



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:19 PM UTC

PDB ID : 3J7B / pdb_00003j7b
EMDB ID : EMD-6314
Title : Catalase solved at 3.2 Angstrom resolution by MicroED
Authors : Nannenga, B.L.; Shi, D.; Hattne, J.; Reyes, F.E.; Gonen, T.
Deposited on : 2014-06-09
Resolution : 3.20 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

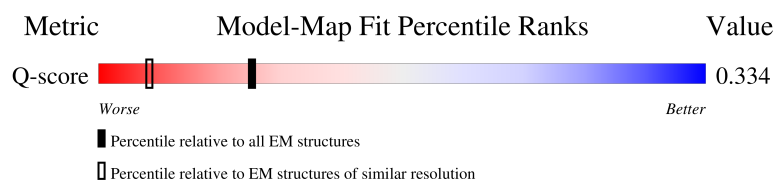
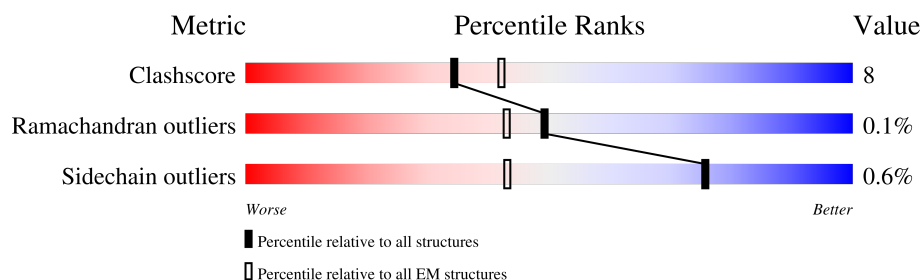
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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	527	19% 77% 17% • 5%
1	B	527	23% 75% 20% 5%
1	C	527	77% 76% 19% 5%
1	D	527	61% 75% 19% • 5%

2 Entry composition [i](#)

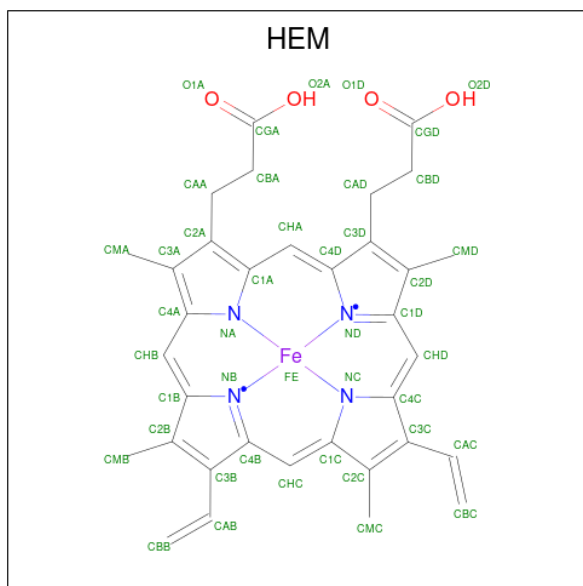
There are 3 unique types of molecules in this entry. The entry contains 16432 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Catalase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	499	Total	C	N	O	S	0	0
			4017	2548	717	738	14		
1	B	499	Total	C	N	O	S	0	0
			4017	2548	717	738	14		
1	C	499	Total	C	N	O	S	0	0
			4017	2548	717	738	14		
1	D	499	Total	C	N	O	S	0	0
			4017	2548	717	738	14		

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
2	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0

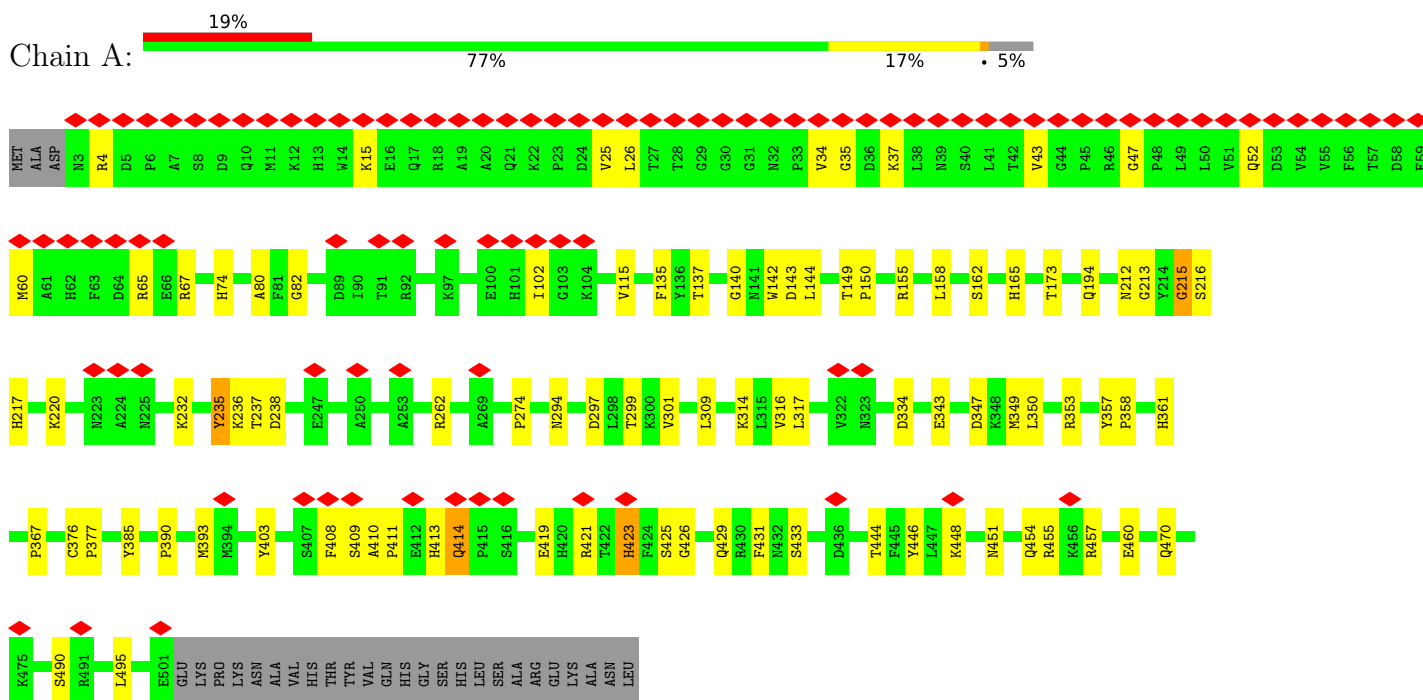
- # NDP

Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0
3	C	1	Total 48	C 21	N 7	O 17	P 3	0
3	D	1	Total 48	C 21	N 7	O 17	P 3	0

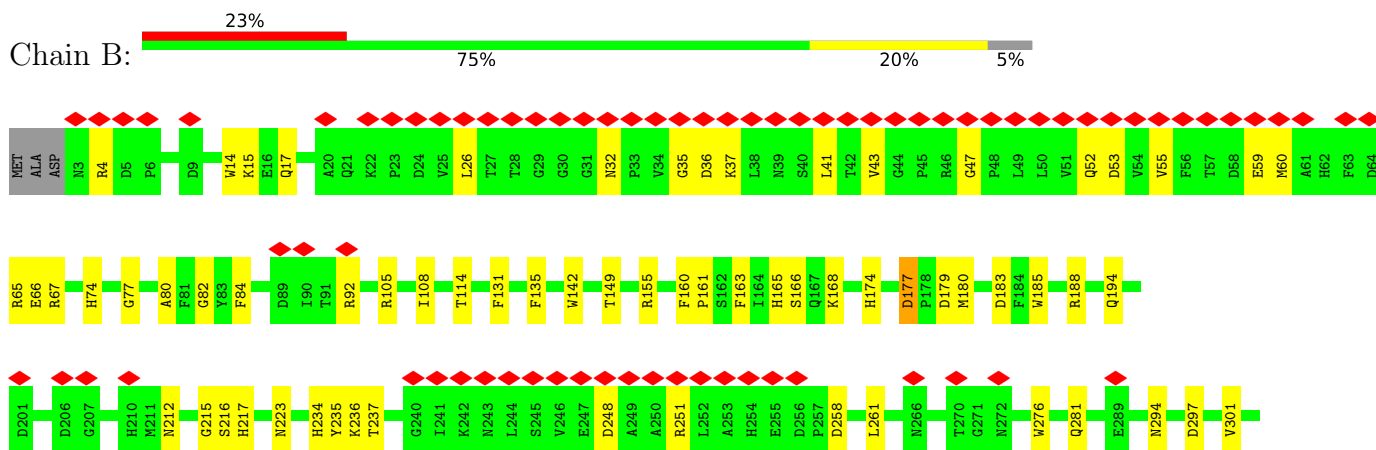
3 Residue-property plots [i](#)

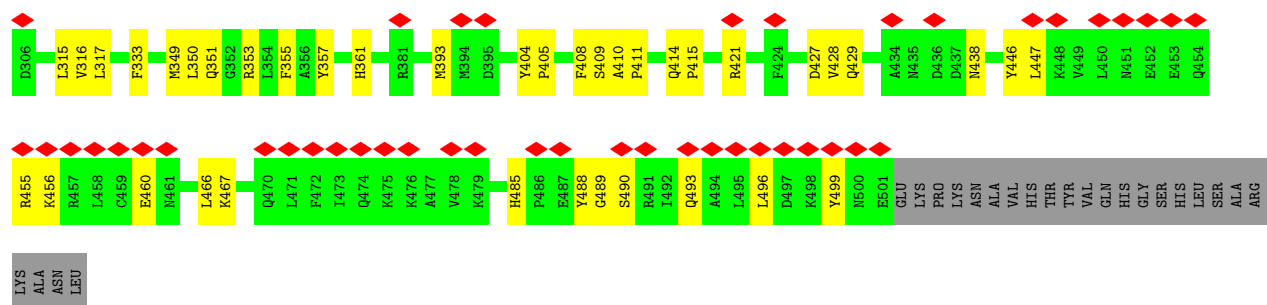
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

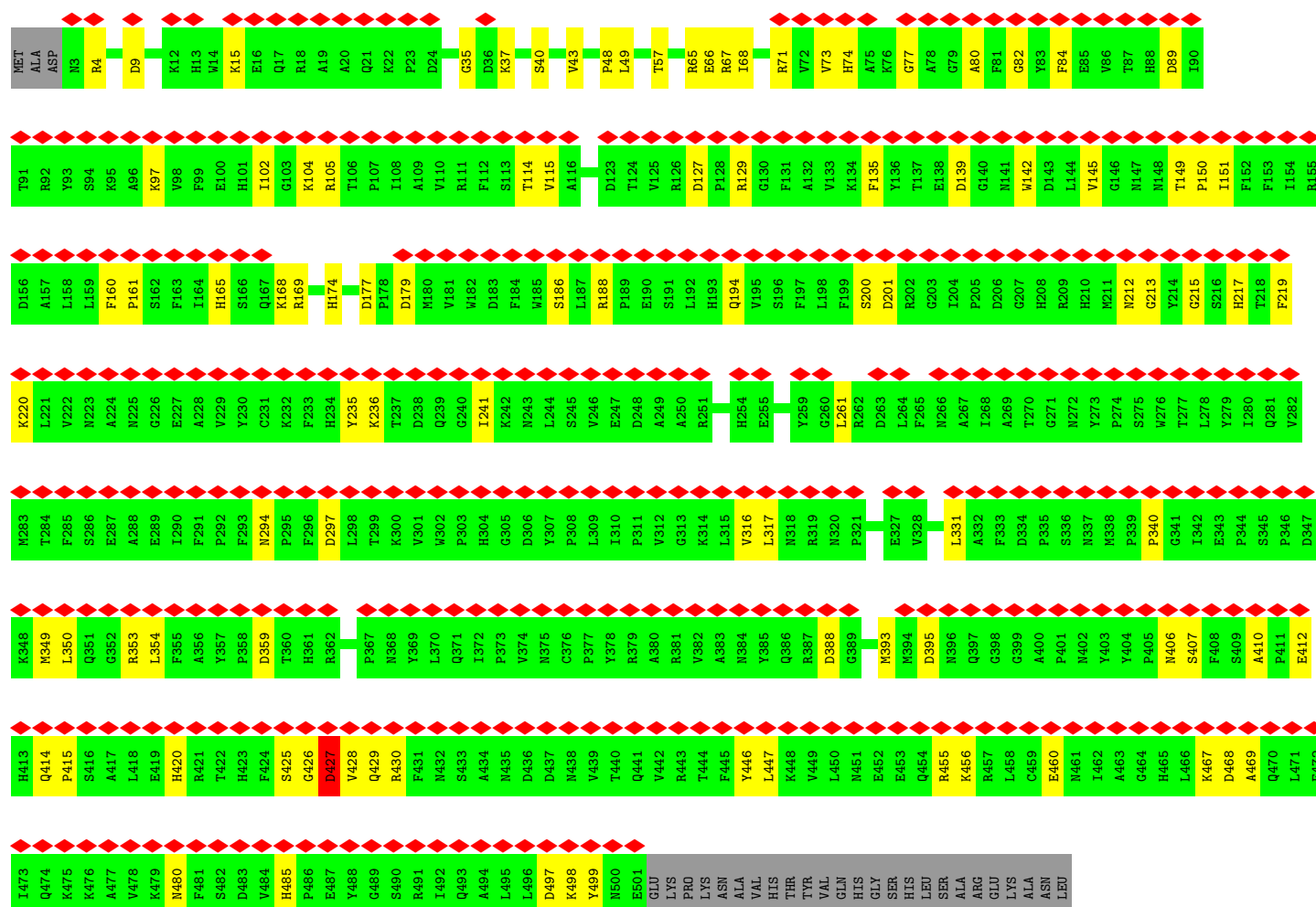
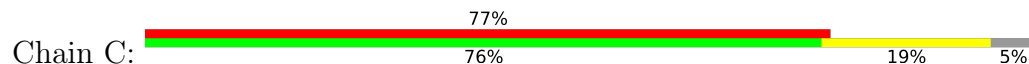


• Molecule 1: Catalase

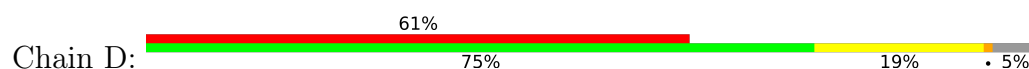




• Molecule 1: Catalase



• Molecule 1: Catalase



GLU LYS ALA ASN LEU	I462	A463	G464	H465	L466	K467	D468	A469	Q470	L471	F472	I473	Q474	K475	K476	A477	V478	K479	N480	F481	S482	D483	V484	H485	P486	E487	Y488	G489	S490	R491	I492	Q493	A494	L495	L496	D497	K498	Y499	N500	E501	GLU	LYS	PRO	LYS	ASN	ALA	VAL	HIS	THR	TYR	VAL	VAL	GLN	HIS	GLY	SER	HIS	LEU	SER	ALA	ARG
	Y403	Y404	P405	N406	S407	F408	S409	A410	P411	E412	H413	Q414	P415	S336	A416	A417	L418	E419	H420	R421	T422	H423	F424	S425	G426	D427	V428	Q429	R430	F431	N432	S433	A434	N435	D436	D437	N438	V439	T440	Q441	V442	R443	T444	F445	Y446	L447	K448	V449	L450	N451	E452	E453	Q454	R455	K456	R457	L458	C459	E460	N461	
	I310	P311	V312	G313	K314	L315	V316	L317	E327	F333	D334	P335	S336	N337	M338	P339	P340	G341	I342	E343	P344	S345	P346	D347	K348	N349	L350	Q351	G352	R353	L354	F355	A356	Y357	P358	D359	T360	H361	R362	G366	P367	N368	V374	R381	V382	A383	N384	Y385	Q386	P390	M393	M394	D395								
	I310	P311	V312	G313	K314	L315	V316	L317	E327	F333	D334	P335	S336	N337	M338	P339	P340	G341	I342	E343	P344	S345	P346	D347	K348	N349	L350	Q351	G352	R353	L354	F355	A356	Y357	P358	D359	T360	H361	R362	G366	P367	N368	V374	R381	V382	A383	N384	Y385	Q386	P390	M393	M394	D395								
	I310	P311	V312	G313	K314	L315	V316	L317	E327	F333	D334	P335	S336	N337	M338	P339	P340	G341	I342	E343	P344	S345	P346	D347	K348	N349	L350	Q351	G352	R353	L354	F355	A356	Y357	P358	D359	T360	H361	R362	G366	P367	N368	V374	R381	V382	A383	N384	Y385	Q386	P390	M393	M394	D395								
GLU LYS ALA ASN LEU	L175	K176	D177	P178	D179	M180	V181	W182	D183	F184	W185	S186	L187	R188	P189	E190	L192	H193	Q194	V195	S196	F197	L198	F199	S200	D201	R202	G203	I204	P205	R209	H210	M211	N212	G213	Y214	G215	S216	H217	T218	F219	K220	L221	V222	N223	A224	N225	G226	E227	A228	V229	Y230	C231	K232	F233	H234	Y235	K236			
	L175	K176	D177	P178	D179	M180	V181	W182	D183	F184	W185	S186	L187	R188	P189	E190	L192	H193	Q194	V195	S196	F197	L198	F199	S200	D201	R202	G203	I204	P205	R209	H210	M211	N212	G213	Y214	G215	S216	H217	T218	F219	K220	L221	V222	N223	A224	N225	G226	E227	A228	V229	Y230	C231	K232	F233	H234	Y235	K236			
	L175	K176	D177	P178	D179	M180	V181	W182	D183	F184	W185	S186	L187	R188	P189	E190	L192	H193	Q194	V195	S196	F197	L198	F199	S200	D201	R202	G203	I204	P205	R209	H210	M211	N212	G213	Y214	G215	S216	H217	T218	F219	K220	L221	V222	N223	A224	N225	G226	E227	A228	V229	Y230	C231	K232	F233	H234	Y235	K236			
	L175	K176	D177	P178	D179	M180	V181	W182	D183	F184	W185	S186	L187	R188	P189	E190	L192	H193	Q194	V195	S196	F197	L198	F199	S200	D201	R202	G203	I204	P205	R209	H210	M211	N212	G213	Y214	G215	S216	H217	T218	F219	K220	L221	V222	N223	A224	N225	G226	E227	A228	V229	Y230	C231	K232	F233	H234	Y235	K236			
	L175	K176	D177	P178	D179	M180	V181	W182	D183	F184	W185	S186	L187	R188	P189	E190	L192	H193	Q194	V195	S196	F197	L198	F199	S200	D201	R202	G203	I204	P205	R209	H210	M211	N212	G213	Y214	G215	S216	H217	T218	F219	K220	L221	V222	N223	A224	N225	G226	E227	A228	V229	Y230	C231	K232	F233	H234	Y235	K236			

4 Experimental information

Property	Value	Source
EM reconstruction method	CRYSTALLOGRAPHY	Depositor
Imposed symmetry	3D CRYSTAL, a =Not provided Å, b =Not provided Å, c =Not provided Å, α =Not provided°, β =Not provided°, γ =Not provided°, space group=Not provided	Depositor
Number of images used	Not provided	
Resolution determination method	DIFFRACTION PATTERN/LAYERLINES	Depositor
CTF correction method	Not provided	
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	0.1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	TVIPS TEMCAM-F416 (4k x 4k)	Depositor
Maximum map value	5.384	Depositor
Minimum map value	-3.715	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	67.64004, 172.08072, 182.0712	wwPDB
Map dimensions	240, 216, 90	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.751556, 0.79667, 0.75863	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.41	0/4137	0.86	5/5619 (0.1%)
1	B	0.42	0/4137	0.88	6/5619 (0.1%)
1	C	0.41	0/4137	0.86	8/5619 (0.1%)
1	D	0.41	0/4137	0.84	5/5619 (0.1%)
All	All	0.41	0/16548	0.86	24/22476 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	426	GLY	N-CA-C	-7.11	101.64	111.09
1	D	77	GLY	N-CA-C	6.81	121.32	110.90
1	A	425	SER	N-CA-C	6.53	119.08	108.76
1	B	489	GLY	N-CA-C	6.41	119.93	112.50
1	B	188	ARG	CA-C-N	6.31	126.01	119.82
1	B	188	ARG	C-N-CA	6.31	126.01	119.82
1	C	177	ASP	CA-C-N	6.29	125.97	119.56
1	C	177	ASP	C-N-CA	6.29	125.97	119.56
1	C	77	GLY	N-CA-C	6.10	120.23	110.90
1	B	77	GLY	N-CA-C	5.97	120.03	110.90
1	B	177	ASP	CA-C-N	5.80	125.66	119.28
1	B	177	ASP	C-N-CA	5.80	125.66	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	215	GLY	N-CA-C	-5.72	107.57	114.66
1	A	414	GLN	CA-C-N	5.32	125.14	119.28
1	A	414	GLN	C-N-CA	5.32	125.14	119.28
1	C	426	GLY	N-CA-C	-5.31	104.64	110.96
1	D	366	GLY	CA-C-N	5.31	125.37	119.32
1	D	366	GLY	C-N-CA	5.31	125.37	119.32
1	C	188	ARG	CA-C-N	5.21	124.92	119.82
1	C	188	ARG	C-N-CA	5.21	124.92	119.82
1	D	177	ASP	CA-C-N	5.07	124.86	119.28
1	D	177	ASP	C-N-CA	5.07	124.86	119.28
1	C	388	ASP	CB-CA-C	-5.01	109.33	116.34
1	A	215	GLY	N-CA-C	-5.00	108.46	114.66

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	200	SER	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	4017	0	3844	66	0
1	B	4017	0	3844	90	0
1	C	4017	0	3844	74	0
1	D	4017	0	3844	73	0
2	A	43	0	30	3	0
2	B	43	0	30	5	0
2	C	43	0	30	1	0
2	D	43	0	30	2	0
3	A	48	0	26	2	0
3	B	48	0	26	3	0
3	C	48	0	26	3	0
3	D	48	0	26	1	0
All	All	16432	0	15600	258	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 8.

All (258) 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:A:150:PRO:HG3	3:A:602:NDP:H41N	1.55	0.87
1:B:235:TYR:CZ	1:B:276:TRP:HB2	2.17	0.79
1:B:174:HIS:HB3	1:C:261:LEU:HD21	1.65	0.78
1:D:251:ARG:O	1:D:254:HIS:CD2	2.38	0.77
1:B:235:TYR:CE1	1:B:315:LEU:HD12	2.20	0.77
1:A:409:SER:OG	1:C:15:LYS:NZ	2.19	0.74
1:D:251:ARG:O	1:D:254:HIS:HD2	1.71	0.72
1:A:149:THR:HG21	1:A:194:GLN:HE22	1.54	0.72
1:A:65:ARG:NH1	1:D:359:ASP:OD2	2.22	0.71
1:D:209:ARG:NH1	1:D:263:ASP:OD2	2.23	0.70
1:B:37:LYS:NZ	1:B:59:GLU:OE2	2.21	0.70
1:B:408:PHE:HA	1:D:15:LYS:HD3	1.74	0.70
1:A:67:ARG:HH21	1:D:168:LYS:HE2	1.58	0.69
1:B:490:SER:HA	1:B:493:GLN:HB3	1.77	0.67
1:C:427:ASP:OD2	1:C:429:GLN:HG2	1.93	0.67
1:A:347:ASP:HB3	1:A:350:LEU:HB3	1.77	0.67
2:A:601:HEM:HMB2	2:A:601:HEM:HBB2	1.78	0.65
1:B:67:ARG:HH21	1:C:168:LYS:HE2	1.60	0.65
1:C:43:VAL:HG11	1:D:43:VAL:HG11	1.79	0.64
1:C:212:ASN:ND2	1:C:241:ILE:HD11	2.13	0.63
1:D:475:LYS:O	1:D:479:LYS:HG2	1.98	0.63
1:B:131:PHE:CZ	1:B:235:TYR:CE2	2.87	0.63
1:C:406:ASN:HD21	1:C:410:ALA:HB3	1.63	0.62
1:D:150:PRO:HG3	3:D:602:NDP:H41N	1.81	0.62
1:B:168:LYS:HE2	1:C:67:ARG:HH21	1.64	0.61
1:C:236:LYS:NZ	3:C:602:NDP:O1X	2.32	0.61
2:B:601:HEM:HBD2	2:B:601:HEM:HMD1	1.82	0.61
2:A:601:HEM:HMC1	2:A:601:HEM:HBC2	1.83	0.60
1:C:139:ASP:HB3	1:C:340:PRO:HD2	1.83	0.60
1:A:444:THR:O	1:A:448:LYS:HG2	2.02	0.60
1:C:40:SER:HB3	1:C:49:LEU:HD13	1.83	0.60
1:D:213:GLY:HA3	1:D:235:TYR:CE1	2.36	0.59
2:D:601:HEM:HBB2	2:D:601:HEM:HMB2	1.84	0.59
1:A:451:ASN:O	1:A:455:ARG:HG3	2.02	0.59
1:B:235:TYR:HE1	1:B:315:LEU:HB2	1.66	0.59
1:D:406:ASN:HD21	1:D:410:ALA:HB3	1.66	0.59
1:C:213:GLY:HA3	1:C:235:TYR:CE1	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:ALA:HB1	1:B:411:PRO:HD2	1.85	0.58
1:B:36:ASP:O	1:C:430:ARG:NH1	2.37	0.58
1:B:258:ASP:OD2	1:C:169:ARG:NH1	2.31	0.58
1:C:150:PRO:HG3	3:C:602:NDP:H41N	1.85	0.57
1:B:53:ASP:OD1	1:C:430:ARG:NH2	2.38	0.57
1:D:258:ASP:HB3	1:D:261:LEU:HB3	1.85	0.57
1:A:216:SER:O	1:A:232:LYS:NZ	2.25	0.57
1:B:52:GLN:HE21	1:D:351:GLN:HE22	1.53	0.57
1:A:15:LYS:NZ	1:C:407:SER:O	2.30	0.57
1:C:71:ARG:NH2	1:C:331:LEU:O	2.37	0.56
1:A:423:HIS:HB2	1:B:427:ASP:HA	1.87	0.56
1:B:235:TYR:CE1	1:B:315:LEU:HB2	2.41	0.56
1:A:274:PRO:HG2	1:A:317:LEU:HB2	1.87	0.56
1:B:43:VAL:O	1:B:47:GLY:HA3	2.05	0.56
1:A:137:THR:OG1	1:A:140:GLY:O	2.16	0.55
1:A:361:HIS:NE2	2:A:601:HEM:O1A	2.29	0.55
1:A:393:MET:HG3	1:C:393:MET:HE3	1.89	0.55
1:A:408:PHE:HA	1:C:15:LYS:HD2	1.88	0.55
1:C:149:THR:HG21	1:C:194:GLN:HE22	1.73	0.55
1:B:351:GLN:NE2	1:D:52:GLN:OE1	2.40	0.54
1:B:236:LYS:NZ	3:B:602:NDP:O1X	2.39	0.54
1:B:65:ARG:NH1	1:C:359:ASP:OD2	2.33	0.54
2:D:601:HEM:HMC1	2:D:601:HEM:HBC2	1.89	0.54
1:D:200:SER:HB2	1:D:458:LEU:HD13	1.90	0.53
1:D:40:SER:HB3	1:D:49:LEU:HD13	1.91	0.53
1:A:236:LYS:HE3	1:A:309:LEU:HD21	1.91	0.53
1:A:82:GLY:HA3	1:A:316:VAL:O	2.08	0.53
1:B:82:GLY:HA3	1:B:316:VAL:O	2.08	0.53
1:B:35:GLY:HA2	1:D:414:GLN:O	2.09	0.53
1:C:429:GLN:HB3	1:D:421:ARG:HG2	1.91	0.52
1:B:80:ALA:HB3	1:B:317:LEU:HD13	1.90	0.52
1:D:347:ASP:O	1:D:351:GLN:HG2	2.08	0.52
1:D:215:GLY:O	1:D:217:HIS:N	2.39	0.52
1:B:4:ARG:NH1	1:C:468:ASP:O	2.42	0.52
1:A:4:ARG:NH2	1:D:179:ASP:OD2	2.42	0.52
1:A:165:HIS:NE2	1:D:66:GLU:OE2	2.30	0.52
1:B:92:ARG:O	1:B:223:ASN:ND2	2.39	0.52
1:C:4:ARG:NE	1:C:9:ASP:OD1	2.39	0.52
1:B:456:LYS:O	1:B:460:GLU:HG3	2.11	0.51
1:B:409:SER:O	1:B:409:SER:OG	2.29	0.51
1:D:368:ASN:ND2	1:D:390:PRO:O	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:TYR:CD1	1:B:405:PRO:HA	2.46	0.51
1:D:222:VAL:HG21	1:D:420:HIS:HB2	1.93	0.51
1:B:237:THR:HA	1:B:276:TRP:CD1	2.45	0.51
1:D:212:ASN:ND2	1:D:241:ILE:HD11	2.26	0.51
1:B:165:HIS:NE2	1:C:66:GLU:OE2	2.35	0.51
1:B:212:ASN:OD1	1:B:237:THR:HG22	2.11	0.50
1:B:135:PHE:HB2	1:B:142:TRP:HB3	1.92	0.50
1:D:327:GLU:HA	1:D:374:VAL:HG11	1.94	0.50
1:B:26:LEU:HD21	1:B:37:LYS:HD3	1.93	0.50
2:C:601:HEM:HMC1	2:C:601:HEM:HBC2	1.93	0.50
1:B:15:LYS:HD2	1:D:408:PHE:HA	1.94	0.50
1:C:429:GLN:OE1	1:D:421:ARG:HD2	2.12	0.50
1:D:285:PHE:O	1:D:289:GLU:HG3	2.12	0.50
1:C:179:ASP:OD1	1:C:469:ALA:HA	2.12	0.50
1:D:447:LEU:HD11	1:D:485:HIS:CD2	2.47	0.49
1:B:149:THR:HG21	1:B:194:GLN:HE22	1.77	0.49
1:D:446:TYR:HD2	1:D:447:LEU:HD12	1.77	0.49
1:D:347:ASP:HB3	1:D:350:LEU:HB3	1.94	0.49
1:C:217:HIS:HB2	1:C:219:PHE:CZ	2.47	0.49
1:B:160:PHE:HB3	1:B:161:PRO:HD3	1.94	0.49
1:D:446:TYR:O	1:D:455:ARG:HD3	2.13	0.49
1:B:261:LEU:HD21	1:C:174:HIS:HB3	1.95	0.48
1:D:404:TYR:CD1	1:D:405:PRO:HA	2.49	0.48
1:C:97:LYS:O	1:C:104:LYS:NZ	2.38	0.48
1:A:155:ARG:NH1	1:A:299:THR:OG1	2.46	0.48
1:A:217:HIS:CD2	1:A:353:ARG:HH11	2.31	0.48
1:B:235:TYR:CZ	1:B:276:TRP:CB	2.91	0.48
1:B:349:MET:HE3	2:B:601:HEM:HAB	1.95	0.48
1:C:43:VAL:HG23	1:C:48:PRO:HD2	1.96	0.48
1:D:80:ALA:HB3	1:D:317:LEU:HD13	1.94	0.48
1:D:217:HIS:CD2	1:D:353:ARG:HH11	2.31	0.48
1:B:258:ASP:HB3	1:B:261:LEU:HB3	1.96	0.47
1:C:467:LYS:HD3	1:C:499:TYR:CD1	2.49	0.47
1:D:179:ASP:OD1	1:D:469:ALA:HA	2.14	0.47
1:A:349:MET:O	1:A:353:ARG:HG3	2.14	0.47
1:D:395:ASP:OD1	1:D:395:ASP:N	2.44	0.47
1:B:446:TYR:O	1:B:455:ARG:HD3	2.13	0.47
1:B:55:VAL:HB	1:C:430:ARG:HH22	1.79	0.47
1:B:74:HIS:HA	1:B:114:THR:O	2.14	0.47
1:A:74:HIS:CE1	1:A:115:VAL:HG22	2.50	0.47
1:A:390:PRO:HG3	1:C:68:ILE:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:VAL:HG22	1:C:43:VAL:HG12	1.95	0.47
1:C:447:LEU:HD11	1:C:485:HIS:CE1	2.50	0.47
1:D:129:ARG:HG3	1:D:205:PRO:HG2	1.97	0.47
1:C:82:GLY:HA3	1:C:316:VAL:O	2.14	0.47
1:B:55:VAL:HB	1:C:430:ARG:NH2	2.30	0.47
1:B:301:VAL:HG21	3:B:602:NDP:H2D	1.96	0.46
1:A:238:ASP:OD2	1:A:314:LYS:HE2	2.15	0.46
1:A:60:MET:HE1	1:D:161:PRO:HD3	1.97	0.46
1:A:144:LEU:HG	1:A:235:TYR:OH	2.14	0.46
1:A:357:TYR:HB2	1:A:358:PRO:HD3	1.97	0.46
1:A:213:GLY:HA3	1:A:235:TYR:CD2	2.50	0.46
1:A:43:VAL:O	1:A:47:GLY:HA3	2.15	0.46
1:A:43:VAL:HG21	1:B:43:VAL:HG21	1.98	0.46
1:B:166:SER:HA	1:B:180:MET:HE2	1.97	0.46
1:D:26:LEU:HD21	1:D:37:LYS:HD3	1.97	0.46
1:D:367:PRO:HG2	1:D:390:PRO:HG2	1.97	0.46
1:A:429:GLN:OE1	1:B:421:ARG:NH1	2.49	0.46
1:B:108:ILE:HD13	1:B:315:LEU:HD22	1.96	0.46
1:C:427:ASP:CG	1:C:429:GLN:HG2	2.41	0.46
1:B:163:PHE:HE1	1:B:185:TRP:HE1	1.64	0.46
1:A:142:TRP:CH2	1:A:144:LEU:HD22	2.51	0.46
1:B:52:GLN:NE2	1:D:351:GLN:HE22	2.14	0.46
1:B:66:GLU:OE2	1:C:165:HIS:NE2	2.48	0.46
1:C:74:HIS:HA	1:C:114:THR:O	2.16	0.46
1:C:151:ILE:HG13	1:C:194:GLN:OE1	2.16	0.46
1:C:161:PRO:O	1:C:165:HIS:ND1	2.49	0.46
1:D:444:THR:HG23	1:D:448:LYS:HD3	1.96	0.46
1:B:84:PHE:HB2	1:B:315:LEU:CD2	2.46	0.45
1:D:77:GLY:HA2	1:D:112:PHE:O	2.15	0.45
1:D:215:GLY:C	1:D:216:SER:HG	2.24	0.45
1:A:421:ARG:HD2	1:B:429:GLN:OE1	2.16	0.45
1:D:346:PRO:HA	1:D:351:GLN:NE2	2.32	0.45
1:A:213:GLY:HA3	1:A:235:TYR:HD2	1.80	0.45
1:B:155:ARG:NH2	1:B:438:ASN:OD1	2.21	0.45
1:B:393:MET:HE3	1:D:393:MET:HG3	1.98	0.45
1:A:294:ASN:HB3	1:A:297:ASP:HB2	1.97	0.45
1:C:160:PHE:HB3	1:C:161:PRO:HD3	1.98	0.45
1:C:349:MET:O	1:C:353:ARG:HG3	2.16	0.45
1:B:446:TYR:CE2	1:B:488:TYR:HB2	2.51	0.45
1:C:294:ASN:HB3	1:C:297:ASP:HB2	1.99	0.45
1:D:110:VAL:HG22	1:D:133:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:PHE:CZ	1:C:57:THR:HG23	2.52	0.45
1:B:179:ASP:OD1	1:B:180:MET:N	2.50	0.45
1:B:456:LYS:HB3	1:B:456:LYS:HE2	1.83	0.44
1:B:41:LEU:HB3	1:B:53:ASP:HB2	1.99	0.44
1:A:454:GLN:HG2	1:A:457:ARG:HH21	1.81	0.44
1:B:217:HIS:CD2	1:B:350:LEU:HD13	2.52	0.44
1:B:32:ASN:ND2	1:D:139:ASP:O	2.36	0.44
1:C:456:LYS:O	1:C:460:GLU:HG3	2.17	0.44
1:D:155:ARG:NH2	1:D:438:ASN:OD1	2.38	0.44
1:A:301:VAL:HG21	3:A:602:NDP:H2D	1.98	0.44
1:C:89:ASP:OD1	1:C:102:ILE:HG13	2.17	0.44
1:B:215:GLY:C	1:B:216:SER:HG	2.25	0.44
1:B:447:LEU:HD11	1:B:485:HIS:CD2	2.53	0.44
1:C:497:ASP:OD1	1:C:498:LYS:N	2.51	0.44
1:D:454:GLN:HG2	1:D:457:ARG:NH2	2.32	0.44
1:A:26:LEU:O	1:A:34:VAL:HG22	2.18	0.44
1:B:215:GLY:O	1:B:216:SER:OG	2.35	0.44
1:B:294:ASN:HB3	1:B:297:ASP:HB2	2.00	0.44
1:D:143:ASP:HB2	1:D:334:ASP:O	2.18	0.44
3:B:602:NDP:H1B	3:B:602:NDP:C5N	2.48	0.44
1:A:52:GLN:HA	1:C:354:LEU:HD13	2.00	0.43
1:D:349:MET:O	1:D:353:ARG:HG3	2.19	0.43
1:D:192:LEU:HD11	1:D:480:ASN:HB3	2.00	0.43
1:B:235:TYR:CE1	1:B:276:TRP:HB2	2.51	0.43
1:B:248:ASP:HB2	1:B:251:ARG:HH21	1.82	0.43
1:C:74:HIS:CE1	1:C:115:VAL:HG22	2.53	0.43
1:C:414:GLN:HA	1:C:415:PRO:HD3	1.80	0.43
1:A:35:GLY:HA2	1:C:414:GLN:O	2.18	0.43
1:A:215:GLY:O	1:A:217:HIS:N	2.45	0.43
3:C:602:NDP:H71N	3:C:602:NDP:H2N	1.63	0.43
1:A:414:GLN:O	1:C:35:GLY:HA2	2.18	0.43
1:C:395:ASP:OD1	1:C:395:ASP:N	2.51	0.43
1:B:467:LYS:HD3	1:B:499:TYR:CG	2.53	0.43
1:C:37:LYS:HB3	1:C:37:LYS:HE3	1.84	0.43
1:D:74:HIS:HA	1:D:114:THR:O	2.19	0.43
1:D:357:TYR:HB2	1:D:358:PRO:HD3	2.01	0.43
1:A:102:ILE:HD12	1:A:102:ILE:H	1.84	0.42
1:B:168:LYS:HE2	1:C:67:ARG:NH2	2.33	0.42
1:D:448:LYS:NZ	1:D:448:LYS:HB3	2.32	0.42
1:A:212:ASN:OD1	1:A:237:THR:HG22	2.19	0.42
1:A:143:ASP:HB2	1:A:334:ASP:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ILE:HG21	1:B:315:LEU:HD22	2.00	0.42
1:B:177:ASP:HB3	1:B:180:MET:SD	2.59	0.42
1:D:338:MET:SD	1:D:344:PRO:HD3	2.59	0.42
1:C:73:VAL:HG12	1:C:74:HIS:CD2	2.54	0.42
1:B:60:MET:HE1	1:C:161:PRO:HD3	2.00	0.42
1:B:248:ASP:HB2	1:B:251:ARG:NH2	2.35	0.42
1:B:414:GLN:HA	1:B:415:PRO:HD3	1.89	0.42
1:D:18:ARG:HG2	1:D:18:ARG:O	2.19	0.42
1:D:95:LYS:HG2	1:D:222:VAL:O	2.20	0.42
1:D:135:PHE:HB2	1:D:142:TRP:HB3	2.00	0.42
1:A:385:TYR:OH	1:A:411:PRO:O	2.36	0.42
2:B:601:HEM:HMB2	2:B:601:HEM:HBB2	2.01	0.42
1:C:217:HIS:ND1	1:C:350:LEU:HB2	2.34	0.42
1:D:131:PHE:HZ	1:D:276:TRP:CE2	2.38	0.42
1:A:173:THR:HG22	1:D:265:PHE:CZ	2.55	0.42
1:A:410:ALA:HB1	1:A:411:PRO:HD2	2.02	0.42
1:A:421:ARG:NH1	1:B:427:ASP:OD2	2.53	0.42
1:D:451:ASN:OD1	1:D:454:GLN:HG3	2.18	0.42
1:C:84:PHE:O	1:C:105:ARG:HA	2.20	0.42
1:A:37:LYS:HG2	1:D:158:LEU:HD22	2.02	0.41
1:A:262:ARG:NH1	1:D:175:LEU:HD13	2.34	0.41
1:A:446:TYR:CZ	1:A:455:ARG:HD2	2.55	0.41
1:C:186:SER:O	1:C:480:ASN:ND2	2.50	0.41
1:D:41:LEU:O	1:D:49:LEU:HD12	2.20	0.41
1:A:135:PHE:HB2	1:A:142:TRP:HB3	2.02	0.41
1:A:236:LYS:HE3	1:A:309:LEU:CD2	2.50	0.41
1:B:466:LEU:HD23	1:B:496:LEU:HD11	2.02	0.41
1:B:349:MET:CE	2:B:601:HEM:HAB	2.50	0.41
2:B:601:HEM:HBD2	2:B:601:HEM:CMD	2.48	0.41
1:A:162:SER:HB3	1:B:404:TYR:H	1.86	0.41
1:B:333:PHE:O	1:B:361:HIS:HE1	2.04	0.41
1:C:127:ASP:O	1:C:129:ARG:NH1	2.54	0.41
1:A:367:PRO:HG3	1:C:65:ARG:HD3	2.03	0.41
1:A:429:GLN:HG2	1:A:431:PHE:CZ	2.55	0.41
1:B:14:TRP:O	1:B:17:GLN:HG2	2.19	0.41
1:B:234:HIS:NE2	1:B:281:GLN:OE1	2.54	0.41
1:C:135:PHE:HB2	1:C:142:TRP:HB3	2.03	0.41
1:C:200:SER:OG	1:C:201:ASP:N	2.54	0.41
1:B:235:TYR:CE2	1:B:276:TRP:CG	3.09	0.41
1:B:353:ARG:NH2	1:B:357:TYR:OH	2.47	0.41
1:C:80:ALA:HB3	1:C:317:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:485:HIS:O	1:D:488:TYR:HB3	2.21	0.41
1:A:460:GLU:HG2	1:A:495:LEU:HD11	2.02	0.41
1:B:217:HIS:ND1	1:B:350:LEU:HB2	2.36	0.41
1:C:145:VAL:HB	1:C:353:ARG:HH22	1.86	0.41
1:C:446:TYR:O	1:C:455:ARG:HD3	2.20	0.41
1:A:158:LEU:HD21	1:D:56:PHE:HA	2.03	0.40
1:A:376:CYS:HA	1:A:377:PRO:HD3	1.94	0.40
1:A:80:ALA:HB3	1:A:317:LEU:HD13	2.03	0.40
1:A:403:TYR:OH	1:B:183:ASP:OD2	2.37	0.40
1:C:220:LYS:NZ	1:C:420:HIS:HB3	2.36	0.40
1:C:427:ASP:OD1	1:C:428:VAL:N	2.53	0.40
1:A:220:LYS:HB3	1:A:343:GLU:HB2	2.03	0.40
1:C:425:SER:HB2	1:D:425:SER:HB2	2.03	0.40
1:A:470:GLN:HE22	1:D:12:LYS:HB2	1.87	0.40
1:B:84:PHE:O	1:B:105:ARG:HA	2.22	0.40
1:D:137:THR:OG1	1:D:140:GLY:O	2.28	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	497/527 (94%)	481 (97%)	16 (3%)	0	100	100
1	B	497/527 (94%)	480 (97%)	17 (3%)	0	100	100
1	C	497/527 (94%)	481 (97%)	15 (3%)	1 (0%)	43	73
1	D	497/527 (94%)	479 (96%)	17 (3%)	1 (0%)	43	73
All	All	1988/2108 (94%)	1921 (97%)	65 (3%)	2 (0%)	49	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	427	ASP
1	D	216	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	431/454 (95%)	424 (98%)	7 (2%)	55	75
1	B	431/454 (95%)	431 (100%)	0	100	100
1	C	431/454 (95%)	429 (100%)	2 (0%)	81	85
1	D	431/454 (95%)	429 (100%)	2 (0%)	81	85
All	All	1724/1816 (95%)	1713 (99%)	11 (1%)	76	84

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	235	TYR
1	A	413	HIS
1	A	419	GLU
1	A	423	HIS
1	A	433	SER
1	A	490	SER
1	C	412	GLU
1	C	427	ASP
1	D	394	MET
1	D	419	GLU

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

Mol	Chain	Res	Type
1	A	32	ASN
1	A	52	GLN
1	B	21	GLN
1	B	39	ASN

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Mol	Chain	Res	Type
1	B	414	GLN
1	C	194	GLN
1	C	243	ASN
1	C	414	GLN
1	D	32	ASN
1	D	39	ASN
1	D	101	HIS
1	D	174	HIS
1	D	351	GLN
1	D	413	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](#)

8 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	HEM	D	601	1	50,50,50	1.89	8 (16%)	67,82,82	1.28	6 (8%)
3	NDP	D	602	-	51,52,52	2.79	10 (19%)	71,80,80	1.51	16 (22%)
2	HEM	C	601	1	50,50,50	1.87	8 (16%)	67,82,82	1.57	12 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	A	601	1	50,50,50	1.87	8 (16%)	67,82,82	1.24	3 (4%)
3	NDP	C	602	-	51,52,52	2.78	8 (15%)	71,80,80	1.57	17 (23%)
2	HEM	B	601	1	50,50,50	1.99	9 (18%)	67,82,82	1.21	5 (7%)
3	NDP	B	602	-	51,52,52	2.48	10 (19%)	71,80,80	1.53	17 (23%)
3	NDP	A	602	-	51,52,52	2.57	8 (15%)	71,80,80	1.54	17 (23%)

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	HEM	D	601	1	-	2/14/54/54	-
3	NDP	D	602	-	-	10/34/77/77	0/5/5/5
2	HEM	C	601	1	-	2/14/54/54	-
2	HEM	A	601	1	-	5/14/54/54	-
3	NDP	C	602	-	-	12/34/77/77	0/5/5/5
2	HEM	B	601	1	-	5/14/54/54	-
3	NDP	B	602	-	-	11/34/77/77	0/5/5/5
3	NDP	A	602	-	-	10/34/77/77	0/5/5/5

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	NDP	P2B-O2B	15.91	1.87	1.59
3	D	602	NDP	P2B-O2B	15.81	1.87	1.59
3	A	602	NDP	P2B-O2B	14.37	1.84	1.59
3	B	602	NDP	P2B-O2B	13.82	1.83	1.59
2	B	601	HEM	C3D-C2D	8.55	1.55	1.36
2	C	601	HEM	C3D-C2D	7.71	1.53	1.36
2	A	601	HEM	C3D-C2D	7.71	1.53	1.36
2	D	601	HEM	C3D-C2D	7.50	1.52	1.36
3	D	602	NDP	PA-O3	6.96	1.67	1.59
3	C	602	NDP	PA-O3	6.45	1.66	1.59
3	A	602	NDP	PA-O3	6.24	1.66	1.59
2	D	601	HEM	FE-NB	5.32	2.11	1.94
3	B	602	NDP	PA-O3	5.24	1.65	1.59
2	C	601	HEM	FE-NB	4.84	2.09	1.94
2	C	601	HEM	FE-ND	4.78	2.09	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	HEM	FE-NB	4.55	2.08	1.94
2	B	601	HEM	FE-ND	4.52	2.08	1.94
3	B	602	NDP	PN-O5D	4.29	1.76	1.59
2	D	601	HEM	FE-ND	4.24	2.08	1.94
2	A	601	HEM	FE-NB	4.16	2.07	1.94
3	C	602	NDP	PN-O5D	4.11	1.75	1.59
2	A	601	HEM	FE-ND	4.08	2.07	1.94
2	D	601	HEM	FE-NA	4.04	2.08	1.95
3	A	602	NDP	PN-O5D	4.00	1.75	1.59
3	D	602	NDP	PN-O5D	3.89	1.74	1.59
2	A	601	HEM	FE-NA	3.63	2.07	1.95
2	A	601	HEM	FE-NC	3.39	2.06	1.95
2	C	601	HEM	FE-NA	3.31	2.06	1.95
2	B	601	HEM	FE-NC	3.27	2.05	1.95
2	B	601	HEM	CAB-C3B	3.18	1.55	1.47
2	A	601	HEM	CAC-C3C	3.14	1.55	1.47
3	B	602	NDP	O2B-C2B	-3.12	1.33	1.44
3	A	602	NDP	O2B-C2B	-3.08	1.33	1.44
2	C	601	HEM	CAC-C3C	3.05	1.55	1.47
2	B	601	HEM	CAC-C3C	3.02	1.55	1.47
2	B	601	HEM	FE-NA	2.99	2.05	1.95
3	D	602	NDP	O2B-C2B	-2.97	1.34	1.44
2	A	601	HEM	CAB-C3B	2.96	1.55	1.47
2	D	601	HEM	CAB-C3B	2.89	1.55	1.47
2	C	601	HEM	CAB-C3B	2.86	1.55	1.47
3	C	602	NDP	O2B-C2B	-2.84	1.34	1.44
3	C	602	NDP	C5A-C4A	2.83	1.44	1.39
2	D	601	HEM	CAC-C3C	2.80	1.54	1.47
3	B	602	NDP	C5A-C4A	2.69	1.43	1.39
3	D	602	NDP	C5A-C4A	2.67	1.43	1.39
3	D	602	NDP	C2A-N1A	2.51	1.38	1.33
3	C	602	NDP	C2A-N1A	2.50	1.38	1.33
2	D	601	HEM	FE-NC	2.47	2.03	1.95
3	D	602	NDP	C2B-C1B	2.46	1.59	1.53
3	A	602	NDP	C5A-C4A	2.42	1.43	1.39
3	B	602	NDP	C2A-N1A	2.42	1.38	1.33
3	B	602	NDP	C8A-N9A	2.29	1.41	1.37
2	B	601	HEM	CMD-C2D	2.29	1.55	1.50
3	A	602	NDP	C2A-N1A	2.28	1.38	1.33
3	C	602	NDP	C2B-C1B	2.25	1.58	1.53
3	B	602	NDP	C4A-N3A	2.20	1.38	1.34
3	C	602	NDP	C8A-N9A	2.20	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	NDP	C8A-N7A	2.17	1.35	1.31
2	C	601	HEM	FE-NC	2.16	2.02	1.95
3	D	602	NDP	O5D-C5D	-2.14	1.36	1.44
3	D	602	NDP	C8A-N9A	2.13	1.41	1.37
3	A	602	NDP	C4A-N3A	2.12	1.38	1.34
2	C	601	HEM	CMA-C3A	2.08	1.55	1.50
3	A	602	NDP	O5D-C5D	-2.06	1.36	1.44
3	B	602	NDP	C7N-N7N	2.05	1.39	1.33
3	D	602	NDP	C4A-N3A	2.03	1.38	1.34
2	A	601	HEM	CMB-C2B	2.02	1.54	1.50
2	B	601	HEM	CMB-C2B	2.02	1.54	1.50
2	D	601	HEM	CMC-C2C	2.01	1.54	1.50

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	HEM	C4D-ND-C1D	5.76	112.03	105.21
2	A	601	HEM	C4D-ND-C1D	5.37	111.57	105.21
2	D	601	HEM	C4D-ND-C1D	5.18	111.34	105.21
2	B	601	HEM	C4D-ND-C1D	4.90	111.01	105.21
3	C	602	NDP	P2B-O2B-C2B	-4.48	111.46	123.43
3	B	602	NDP	P2B-O2B-C2B	-4.41	111.65	123.43
3	A	602	NDP	P2B-O2B-C2B	-4.24	112.10	123.43
3	D	602	NDP	P2B-O2B-C2B	-4.18	112.26	123.43
3	C	602	NDP	O3-PA-O1A	-3.65	99.73	110.70
2	C	601	HEM	C3B-C2B-C1B	3.41	108.97	106.41
3	D	602	NDP	O3-PA-O1A	-3.39	100.51	110.70
3	A	602	NDP	O3-PA-O1A	-3.35	100.64	110.70
3	A	602	NDP	O2B-P2B-O1X	-3.33	97.48	109.33
3	B	602	NDP	O2B-P2B-O1X	-3.31	97.52	109.33
3	B	602	NDP	O3-PA-O1A	-3.30	100.76	110.70
3	A	602	NDP	PA-O5B-C5B	-3.30	102.43	121.35
3	C	602	NDP	O2B-P2B-O1X	-3.29	97.61	109.33
3	D	602	NDP	O2B-P2B-O1X	-3.07	98.38	109.33
3	B	602	NDP	PA-O5B-C5B	-3.04	103.95	121.35
3	C	602	NDP	PA-O5B-C5B	-3.01	104.08	121.35
3	C	602	NDP	O2N-PN-O3	2.98	115.33	107.27
3	A	602	NDP	O2N-PN-O3	2.95	115.24	107.27
3	D	602	NDP	PA-O5B-C5B	-2.94	104.52	121.35
3	D	602	NDP	O2N-PN-O3	2.93	115.20	107.27
2	C	601	HEM	C3B-C4B-NB	-2.93	107.37	109.47
3	C	602	NDP	PN-O5D-C5D	-2.80	105.30	121.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	NDP	PN-O5D-C5D	-2.77	105.50	121.35
2	C	601	HEM	C1B-NB-C4B	2.75	108.46	105.21
2	C	601	HEM	C2A-C1A-NA	-2.66	107.20	110.15
3	B	602	NDP	O2N-PN-O3	2.62	114.37	107.27
3	A	602	NDP	O3X-P2B-O2X	2.60	117.55	107.80
3	D	602	NDP	C2A-N1A-C6A	-2.60	114.47	118.73
3	B	602	NDP	O3X-P2B-O2X	2.59	117.51	107.80
3	B	602	NDP	PN-O5D-C5D	-2.59	106.52	121.35
3	A	602	NDP	PN-O5D-C5D	-2.56	106.66	121.35
3	C	602	NDP	C2A-N1A-C6A	-2.54	114.56	118.73
3	D	602	NDP	O3X-P2B-O2X	2.52	117.27	107.80
3	C	602	NDP	O3X-P2B-O2X	2.51	117.21	107.80
2	C	601	HEM	CAD-CBD-CGD	-2.46	107.14	113.67
2	D	601	HEM	C2A-C1A-NA	-2.45	107.44	110.15
3	A	602	NDP	C2A-N1A-C6A	-2.44	114.72	118.73
3	C	602	NDP	O5D-PN-O1N	-2.44	99.26	108.94
2	D	601	HEM	CAD-CBD-CGD	-2.44	107.20	113.67
3	A	602	NDP	C5D-C4D-C3D	-2.44	106.44	115.21
3	B	602	NDP	C4B-O4B-C1B	-2.44	104.09	109.47
3	B	602	NDP	C2A-N1A-C6A	-2.41	114.78	118.73
3	B	602	NDP	O2X-P2B-O2B	-2.36	96.64	105.85
3	B	602	NDP	O2N-PN-O1N	2.36	123.42	112.44
3	D	602	NDP	O5D-PN-O1N	-2.34	99.67	108.94
2	D	601	HEM	CAD-C3D-C4D	2.34	128.77	124.70
3	D	602	NDP	O2X-P2B-O2B	-2.34	96.74	105.85
3	A	602	NDP	O2X-P2B-O2B	-2.32	96.80	105.85
3	A	602	NDP	N3A-C4A-N9A	2.32	131.12	127.17
3	C	602	NDP	O2N-PN-O1N	2.31	123.19	112.44
2	C	601	HEM	CAD-C3D-C4D	2.30	128.71	124.70
3	D	602	NDP	N3A-C4A-N9A	2.30	131.08	127.17
3	C	602	NDP	O2X-P2B-O2B	-2.30	96.90	105.85
3	D	602	NDP	O2N-PN-O1N	2.27	123.01	112.44
3	B	602	NDP	C5D-C4D-C3D	-2.26	107.06	115.21
2	A	601	HEM	C1B-NB-C4B	2.26	107.88	105.21
3	B	602	NDP	N3A-C4A-N9A	2.25	131.00	127.17
3	A	602	NDP	O2N-PN-O1N	2.22	122.77	112.44
3	C	602	NDP	O7N-C7N-C3N	2.21	125.06	120.90
2	C	601	HEM	CAA-CBA-CGA	-2.20	107.82	113.67
3	A	602	NDP	C5B-C4B-C3B	-2.20	107.30	115.21
3	C	602	NDP	C5A-C4A-N3A	-2.19	123.69	126.72
3	C	602	NDP	C4B-O4B-C1B	-2.19	104.63	109.47
3	D	602	NDP	C5A-C4A-N3A	-2.18	123.71	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	NDP	C5A-C4A-N3A	-2.18	123.71	126.72
3	A	602	NDP	C5A-C4A-N3A	-2.18	123.71	126.72
3	B	602	NDP	C3B-C2B-C1B	-2.18	98.64	102.81
3	C	602	NDP	O4B-C4B-C3B	2.16	109.44	105.15
2	D	601	HEM	C3B-C2B-C1B	2.15	108.03	106.41
3	B	602	NDP	O7N-C7N-C3N	2.14	124.93	120.90
3	D	602	NDP	O7N-C7N-C3N	2.14	124.93	120.90
2	C	601	HEM	C3D-C4D-ND	-2.14	107.83	110.17
2	B	601	HEM	C3B-C2B-C1B	2.13	108.01	106.41
3	D	602	NDP	O4B-C4B-C3B	2.12	109.36	105.15
2	C	601	HEM	CHD-C1D-ND	2.10	126.69	124.42
3	C	602	NDP	N3A-C4A-N9A	2.09	130.73	127.17
3	B	602	NDP	O5D-PN-O1N	-2.09	100.64	108.94
2	D	601	HEM	C1B-NB-C4B	2.09	107.68	105.21
3	C	602	NDP	C5B-C4B-C3B	-2.09	107.69	115.21
2	B	601	HEM	C1D-C2D-C3D	-2.08	104.79	106.98
3	D	602	NDP	C5B-C4B-C3B	-2.08	107.73	115.21
2	C	601	HEM	CHC-C4B-C3B	2.06	129.19	125.07
2	C	601	HEM	C2B-C1B-NB	-2.04	107.49	109.84
3	A	602	NDP	O4B-C4B-C3B	2.04	109.20	105.15
3	A	602	NDP	C3N-C2N-N1N	-2.04	120.21	123.20
2	A	601	HEM	C3B-C2B-C1B	2.03	107.94	106.41
2	B	601	HEM	C1B-NB-C4B	2.02	107.60	105.21
3	A	602	NDP	O5D-PN-O1N	-2.02	100.95	108.94
2	B	601	HEM	CAD-C3D-C2D	2.01	131.62	127.87

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	HEM	C1A-C2A-CAA-CBA
2	B	601	HEM	C4D-C3D-CAD-CBD
3	A	602	NDP	C5B-O5B-PA-O3
3	B	602	NDP	C2N-C3N-C7N-N7N
3	C	602	NDP	C5B-O5B-PA-O1A
3	C	602	NDP	C5B-O5B-PA-O2A
3	C	602	NDP	C5B-O5B-PA-O3
3	D	602	NDP	C5B-O5B-PA-O2A
3	D	602	NDP	C5B-O5B-PA-O3
3	D	602	NDP	PN-O3-PA-O5B
3	D	602	NDP	C3B-C4B-C5B-O5B
2	B	601	HEM	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
3	A	602	NDP	C3B-C4B-C5B-O5B
3	B	602	NDP	C3B-C4B-C5B-O5B
3	C	602	NDP	O4B-C4B-C5B-O5B
3	C	602	NDP	C3B-C4B-C5B-O5B
3	D	602	NDP	O4B-C4B-C5B-O5B
3	A	602	NDP	C3B-C2B-O2B-P2B
3	A	602	NDP	O4B-C4B-C5B-O5B
3	B	602	NDP	O4B-C4B-C5B-O5B
3	A	602	NDP	C1B-C2B-O2B-P2B
2	B	601	HEM	C3A-C2A-CAA-CBA
3	B	602	NDP	C2D-C1D-N1N-C2N
3	B	602	NDP	C2D-C1D-N1N-C6N
3	A	602	NDP	PN-O3-PA-O5B
3	B	602	NDP	PN-O3-PA-O5B
2	A	601	HEM	C1A-C2A-CAA-CBA
2	B	601	HEM	C3D-CAD-CBD-CGD
3	B	602	NDP	O4D-C1D-N1N-C6N
3	B	602	NDP	O4D-C1D-N1N-C2N
3	C	602	NDP	O4D-C1D-N1N-C6N
3	B	602	NDP	C5D-O5D-PN-O1N
3	C	602	NDP	C5D-O5D-PN-O1N
3	D	602	NDP	C5D-O5D-PN-O1N
3	C	602	NDP	PA-O3-PN-O2N
3	A	602	NDP	O4D-C1D-N1N-C6N
3	D	602	NDP	O4D-C1D-N1N-C6N
3	C	602	NDP	C1B-C2B-O2B-P2B
3	A	602	NDP	C2B-O2B-P2B-O1X
3	C	602	NDP	C2B-O2B-P2B-O1X
3	A	602	NDP	C2D-C1D-N1N-C6N
3	C	602	NDP	C3B-C2B-O2B-P2B
2	A	601	HEM	C2A-CAA-CBA-CGA
3	D	602	NDP	C2D-C1D-N1N-C6N
2	D	601	HEM	CAD-CBD-CGD-O1D
3	B	602	NDP	C2B-O2B-P2B-O3X
3	B	602	NDP	C1B-C2B-O2B-P2B
2	A	601	HEM	C3A-C2A-CAA-CBA
2	A	601	HEM	CAA-CBA-CGA-O2A
2	D	601	HEM	CAD-CBD-CGD-O2D
3	D	602	NDP	C3B-C2B-O2B-P2B
3	A	602	NDP	O4D-C1D-N1N-C2N
2	C	601	HEM	CAD-CBD-CGD-O2D
2	A	601	HEM	CAA-CBA-CGA-O1A

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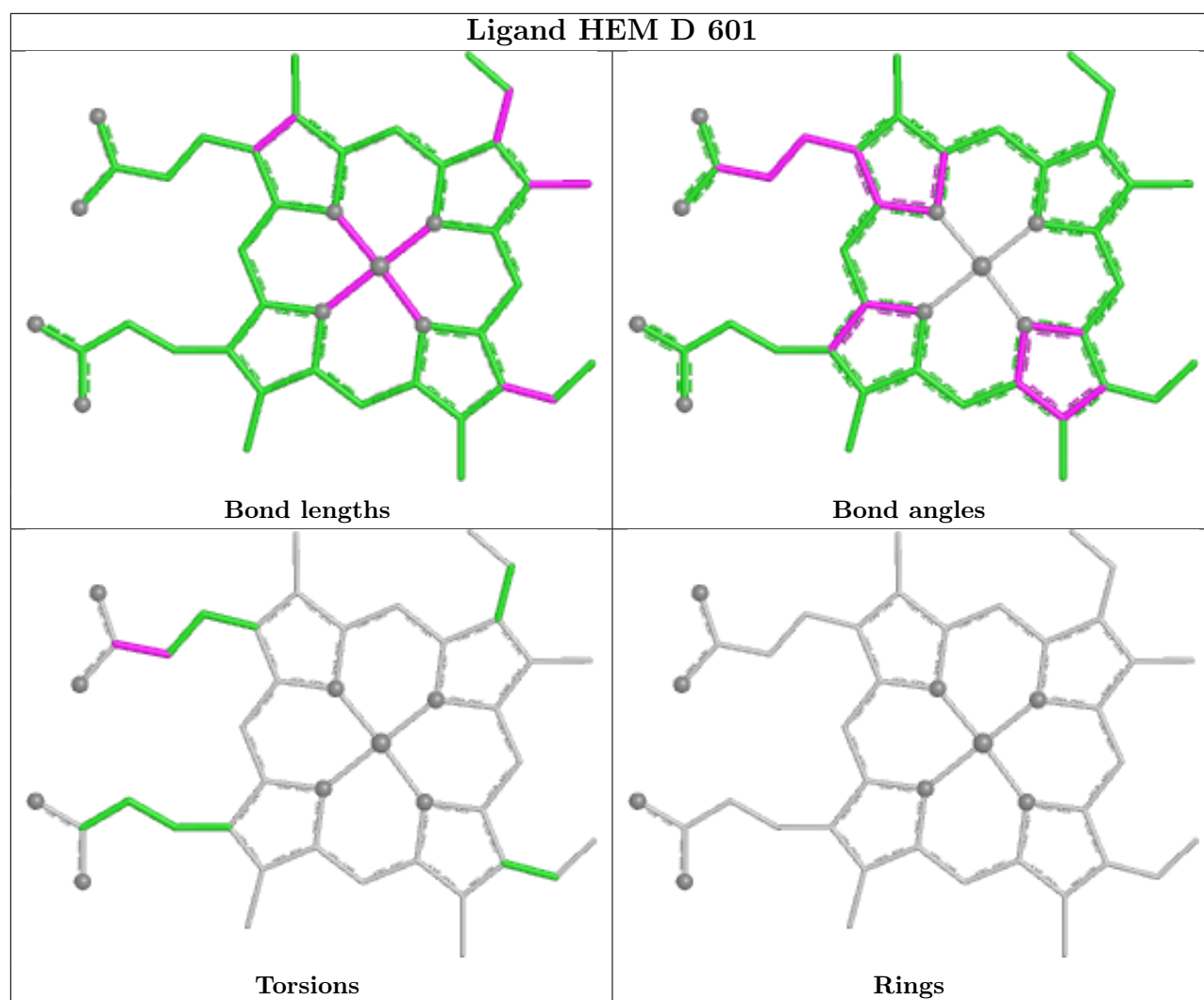
Mol	Chain	Res	Type	Atoms
2	C	601	HEM	CAD-CBD-CGD-O1D
3	C	602	NDP	PA-O3-PN-O1N
3	D	602	NDP	PA-O3-PN-O2N

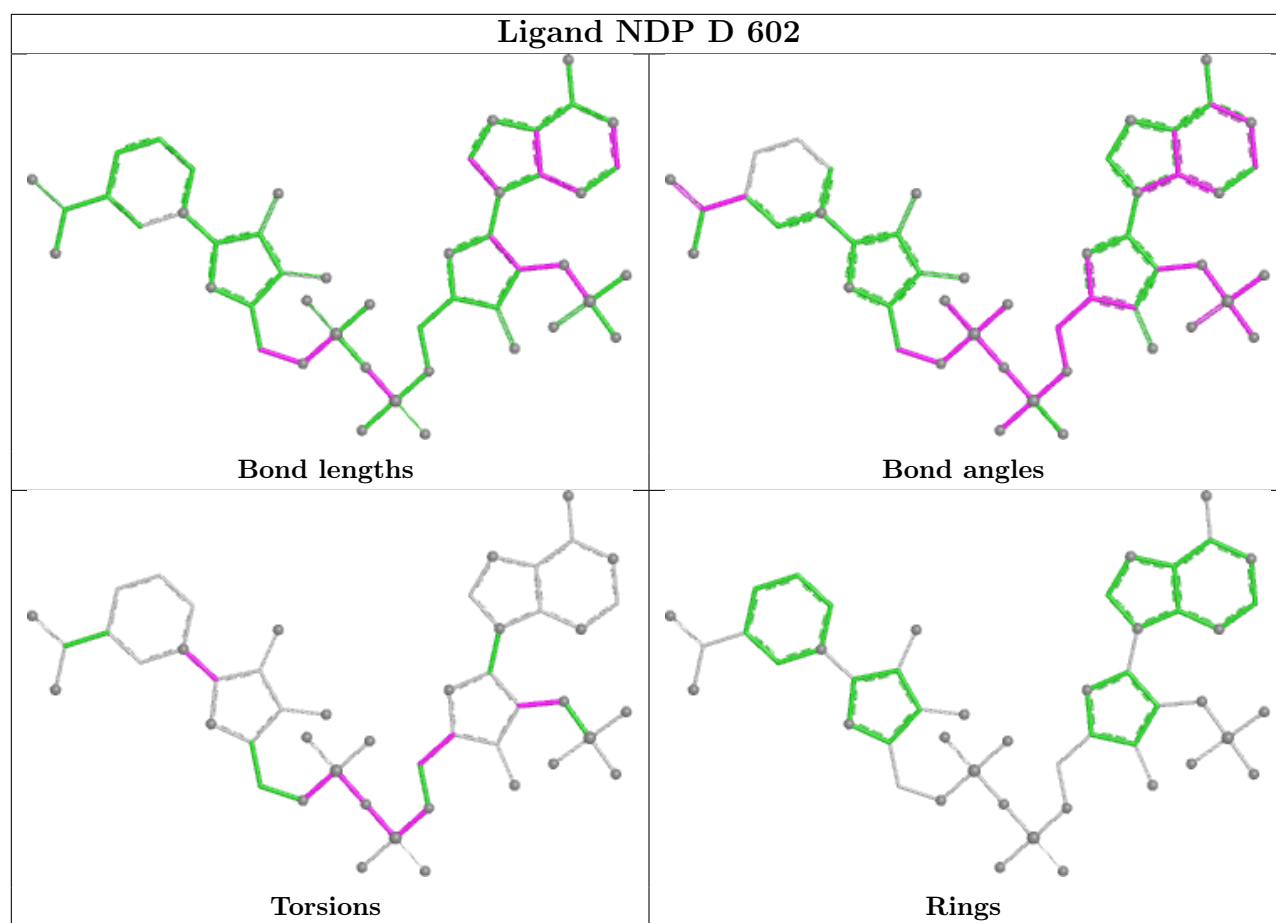
There are no ring outliers.

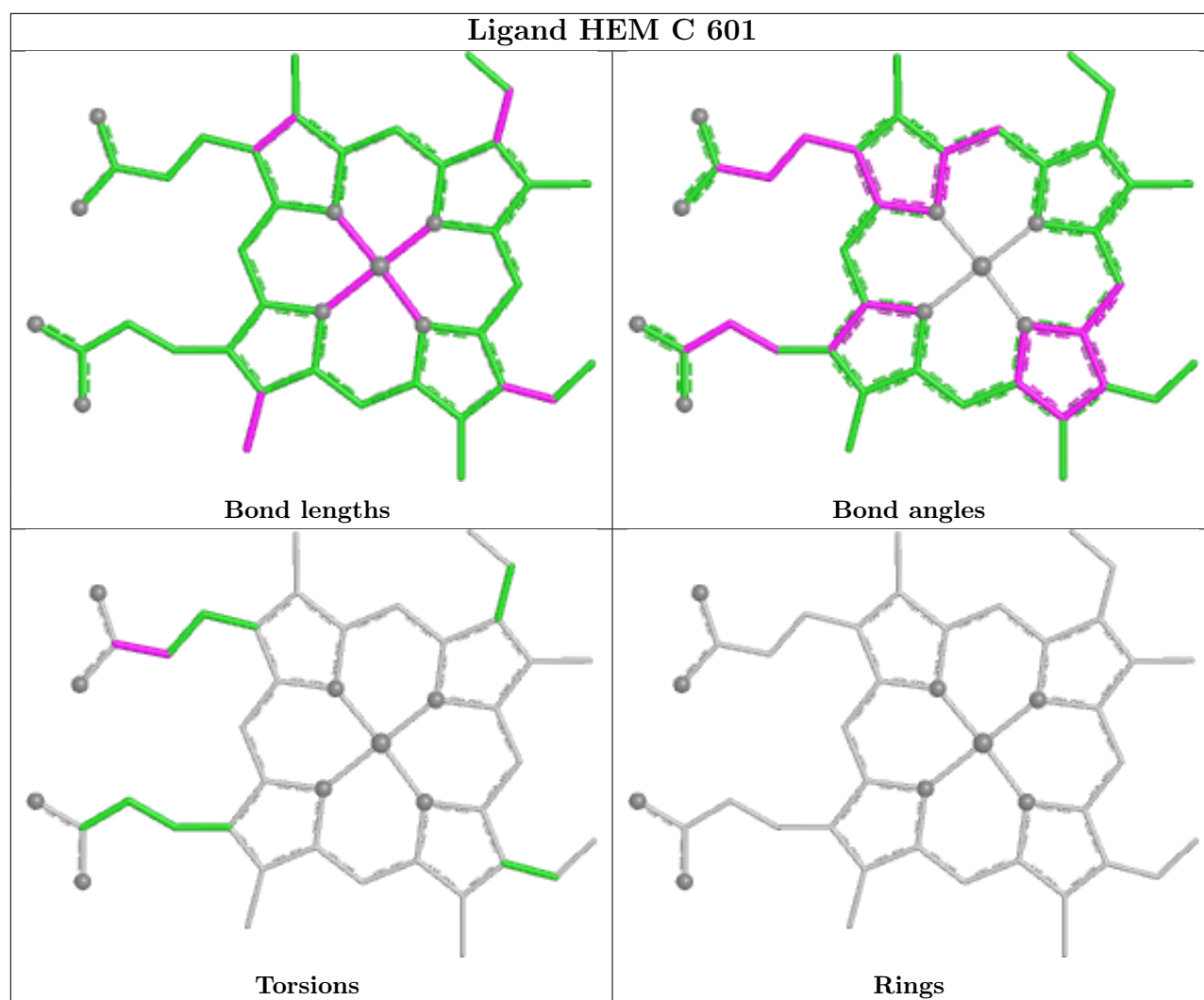
8 monomers are involved in 20 short contacts:

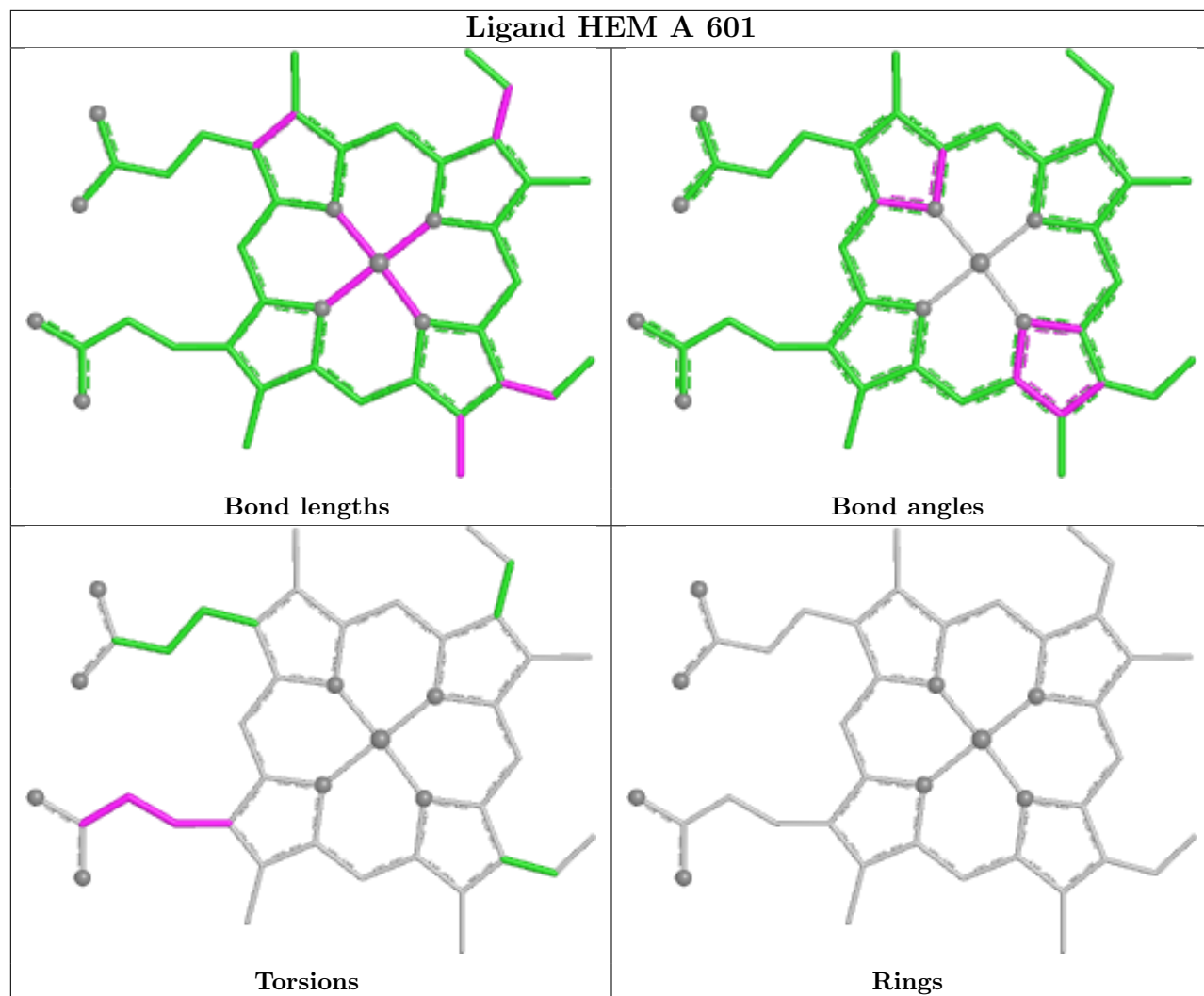
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	HEM	2	0
3	D	602	NDP	1	0
2	C	601	HEM	1	0
2	A	601	HEM	3	0
3	C	602	NDP	3	0
2	B	601	HEM	5	0
3	B	602	NDP	3	0
3	A	602	NDP	2	0

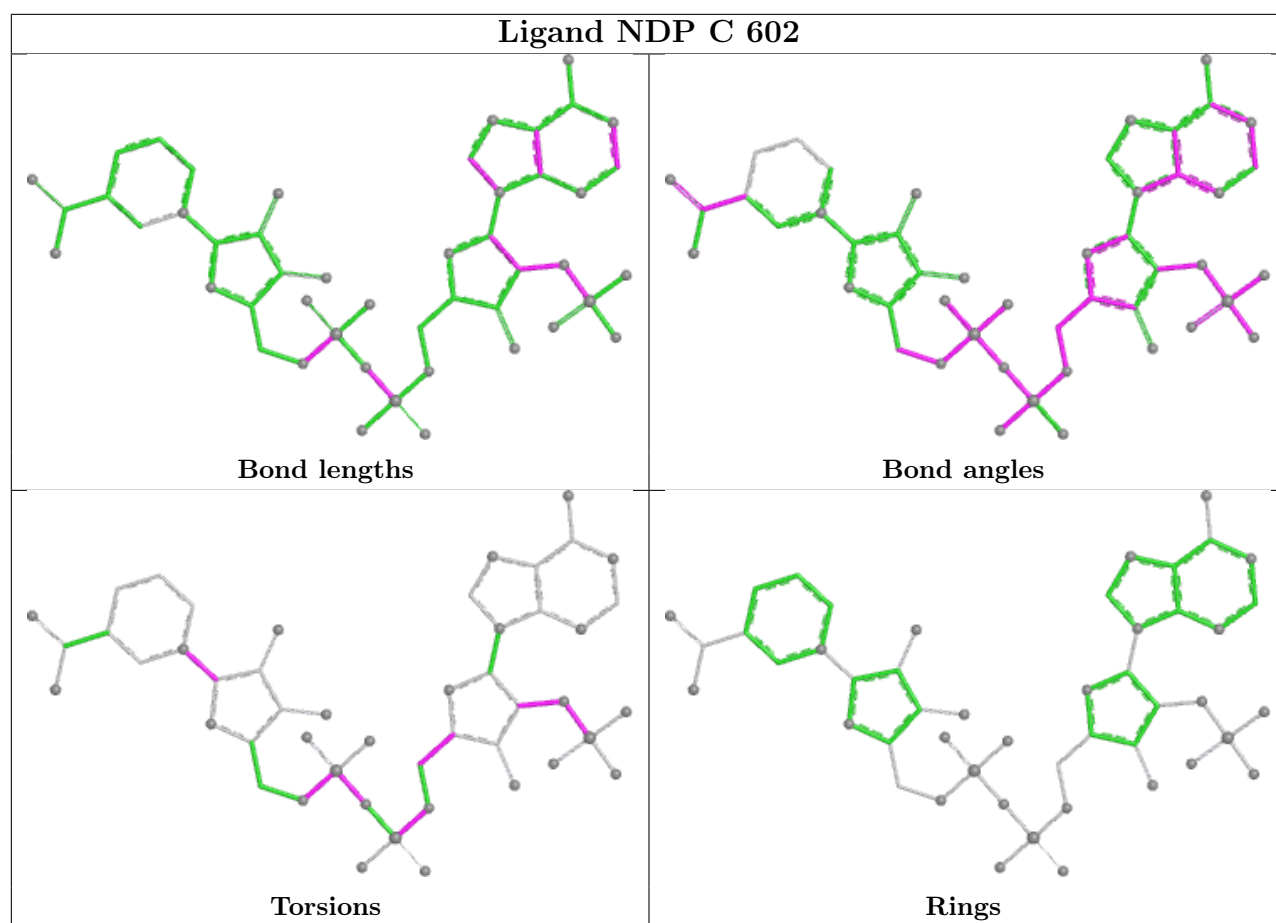
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

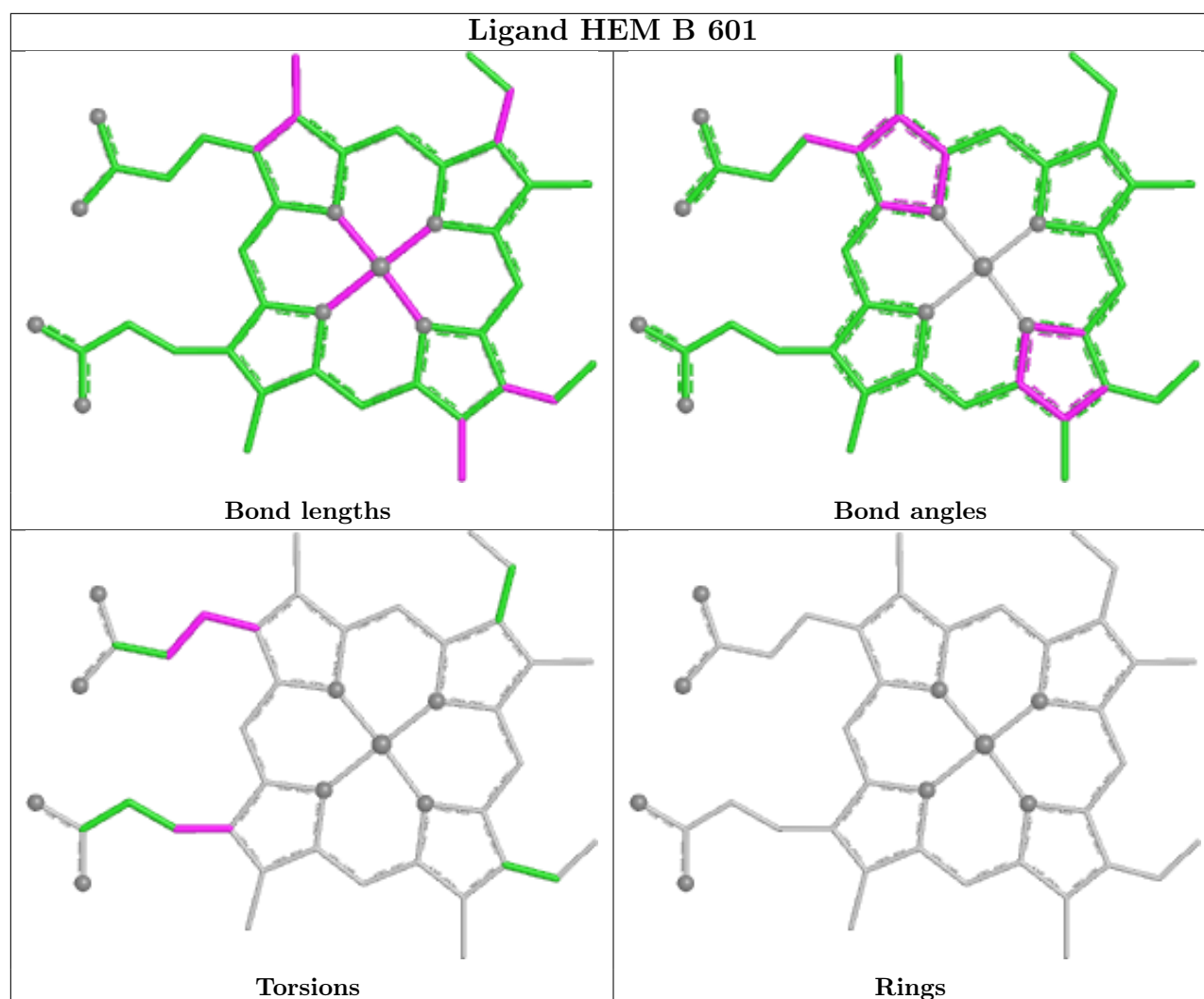


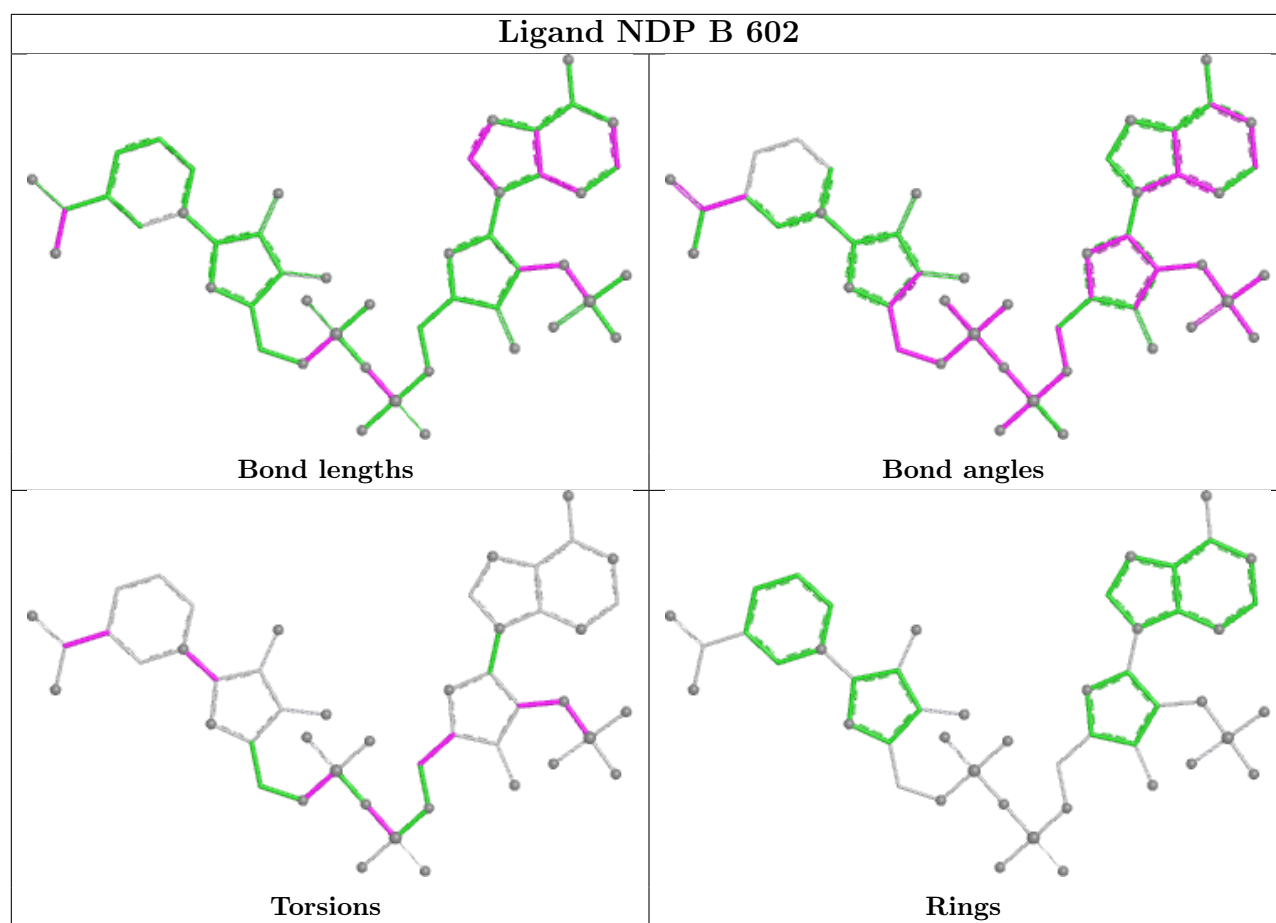


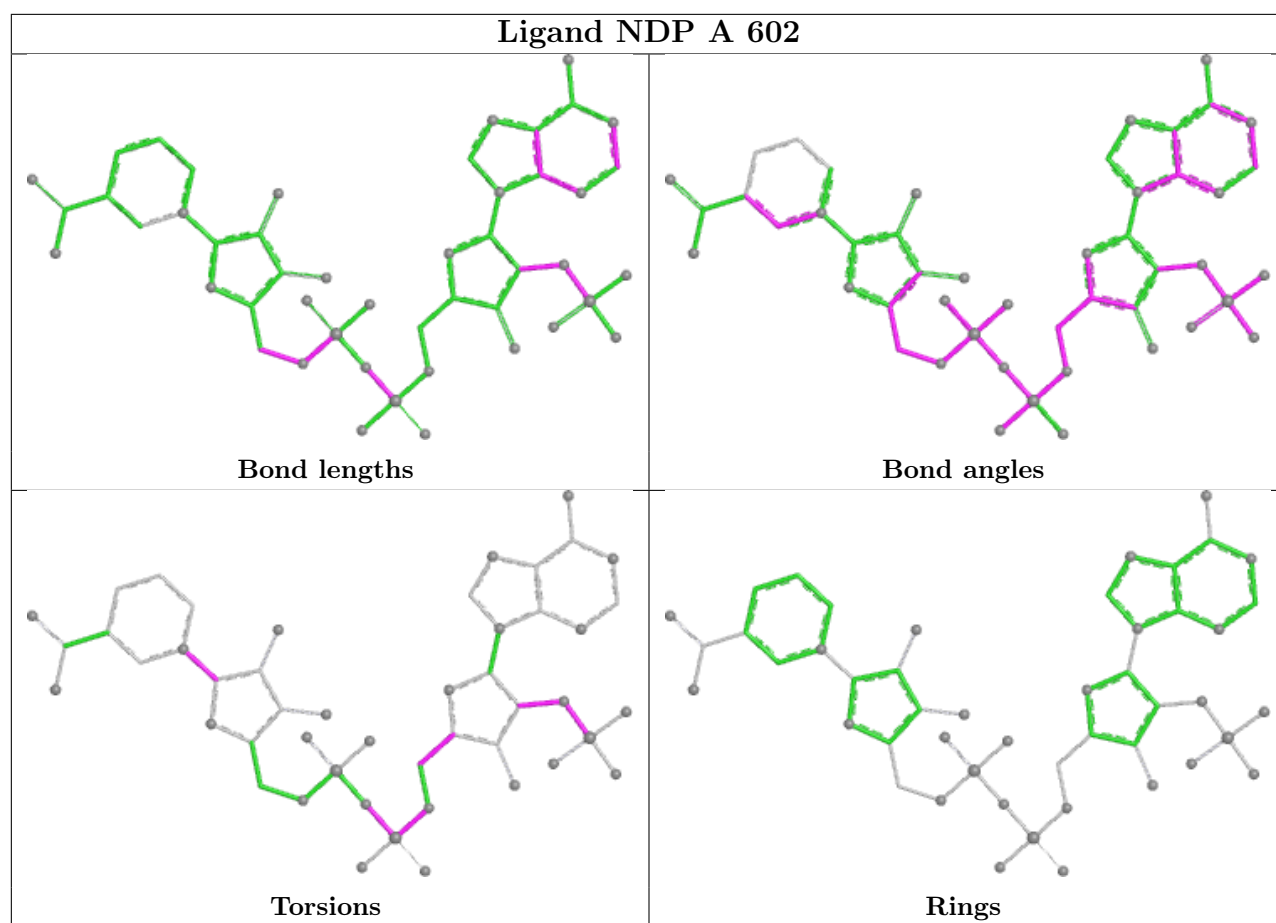












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

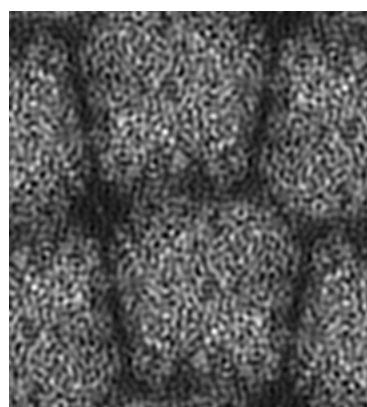
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6314. These allow visual inspection of the internal detail of the map and identification of artifacts.

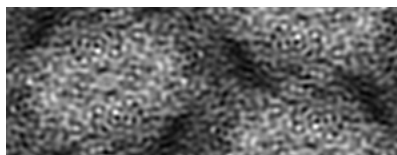
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

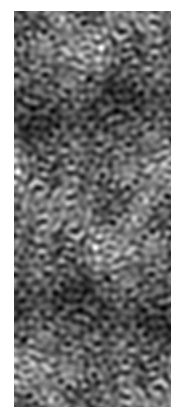
6.1.1 Primary map



X



Y

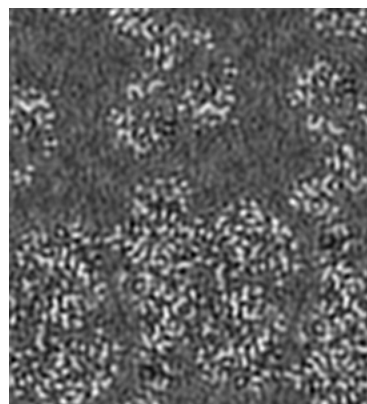


Z

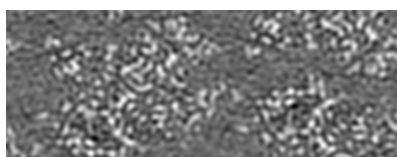
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

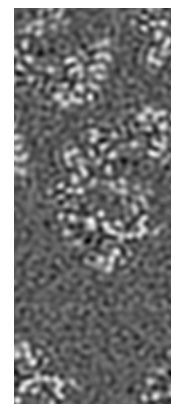
6.2.1 Primary map



X Index: 45



Y Index: 108

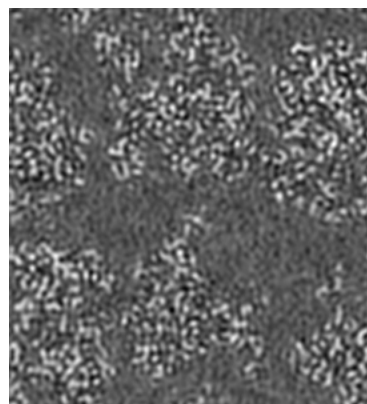


Z Index: 120

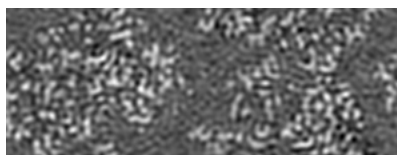
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

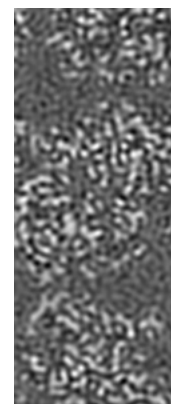
6.3.1 Primary map



X Index: 19



Y Index: 202

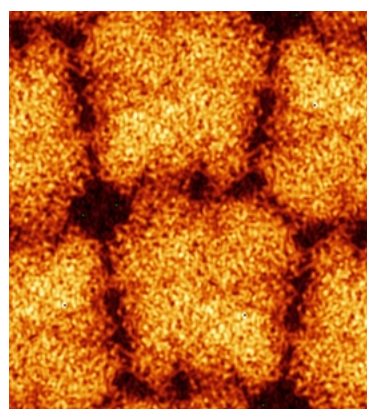


Z Index: 56

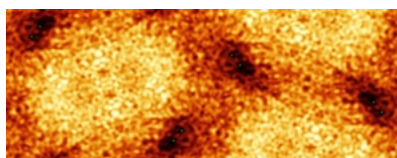
The images above show the largest variance slices of the map in three orthogonal directions.

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

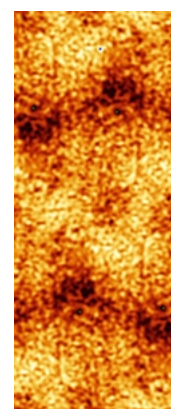
6.4.1 Primary map



X



Y

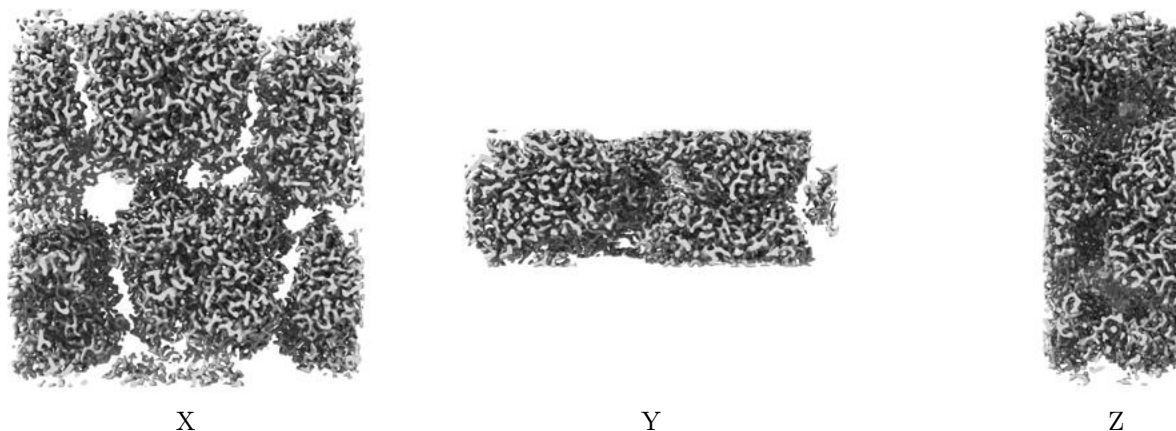


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

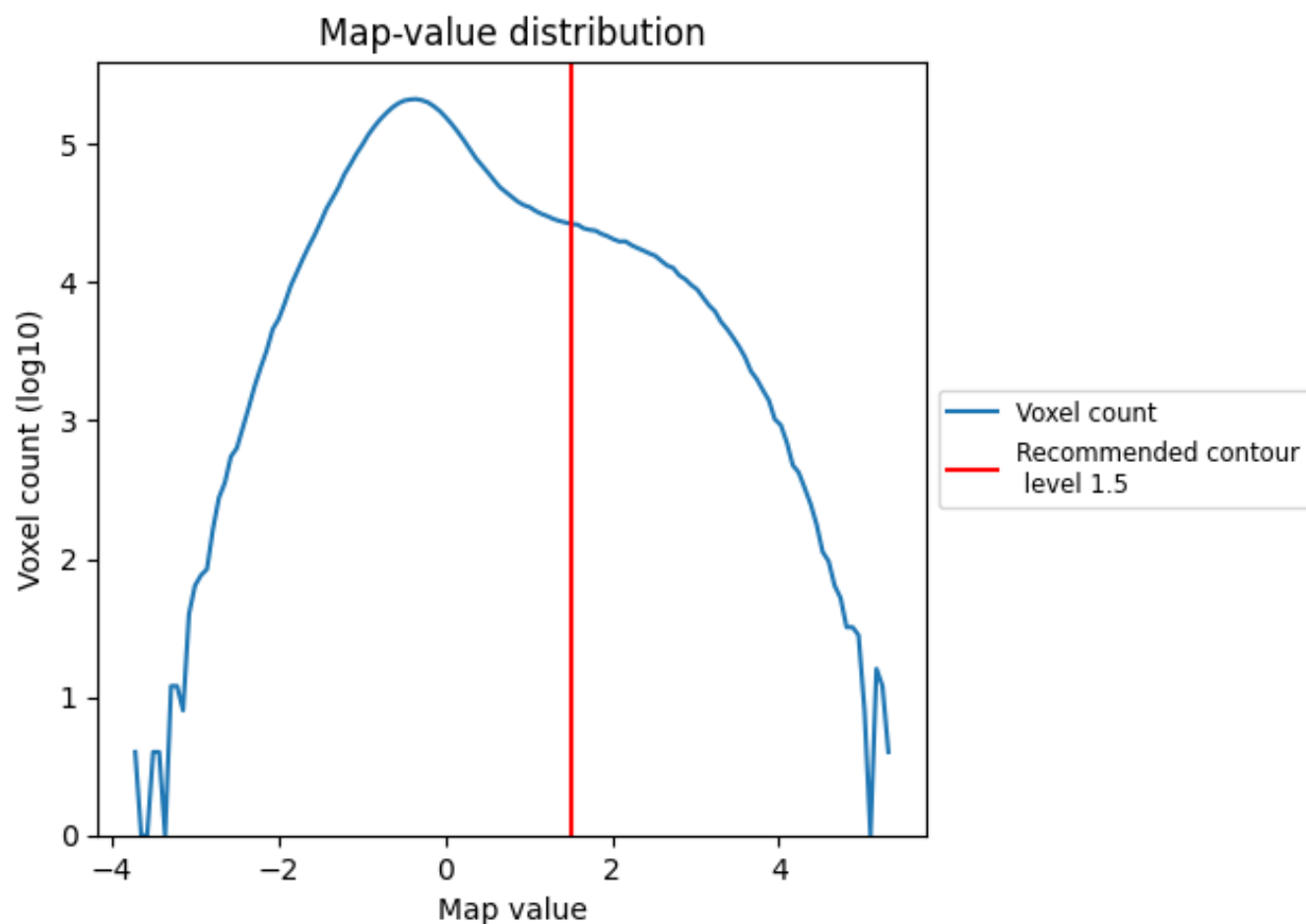
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

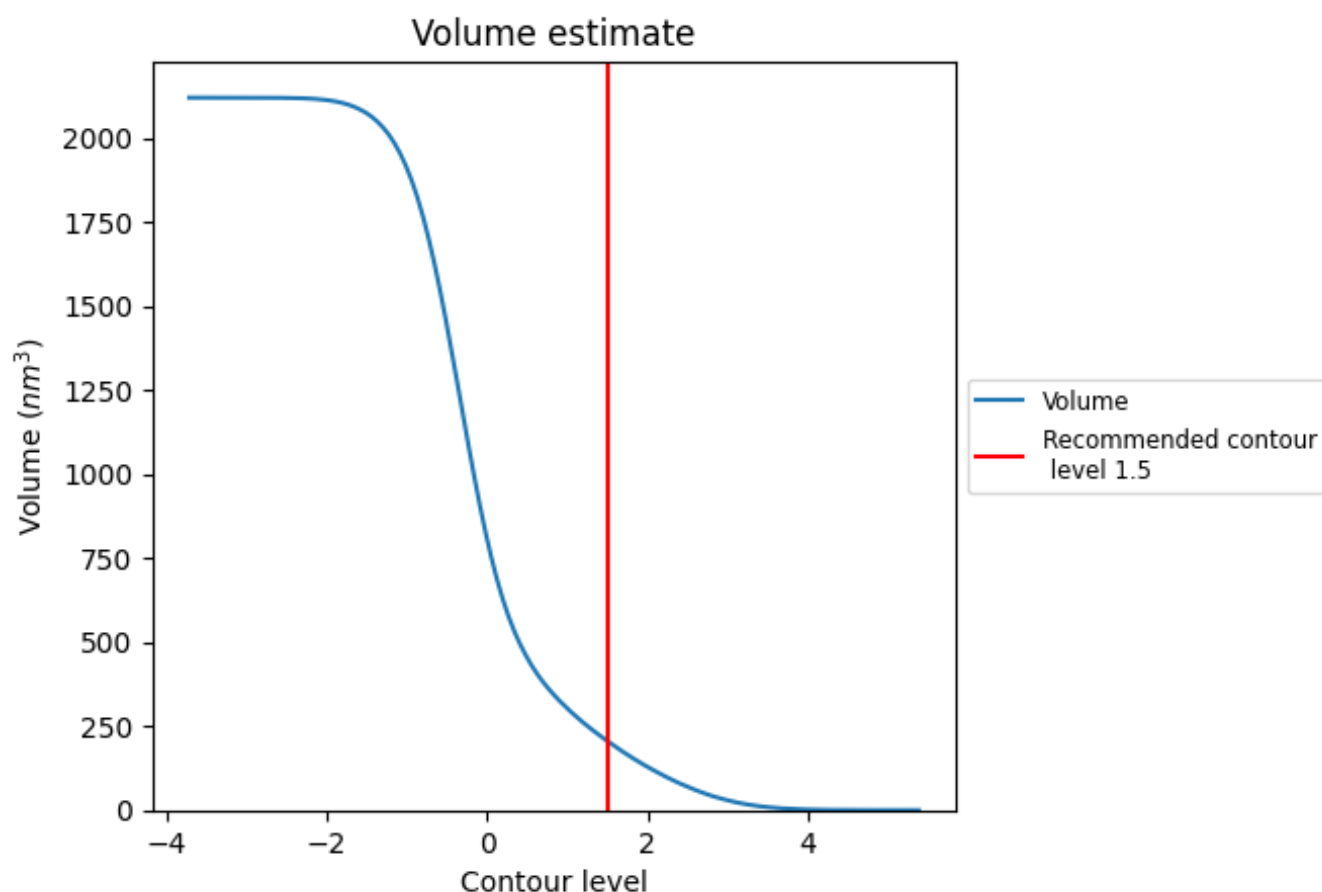
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 206 nm³; this corresponds to an approximate mass of 186 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 [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

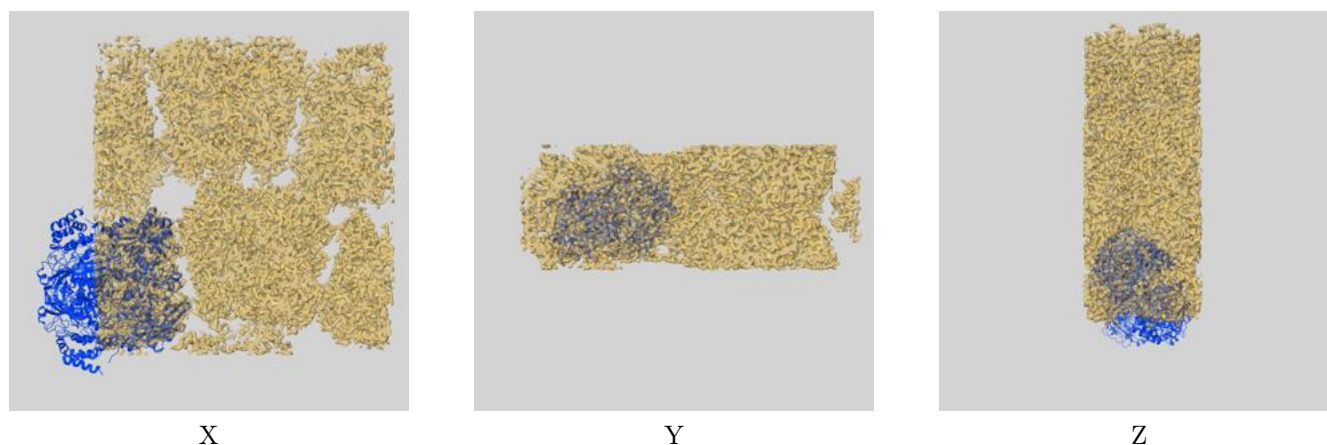
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

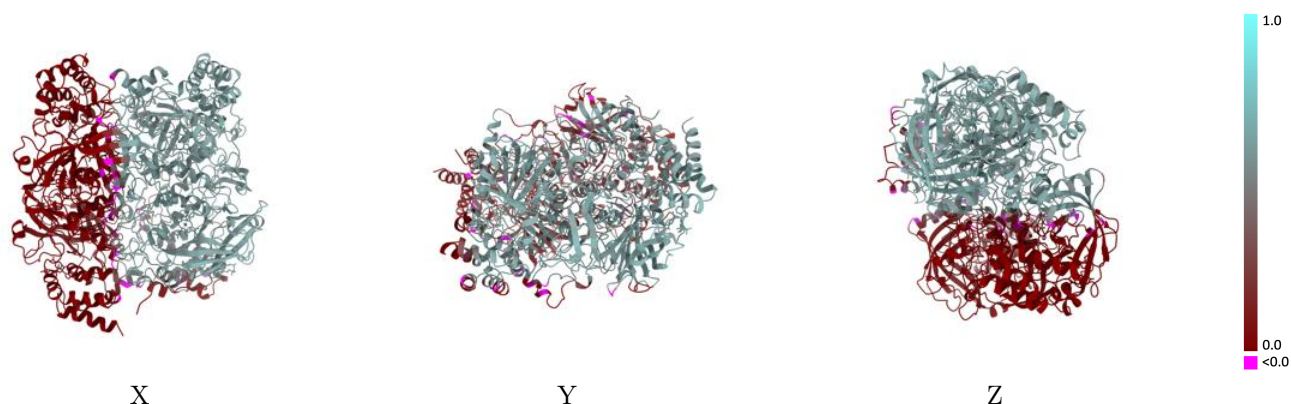
This section contains information regarding the fit between EMDB map EMD-6314 and PDB model 3J7B. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



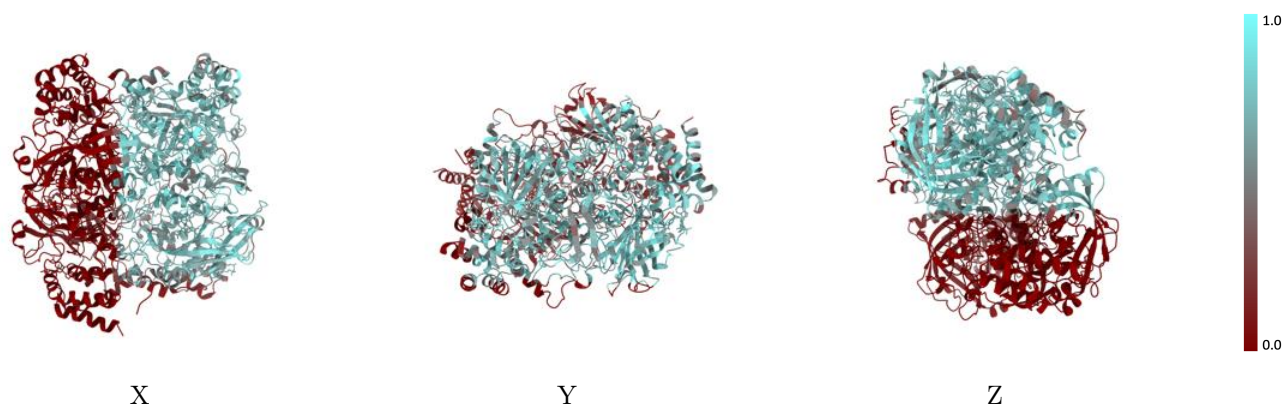
The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



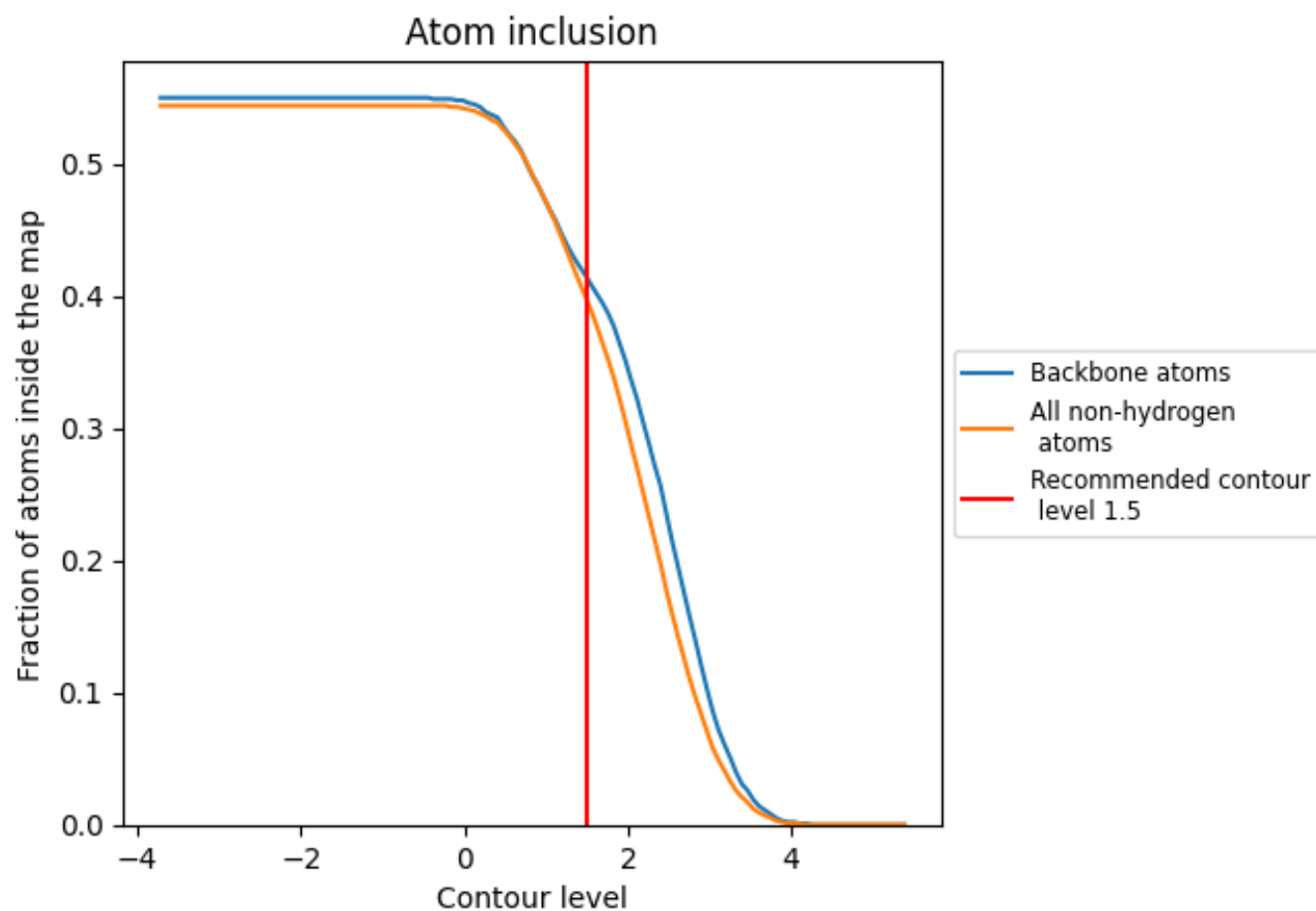
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.5).

9.4 Atom inclusion ⓘ



At the recommended contour level, 41% of all backbone atoms, 40% 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 (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3970	0.3340
A	0.6260	0.5130
B	0.5800	0.4880
C	0.1300	0.1150
D	0.2540	0.2190

