C07-N09	3.26	120.27	114.23
3	D	1102	A1A4L	C22-S21-C20	3.25	98.17	92.33
3	A	1102	A1A4L	C19-C20-S21	3.19	148.53	135.34
4	D	1103	CPS	C26-C27-N2	3.18	121.82	115.35
3	D	1102	A1A4L	C12-N13-C14	3.18	121.71	115.35
4	B	1103	CPS	C27-C26-C25	3.11	117.04	110.95
3	B	1102	A1A4L	N09-C10-N15	3.06	124.05	114.87
3	C	1102	A1A4L	C06-C07-N09	3.04	119.85	114.23
4	A	1103	CPS	C26-C27-N2	3.01	121.46	115.35
3	B	1102	A1A4L	C23-C24-N25	3.00	139.26	136.00
3	D	1102	A1A4L	C06-N05-N04	2.99	118.12	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1102	A1A4L	C19-C20-S21	2.89	147.31	135.34
4	B	1103	CPS	C26-C27-N2	2.87	121.18	115.35
4	C	1103	CPS	C23-C24-N1	-2.86	111.13	116.34
4	B	1103	CPS	C30-C31-C32	2.85	117.26	109.43
3	D	1102	A1A4L	C11-C12-N13	-2.85	118.74	123.60
3	A	1102	A1A4L	C12-N13-C14	2.83	121.00	115.35
3	A	1102	A1A4L	C11-C12-N13	-2.82	118.78	123.60
4	C	1103	CPS	C25-N1-C24	2.77	127.98	122.82
3	B	1102	A1A4L	C06-N05-N04	2.75	117.81	114.27
4	A	1103	CPS	C27-C26-C25	2.73	116.30	110.95
3	C	1102	A1A4L	N09-C10-N15	2.70	122.99	114.87
3	B	1102	A1A4L	C11-C12-N13	-2.70	119.00	123.60
4	D	1103	CPS	C27-C26-C25	2.68	116.20	110.95
4	A	1103	CPS	C30-C31-C32	2.64	116.68	109.43
3	C	1102	A1A4L	C11-C10-N15	-2.53	118.76	122.61
4	D	1103	CPS	C25-N1-C24	2.52	127.51	122.82
4	D	1103	CPS	C30-C31-C32	2.48	116.25	109.43
3	D	1102	A1A4L	C19-C20-S21	2.46	145.52	135.34
4	C	1103	CPS	C30-C31-C32	2.43	116.10	109.43
3	A	1102	A1A4L	C10-N09-C07	-2.41	123.80	128.22
3	D	1102	A1A4L	C11-C10-N09	-2.37	116.00	123.02
3	B	1102	A1A4L	C11-C10-N09	-2.35	116.07	123.02
3	B	1102	A1A4L	C07-C06-N05	-2.35	107.51	111.89
3	A	1102	A1A4L	C20-C24-N25	2.31	111.84	109.32
3	A	1102	A1A4L	N09-C10-N15	2.31	121.79	114.87
3	A	1102	A1A4L	C11-C10-N15	-2.28	119.14	122.61
4	B	1103	CPS	C22-C23-C24	-2.26	108.01	113.06
3	B	1102	A1A4L	C06-C07-N09	2.25	118.39	114.23
3	D	1102	A1A4L	C11-C10-N15	-2.23	119.22	122.61
4	C	1103	CPS	C10-C5-C6	2.22	114.68	111.20
3	D	1102	A1A4L	C02-C03-N04	-2.21	115.17	119.43
4	B	1103	CPS	C10-C5-C6	2.20	114.65	111.20
3	C	1102	A1A4L	C19-C18-C16	2.15	133.91	130.50
4	A	1103	CPS	C10-C5-C6	2.13	114.54	111.20
3	A	1102	A1A4L	C18-C16-N05	2.09	120.80	115.83
4	A	1103	CPS	C25-N1-C24	2.07	126.68	122.82
3	B	1102	A1A4L	C01-C02-C03	-2.07	108.48	113.52
4	B	1103	CPS	C23-C24-N1	-2.05	112.60	116.34
3	C	1102	A1A4L	C12-N13-C14	2.04	119.44	115.35
4	D	1103	CPS	C10-C5-C6	2.04	114.39	111.20
3	B	1102	A1A4L	N13-C14-N15	-2.04	123.87	127.33
4	B	1103	CPS	C23-C22-C20	2.03	118.26	114.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1102	A1A4L	O17-C16-C18	-2.03	119.49	122.45
3	D	1102	A1A4L	O08-C07-N09	-2.03	120.00	123.64
3	D	1102	A1A4L	C19-C20-C24	-2.03	106.67	108.13

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	ADP	C5'-O5'-PA-O1A
2	B	1101	ADP	C5'-O5'-PA-O1A
2	C	1101	ADP	C5'-O5'-PA-O1A
2	D	1101	ADP	C5'-O5'-PA-O1A
2	D	1101	ADP	C5'-O5'-PA-O3A
2	D	1101	ADP	O4'-C1'-N9-C8
2	D	1101	ADP	O4'-C1'-N9-C4
3	B	1102	A1A4L	C07-C06-N05-C16
3	D	1102	A1A4L	N05-C06-C07-O08
4	A	1103	CPS	C21-C20-C9-C5
4	A	1103	CPS	C30-C31-C32-S
4	B	1103	CPS	C30-C31-C32-S
4	C	1103	CPS	C21-C20-C9-C5
4	C	1103	CPS	C30-C31-C32-S
4	B	1103	CPS	C21-C20-C9-C5
4	A	1103	CPS	C26-C25-N1-C24
4	C	1103	CPS	C26-C25-N1-C24
4	C	1103	CPS	C22-C20-C9-C8
4	C	1103	CPS	C22-C20-C9-C5
4	C	1103	CPS	C21-C20-C9-C8
4	D	1103	CPS	C21-C20-C9-C5
4	A	1103	CPS	C22-C20-C9-C8
4	B	1103	CPS	C26-C25-N1-C24
4	D	1103	CPS	C26-C25-N1-C24
4	A	1103	CPS	N1-C25-C26-C27
4	B	1103	CPS	N1-C25-C26-C27
4	D	1103	CPS	N1-C25-C26-C27
2	B	1101	ADP	O4'-C1'-N9-C4
4	C	1103	CPS	N1-C25-C26-C27
3	D	1102	A1A4L	N15-C10-N09-C07
4	D	1103	CPS	C30-C31-C32-S
4	B	1103	CPS	C22-C20-C9-C8
4	A	1103	CPS	C22-C20-C9-C5
3	B	1102	A1A4L	C11-C10-N09-C07

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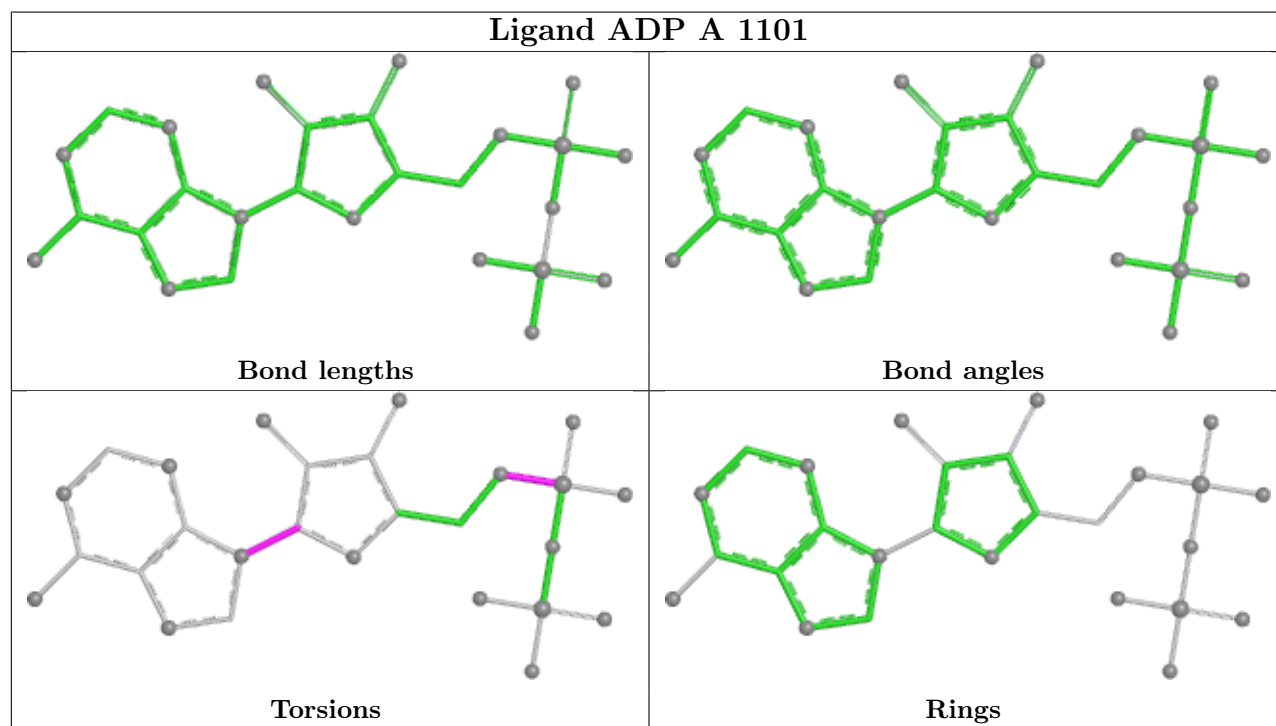
Mol	Chain	Res	Type	Atoms
3	D	1102	A1A4L	C11-C10-N09-C07
3	B	1102	A1A4L	N05-C06-C07-O08
3	A	1102	A1A4L	N15-C10-N09-C07
3	A	1102	A1A4L	C11-C10-N09-C07
3	C	1102	A1A4L	C11-C10-N09-C07
4	D	1103	CPS	C25-C26-C27-N2
3	B	1102	A1A4L	N15-C10-N09-C07
3	C	1102	A1A4L	N15-C10-N09-C07
4	A	1103	CPS	C21-C20-C9-C8
4	D	1103	CPS	C20-C22-C23-C24
3	B	1102	A1A4L	N05-C06-C07-N09
3	D	1102	A1A4L	N05-C06-C07-N09
2	A	1101	ADP	O4'-C1'-N9-C4
4	B	1103	CPS	C22-C20-C9-C5
4	B	1103	CPS	C21-C20-C9-C8
2	A	1101	ADP	O4'-C1'-N9-C8
2	B	1101	ADP	O4'-C1'-N9-C8
4	C	1103	CPS	C25-C26-C27-N2
4	D	1103	CPS	C22-C20-C9-C8
4	D	1103	CPS	C22-C20-C9-C5
2	C	1101	ADP	O4'-C1'-N9-C8
3	A	1102	A1A4L	C07-C06-N05-C16
3	B	1102	A1A4L	C07-C06-N05-N04
4	A	1103	CPS	C25-C26-C27-N2
4	B	1103	CPS	C25-C26-C27-N2
4	D	1103	CPS	C21-C20-C9-C8
2	C	1101	ADP	C5'-O5'-PA-O3A
2	C	1101	ADP	O4'-C1'-N9-C4
4	A	1103	CPS	C20-C22-C23-C24
4	B	1103	CPS	C20-C22-C23-C24
4	A	1103	CPS	C26-C27-N2-C30
2	C	1101	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

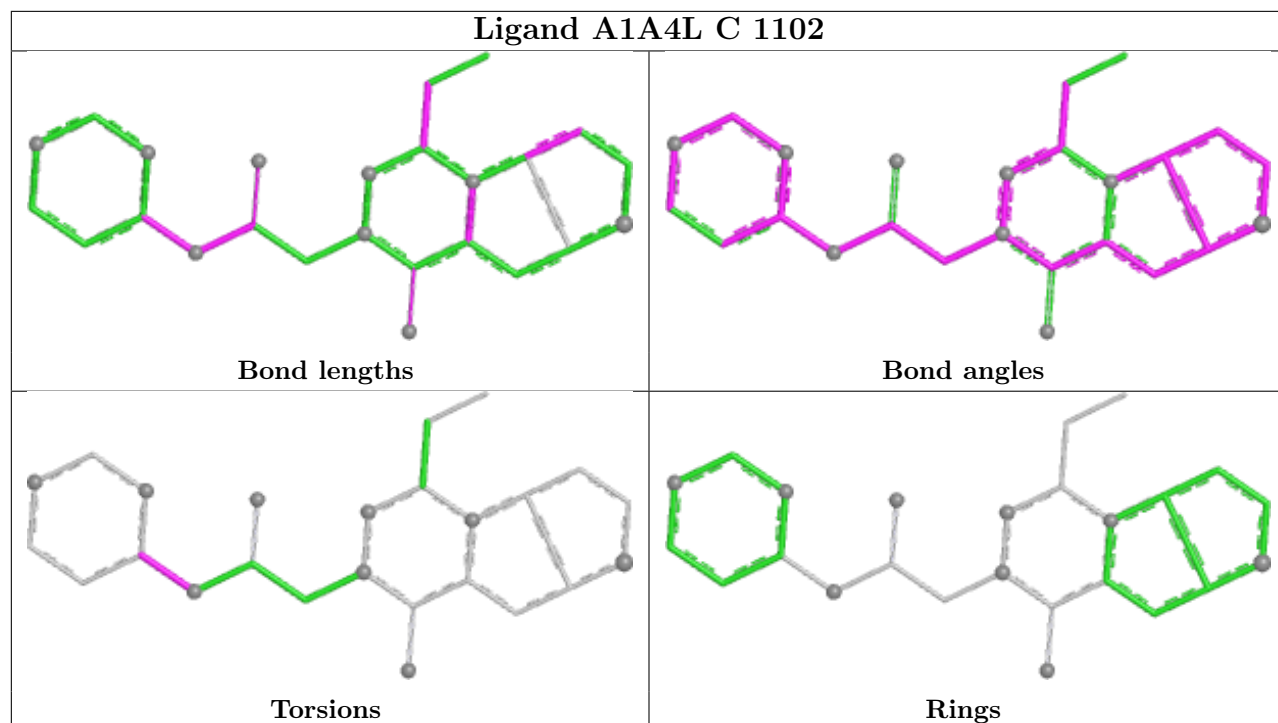
5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	ADP	1	0
3	B	1102	A1A4L	1	0
4	C	1103	CPS	1	0
2	C	1101	ADP	1	0
2	D	1101	ADP	1	0

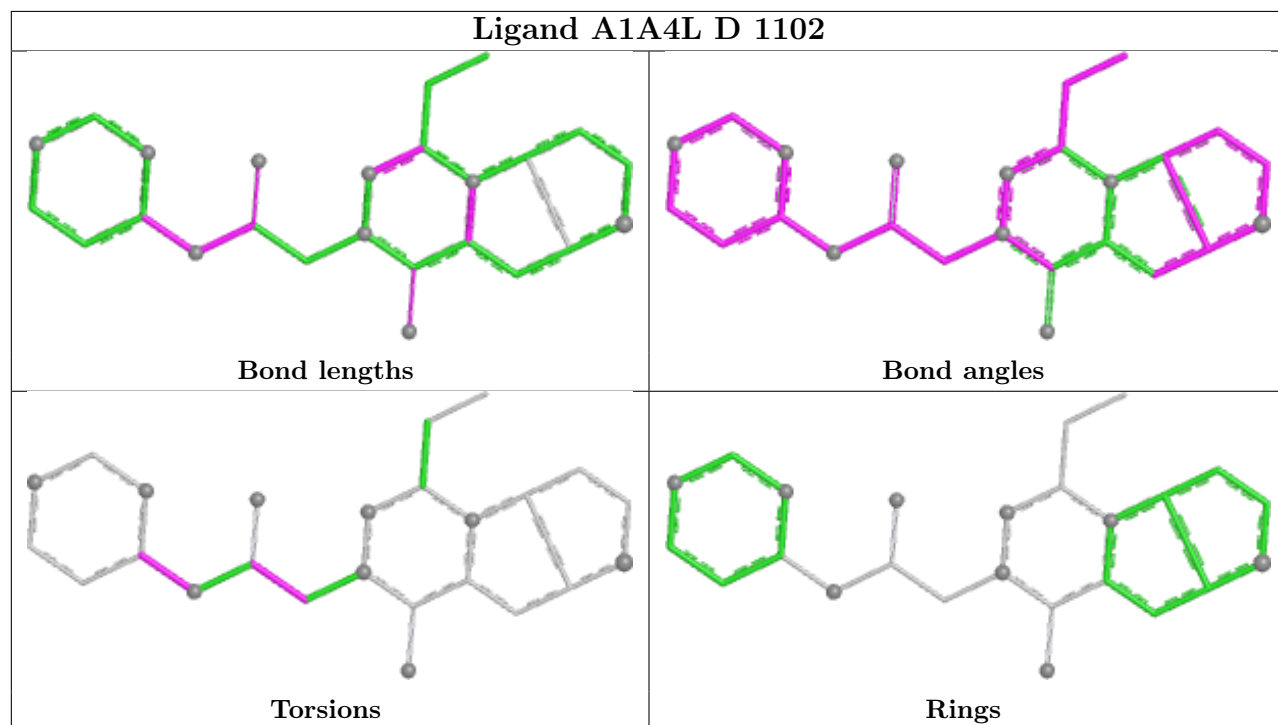
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

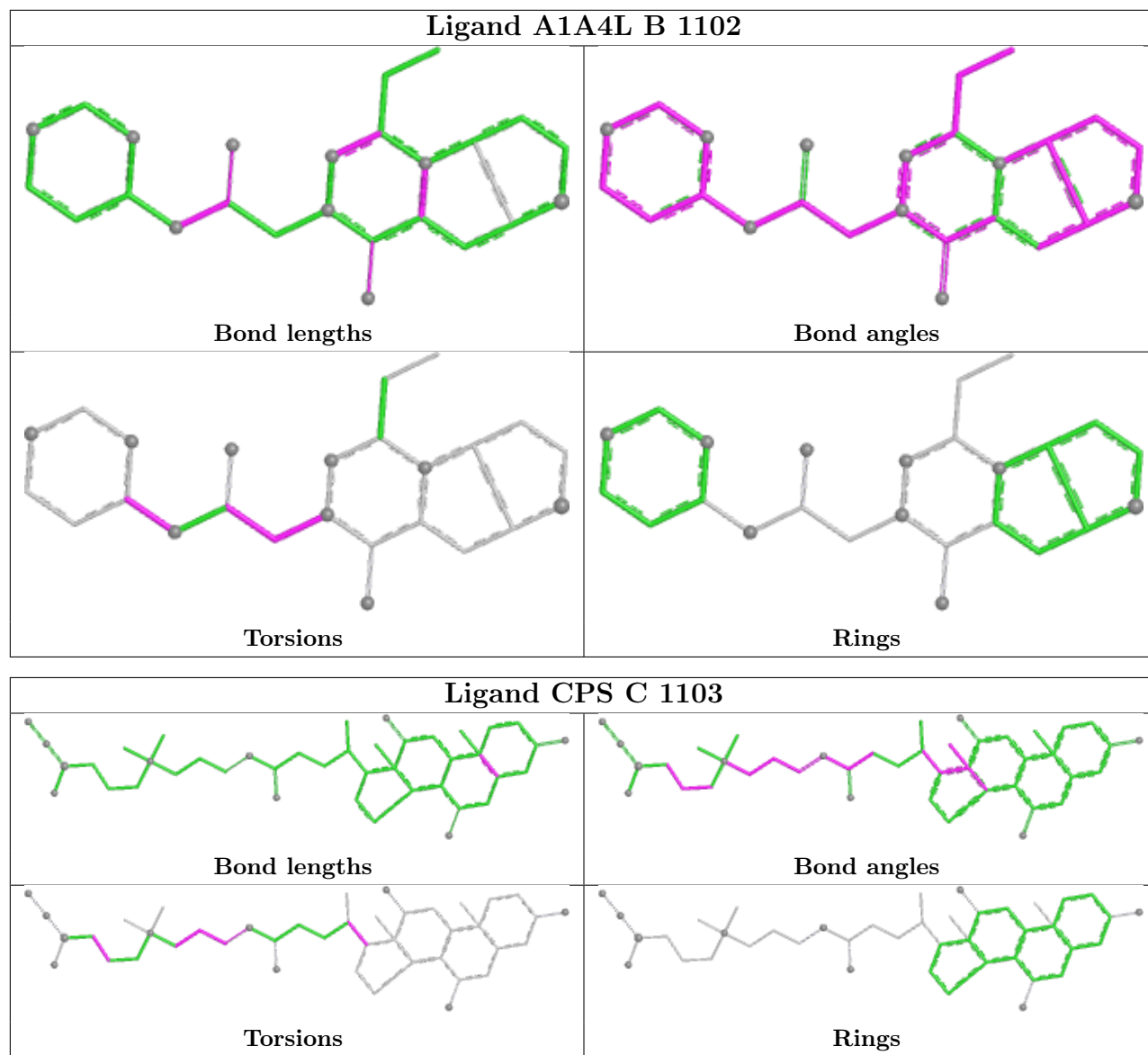


Ligand A1A4L C 1102

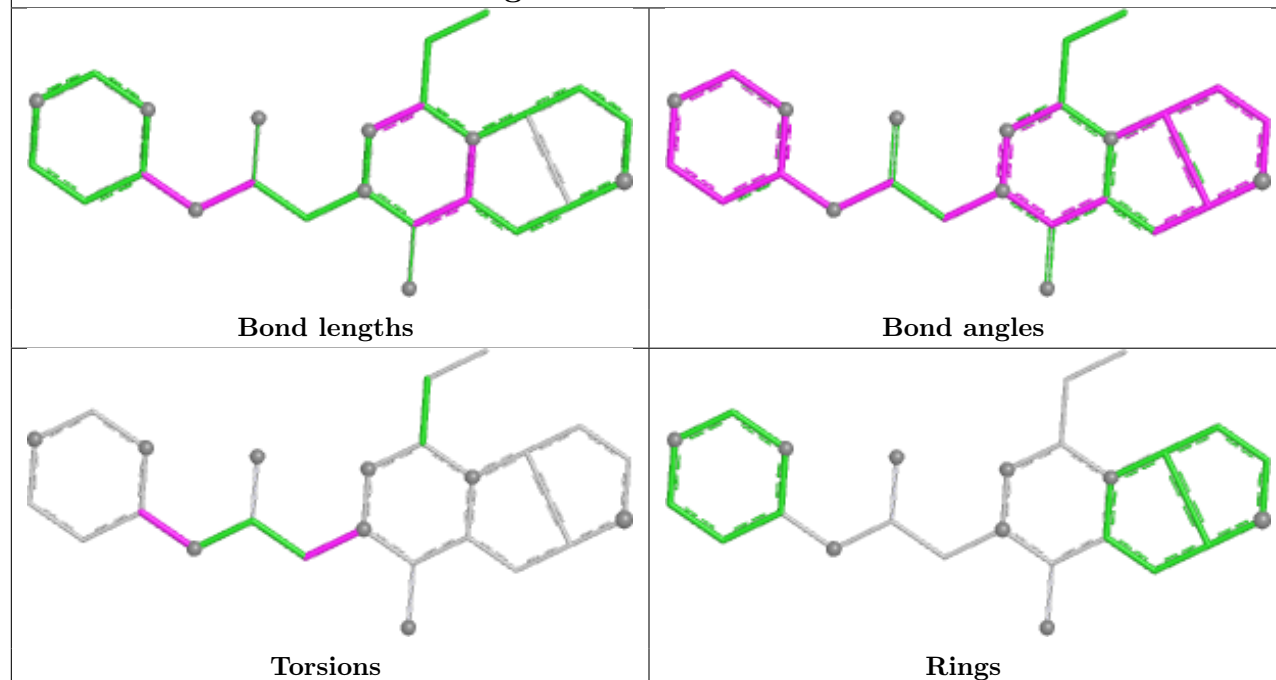


Ligand A1A4L D 1102

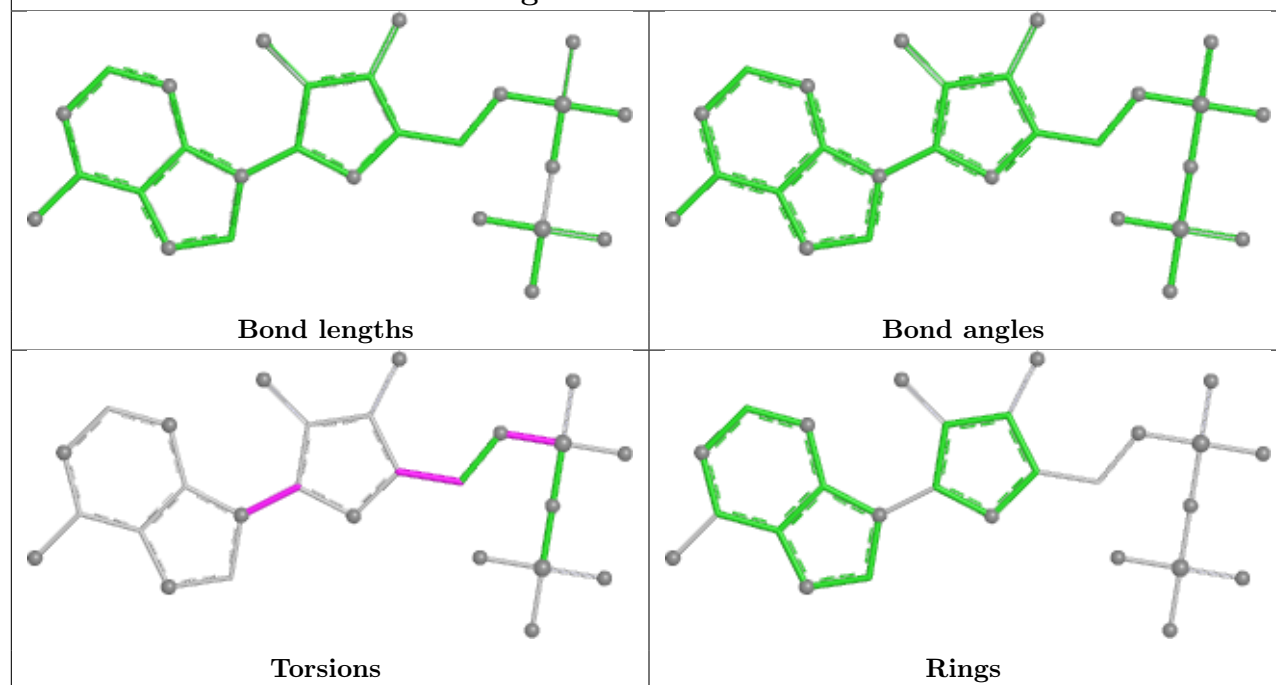


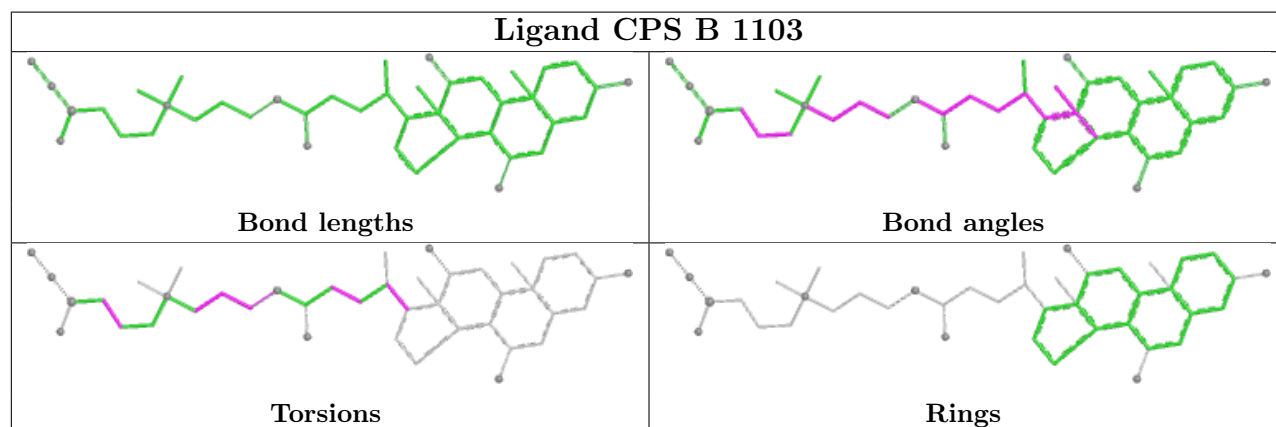
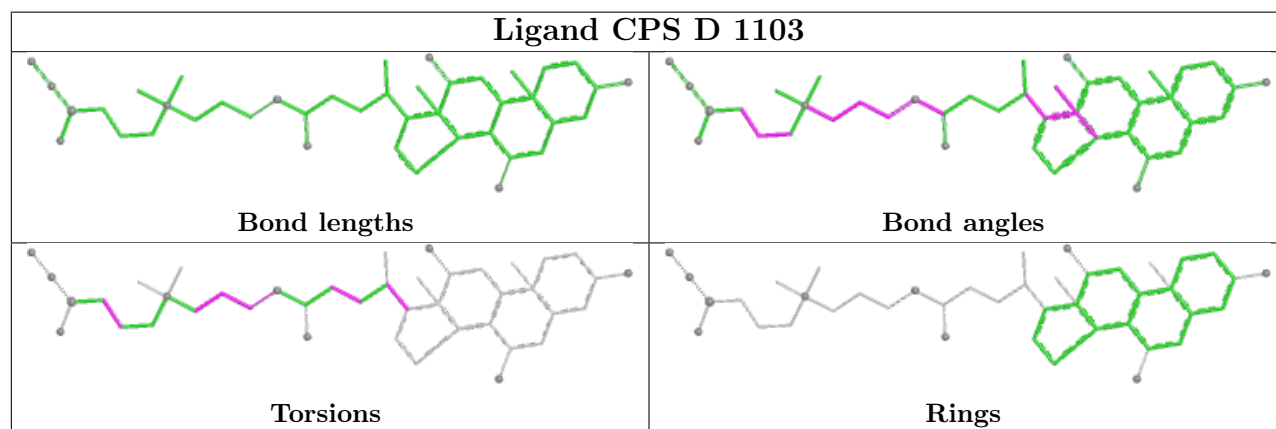
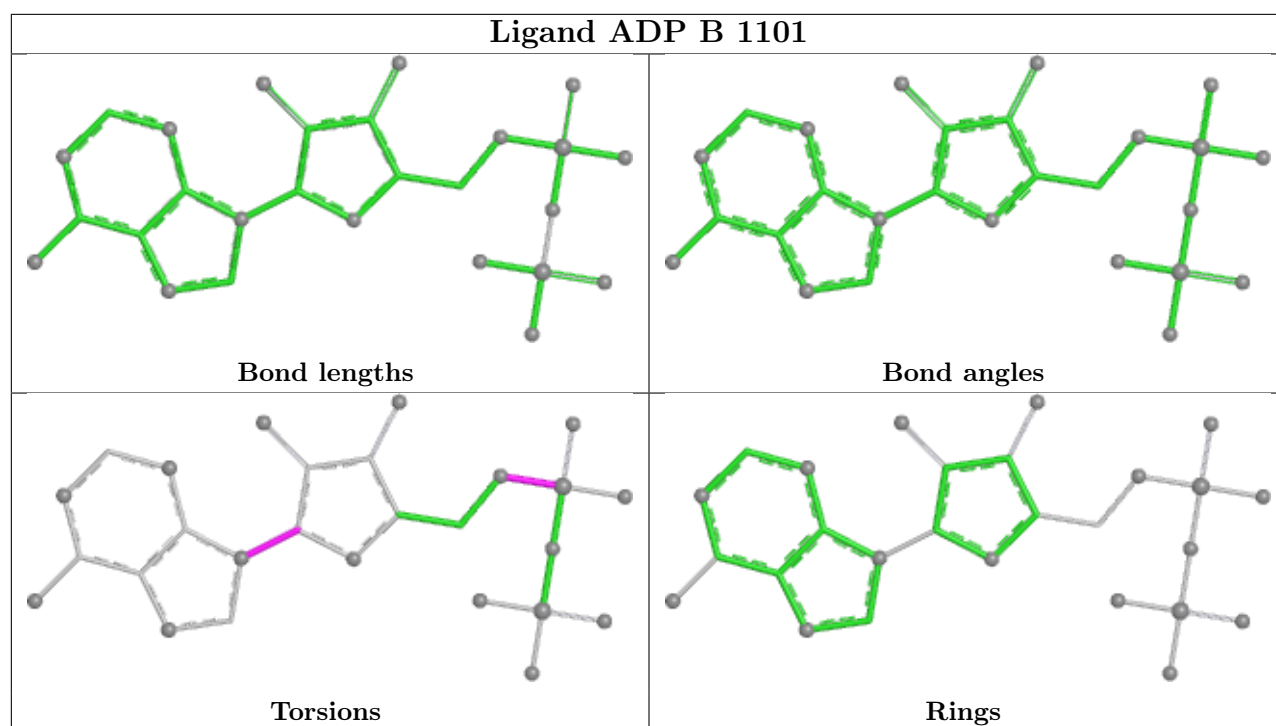


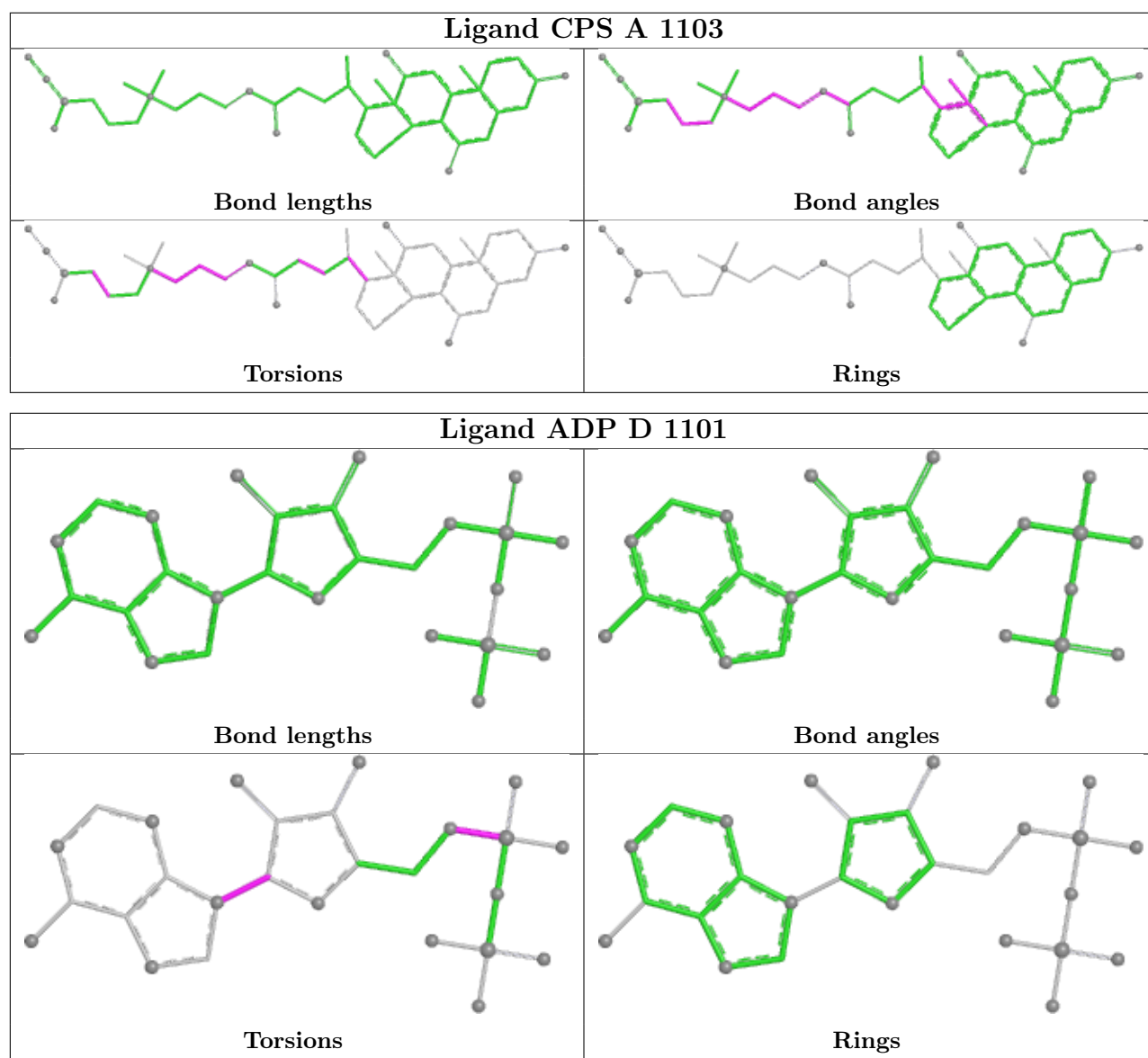
Ligand A1A4L A 1102



Ligand ADP C 1101







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.

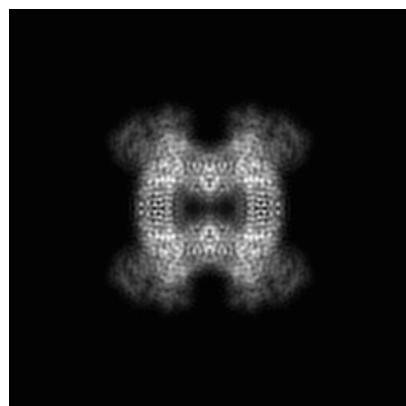
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46855. These allow visual inspection of the internal detail of the map and identification of artifacts.

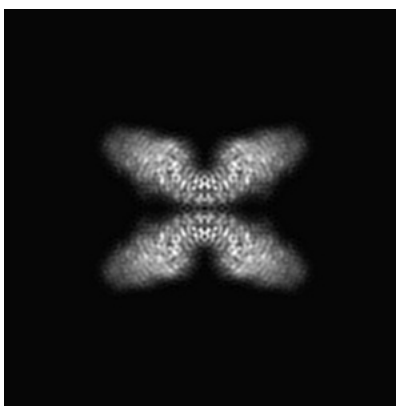
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

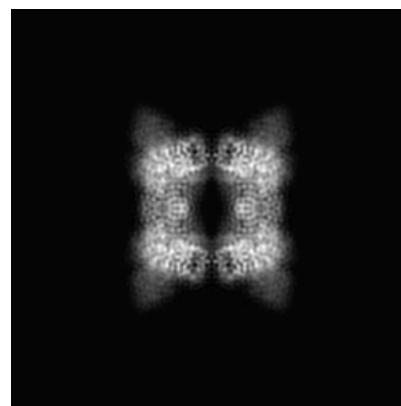
6.1.1 Primary map



X

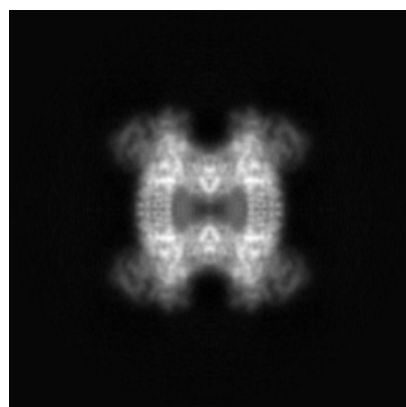


Y

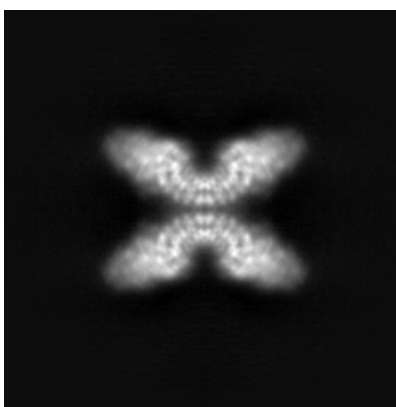


Z

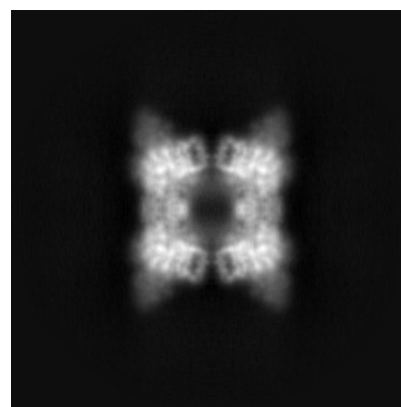
6.1.2 Raw map



X



Y

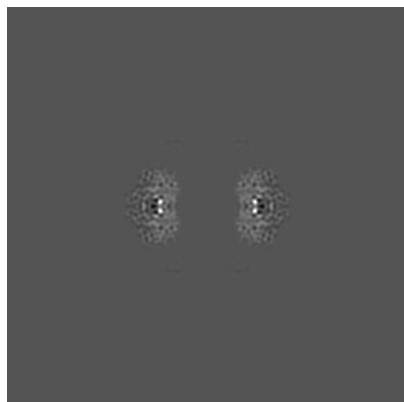


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 150

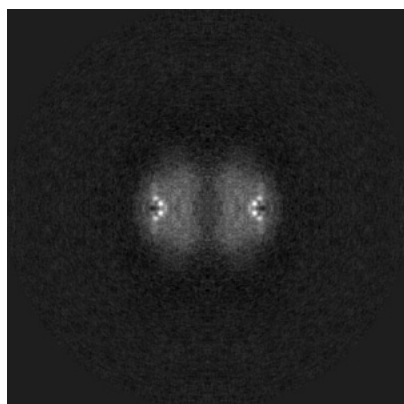


Y Index: 150

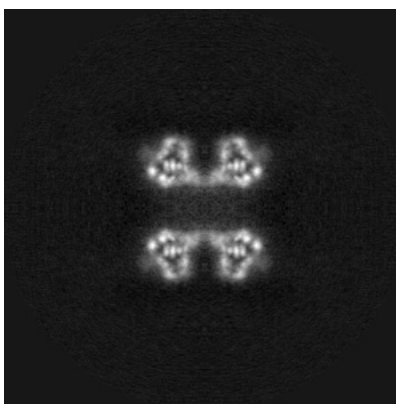


Z Index: 150

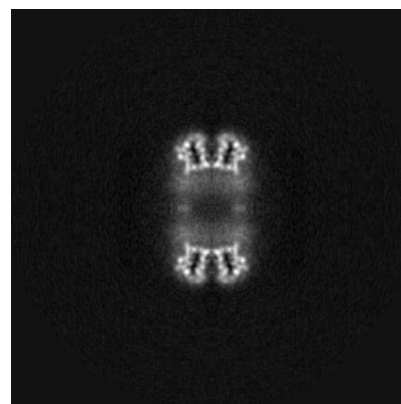
6.2.2 Raw map



X Index: 150



Y Index: 150

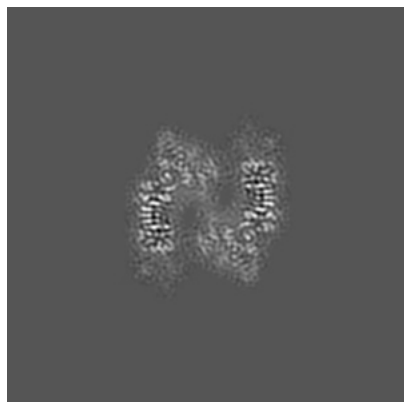


Z Index: 150

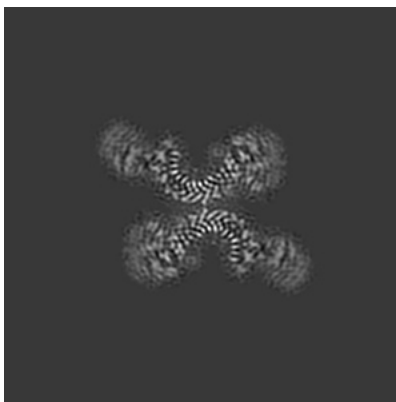
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

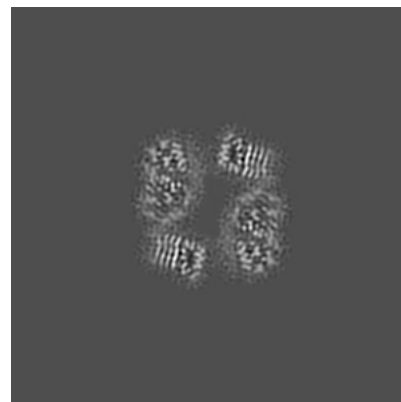
6.3.1 Primary map



X Index: 130

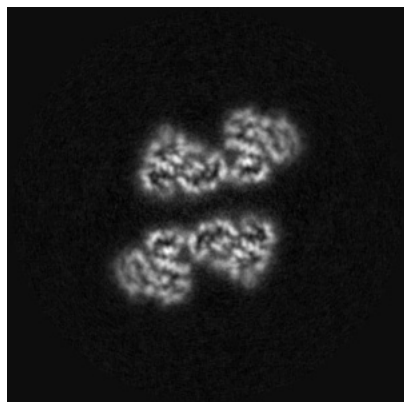


Y Index: 182

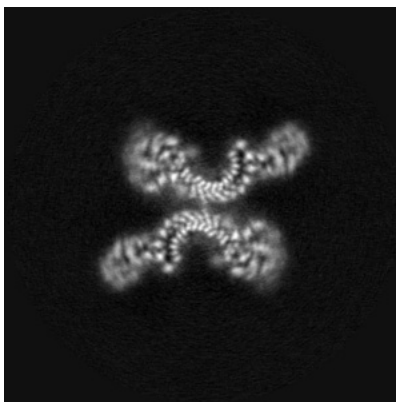


Z Index: 129

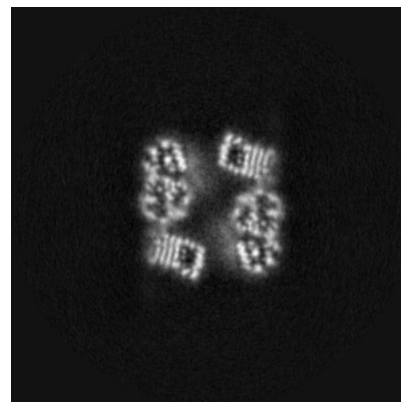
6.3.2 Raw map



X Index: 113



Y Index: 119

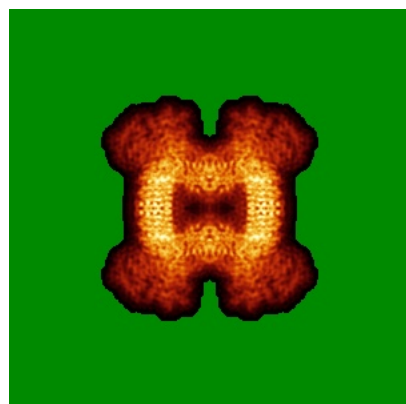


Z Index: 128

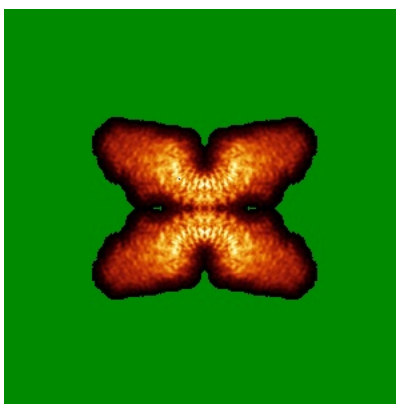
The images above show the largest variance slices of the map in three orthogonal directions.

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

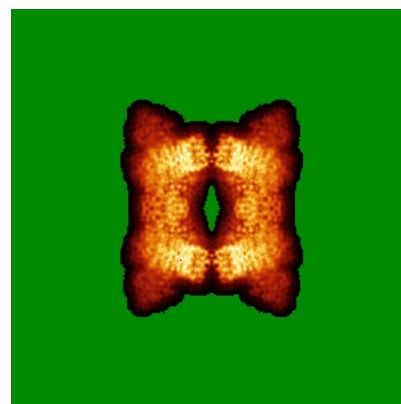
6.4.1 Primary map



X



Y



Z

6.4.2 Raw map



X



Y

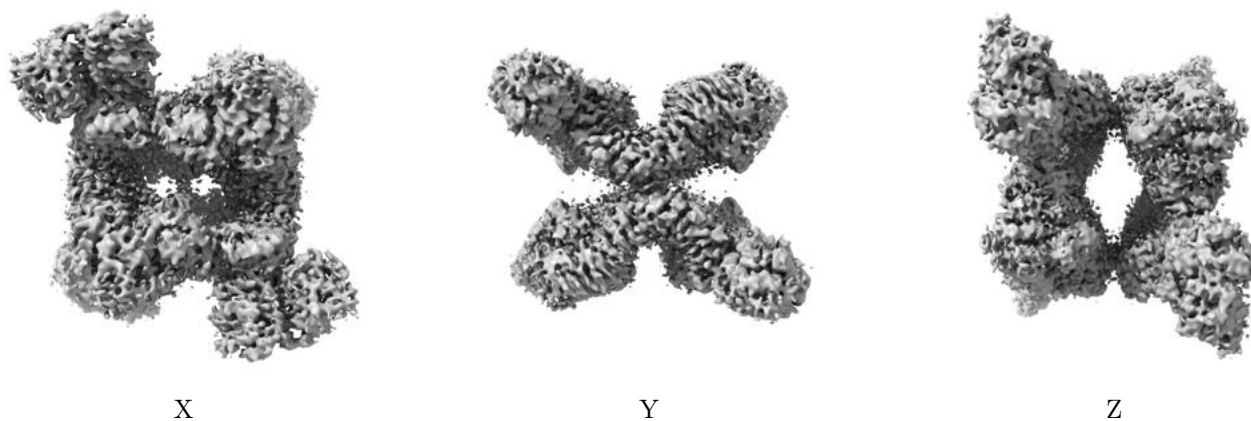


Z

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.

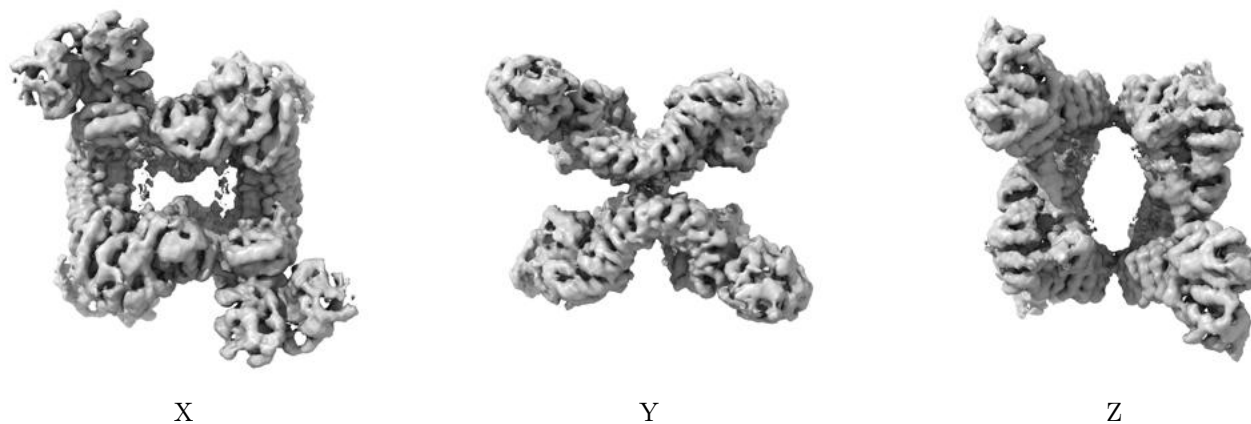
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.016. 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.

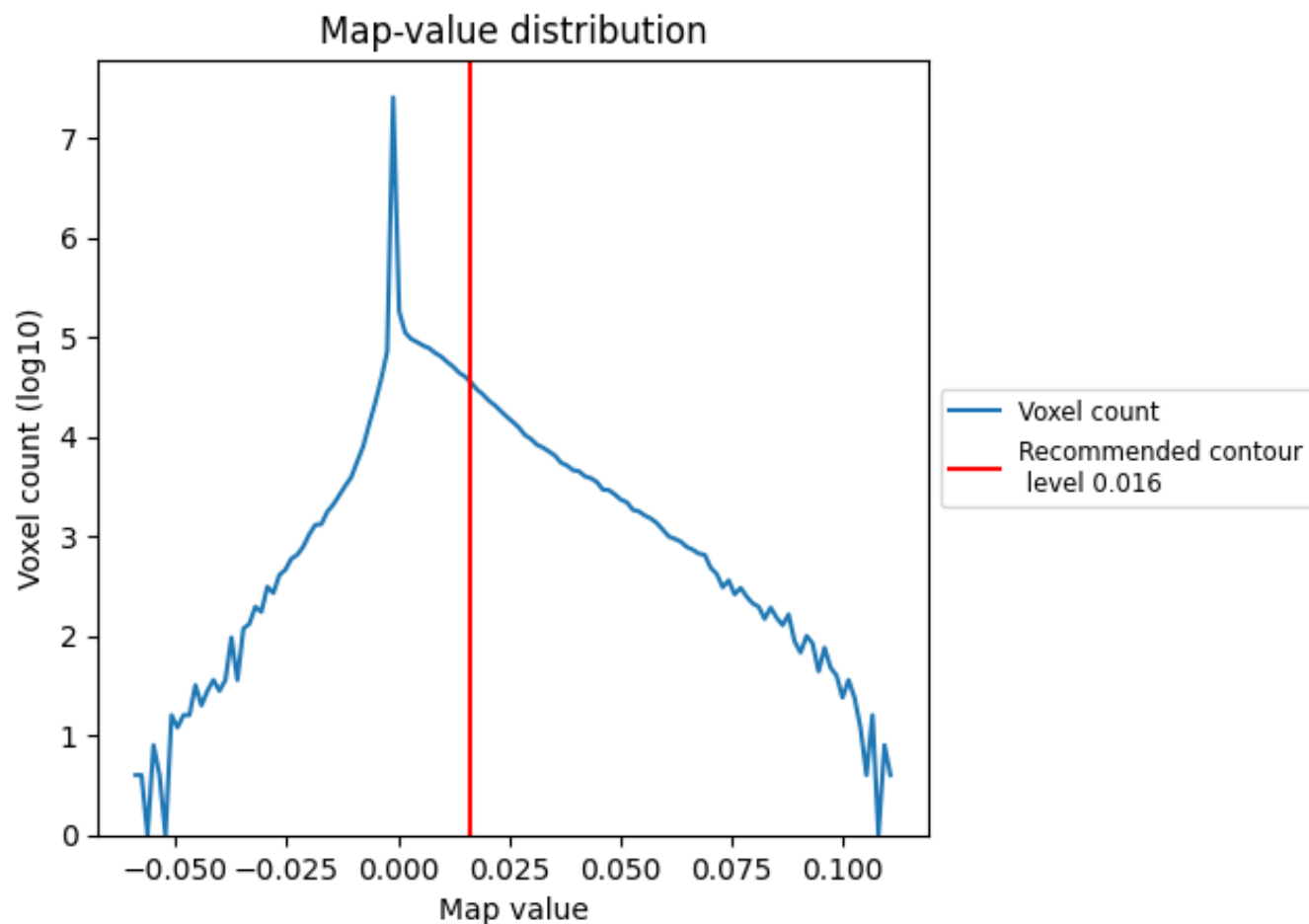
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

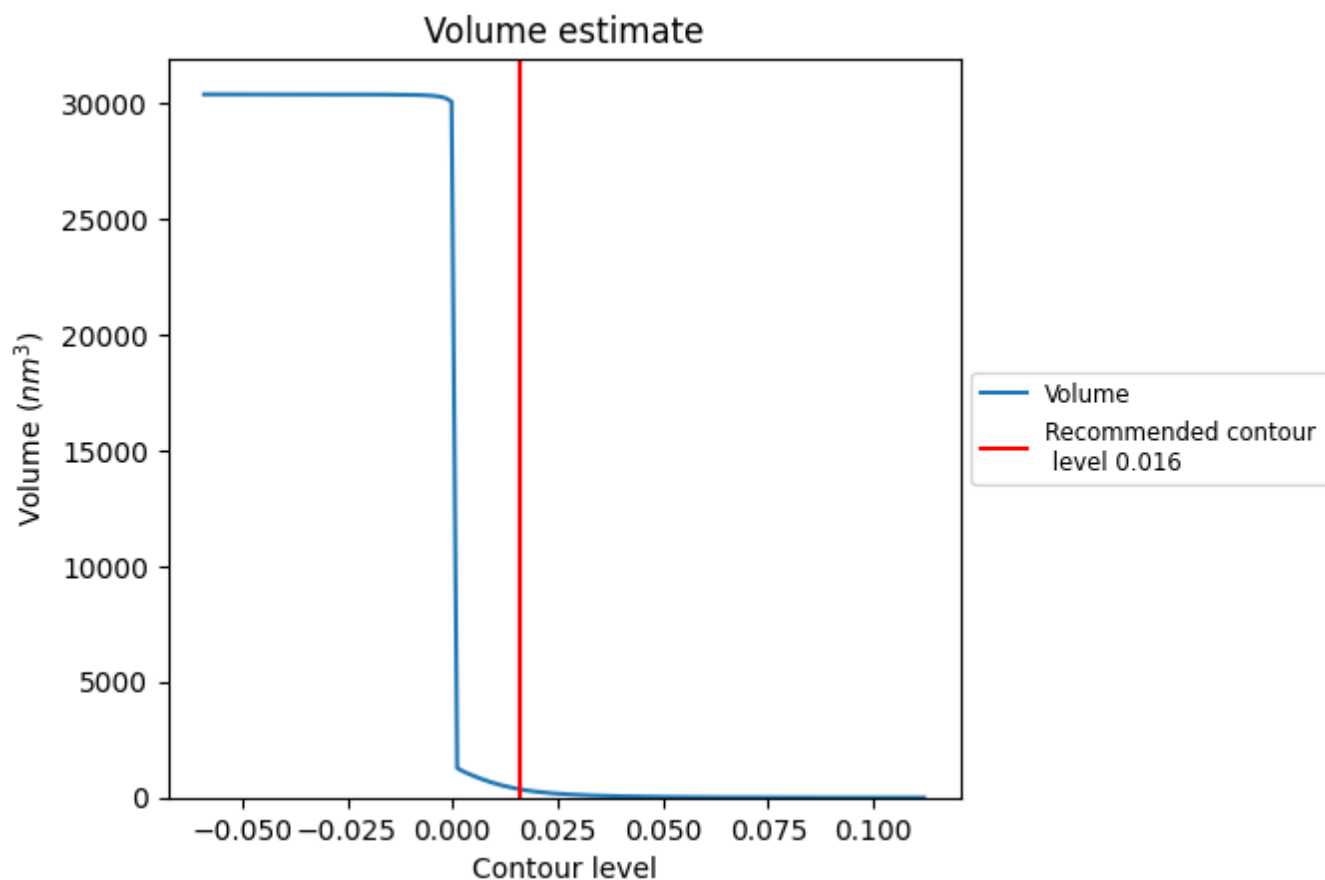
This section contains the results of statistical analysis of the map.

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.

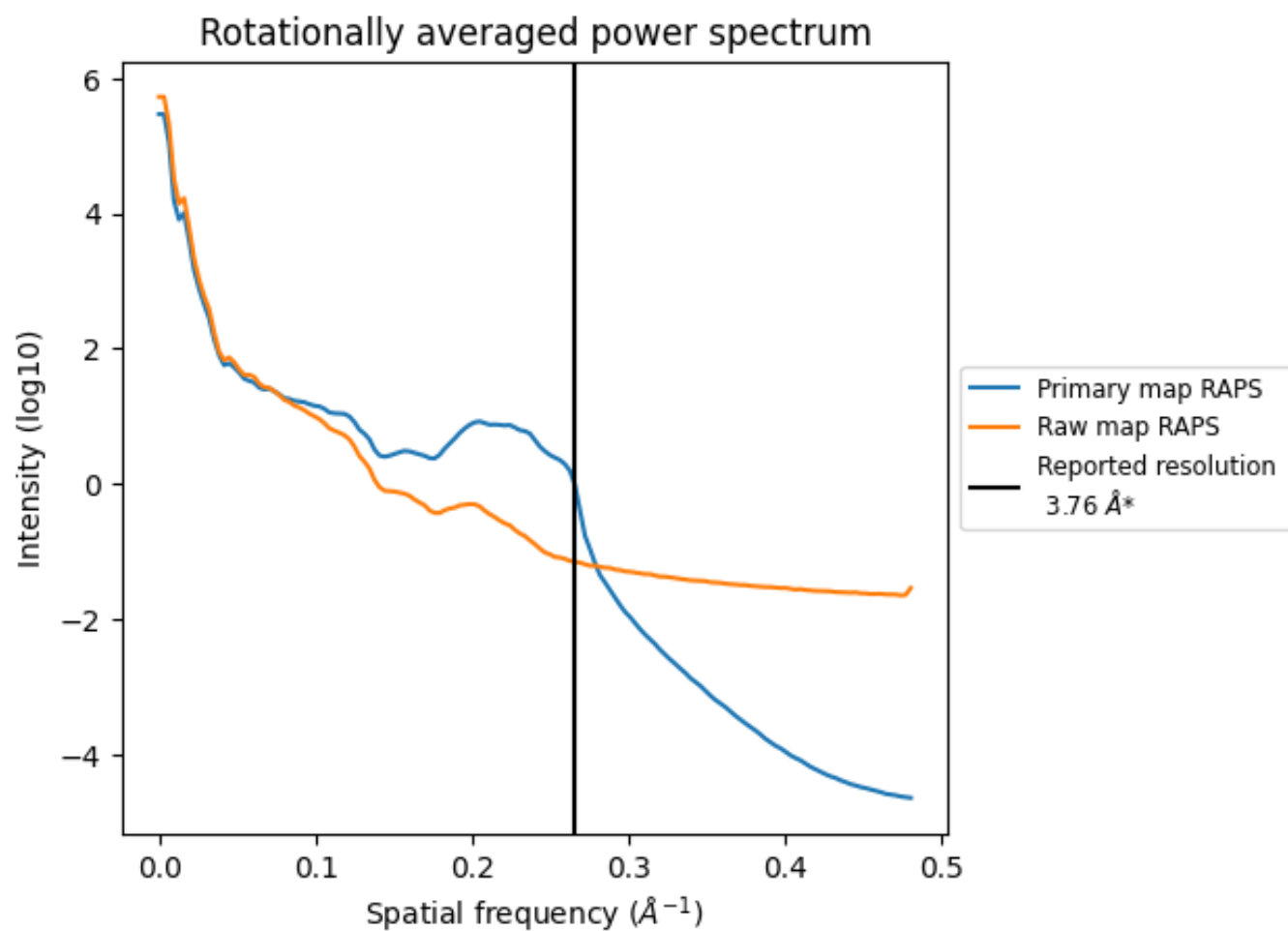
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 359 nm³; this corresponds to an approximate mass of 324 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 ⓘ

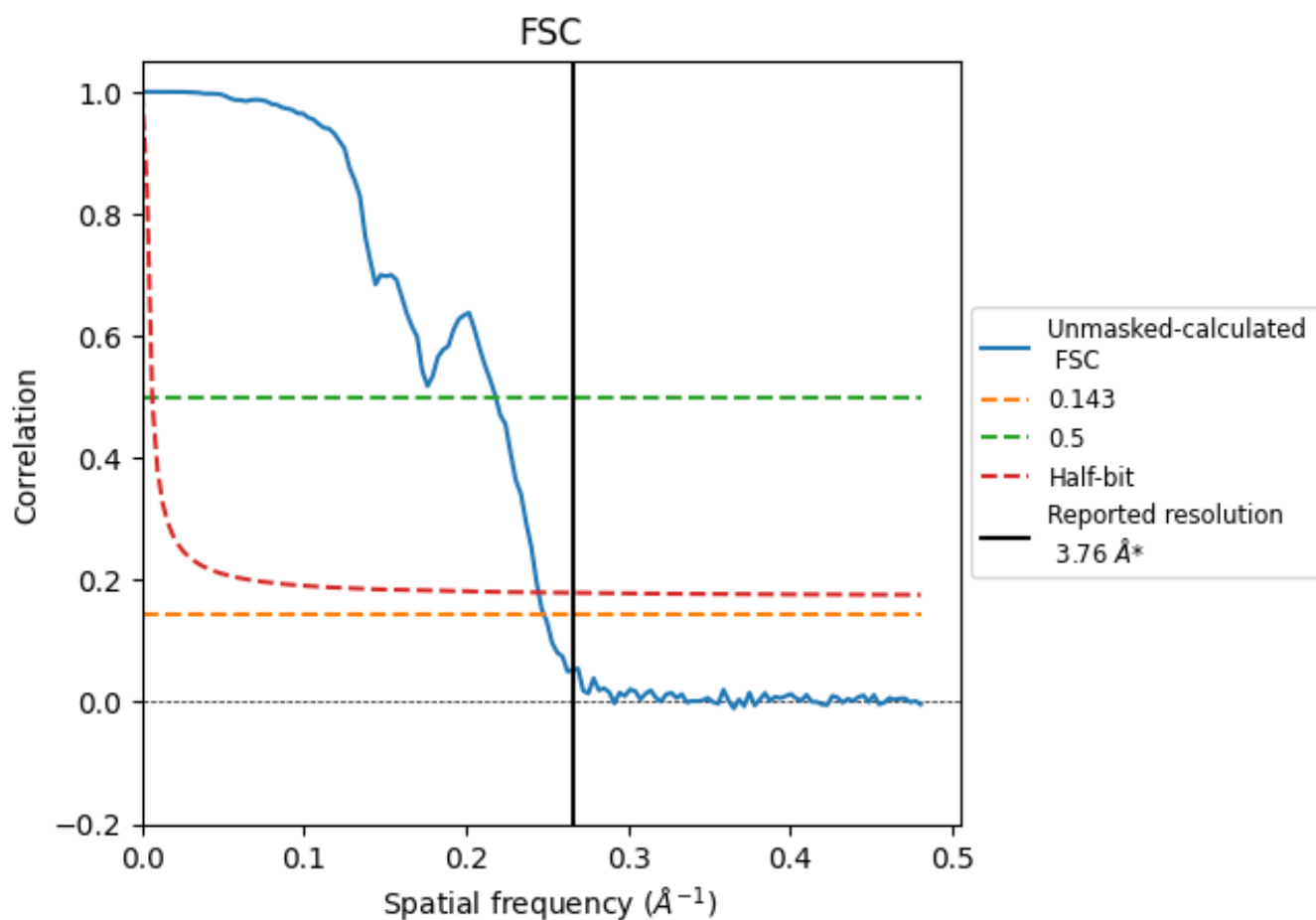


*Reported resolution corresponds to spatial frequency of 0.266 Å⁻¹

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 $0.266 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

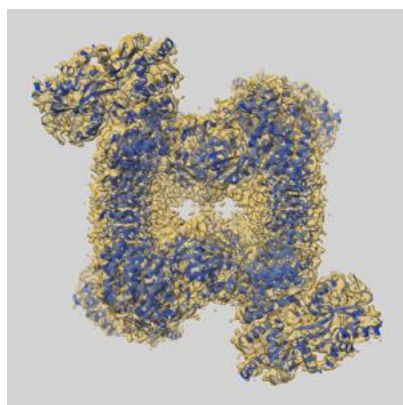
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.76	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.03	4.58	4.08

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

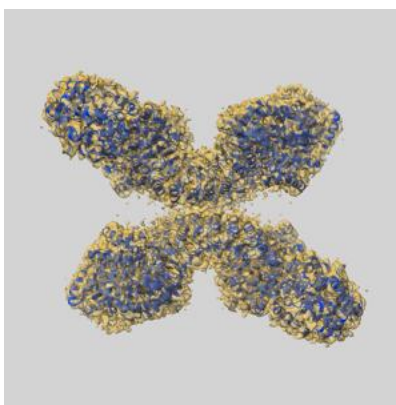
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-46855 and PDB model 9DH3. Per-residue inclusion information can be found in section [3](#) on page [7](#).

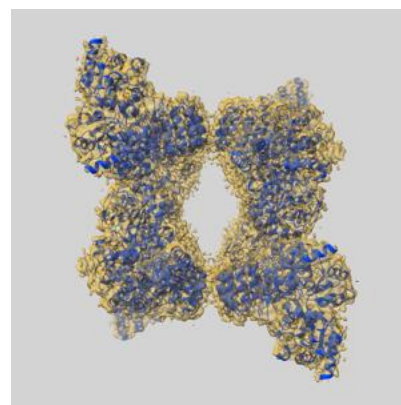
9.1 Map-model overlay [i](#)



X



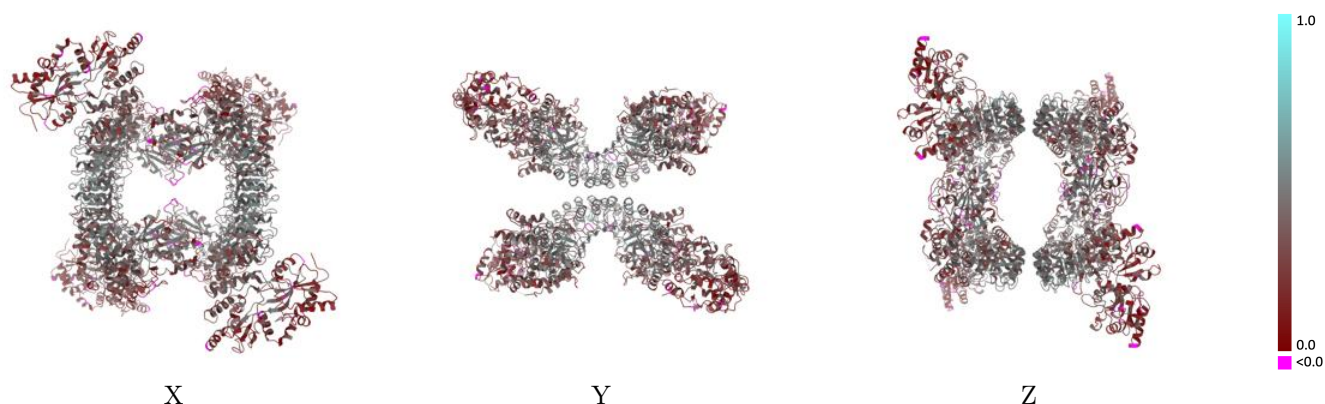
Y



Z

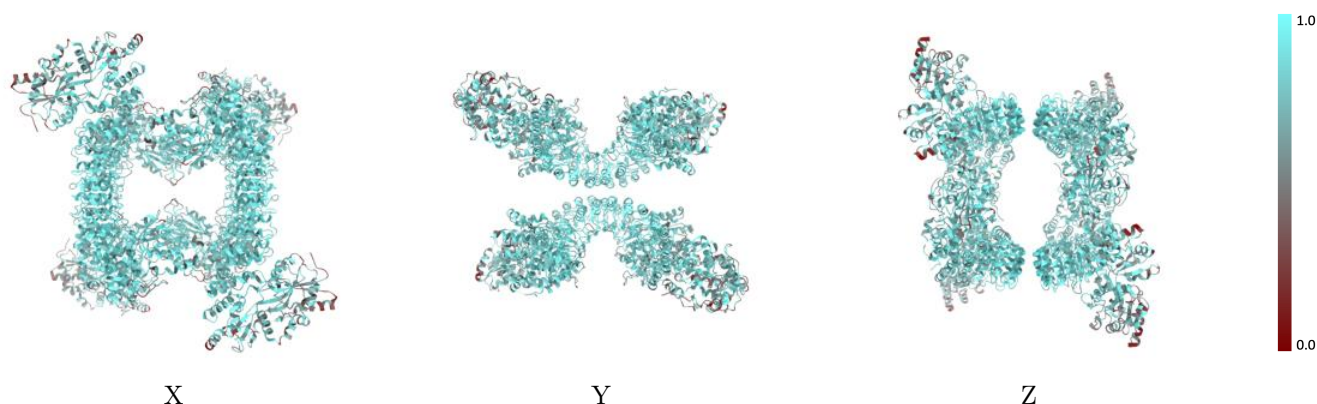
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



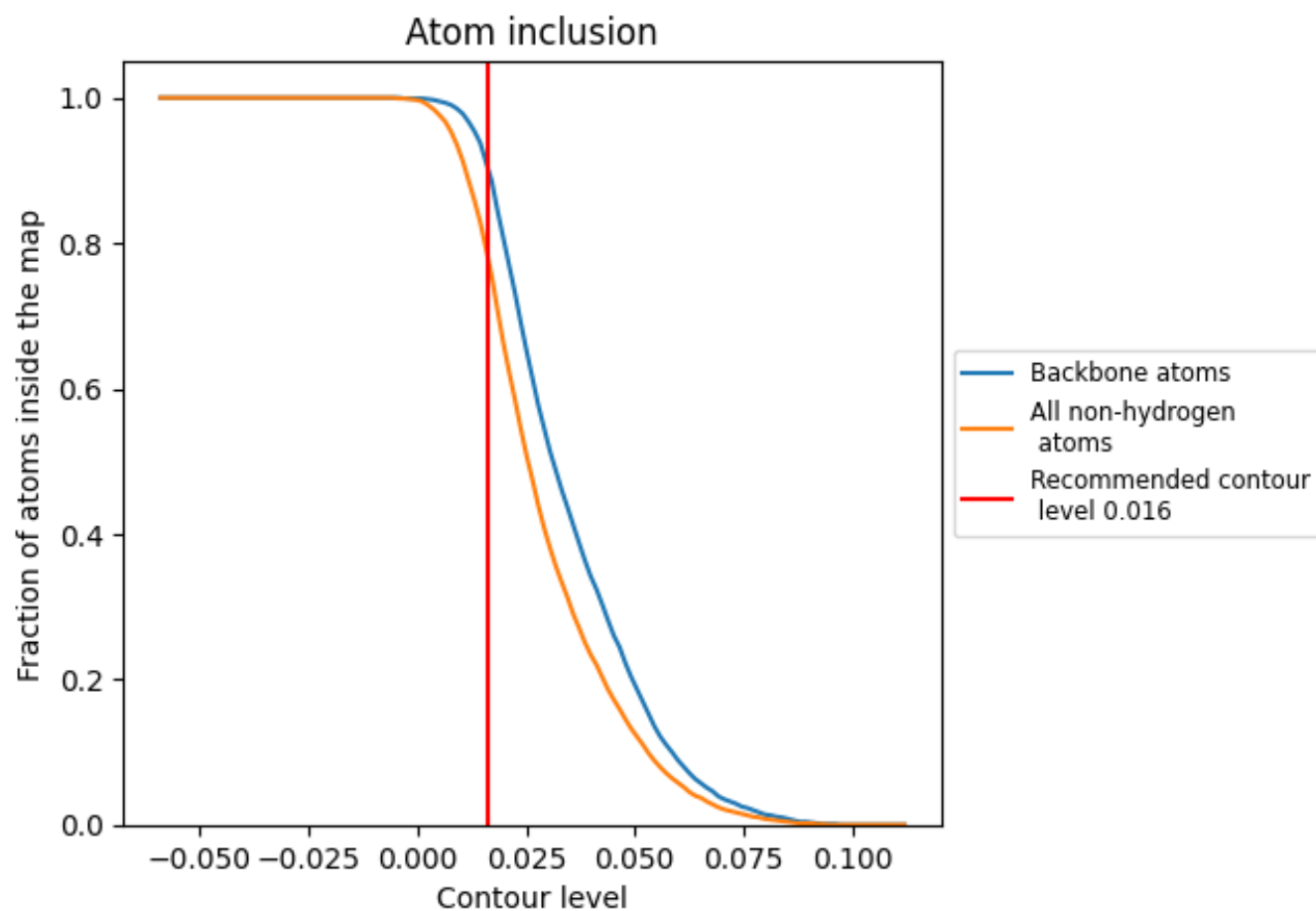
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.016).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 79% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7870	0.3480
A	0.7870	0.3490
B	0.7870	0.3490
C	0.7880	0.3480
D	0.7870	0.3480

