



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 10:51 AM UTC

PDB ID : 1DGG / pdb_00001dgg
Title : HUMAN ERYTHROCYTE CATALASE CYANIDE COMPLEX
Authors : Putnam, C.D.; Arvai, A.S.; Bourne, Y.; Tainer, J.A.
Deposited on : 1999-11-24
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

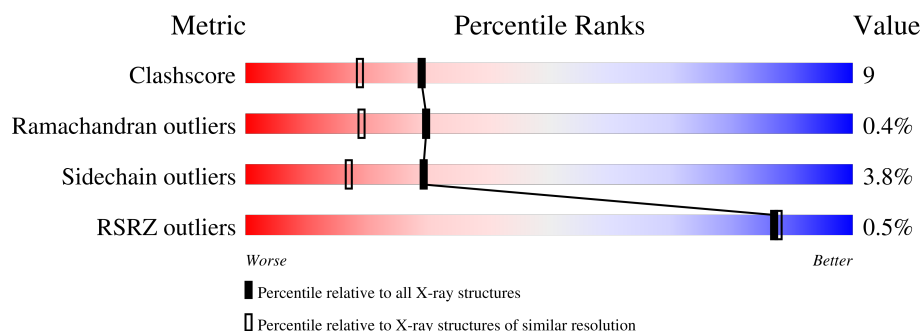
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	497	
1	B	497	
1	C	497	
1	D	497	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CYN	A	4000	-	-	X	-
2	CYN	B	4001	-	-	X	-
2	CYN	C	4002	-	-	X	-
2	CYN	D	4003	-	-	X	-

2 Entry composition [i](#)

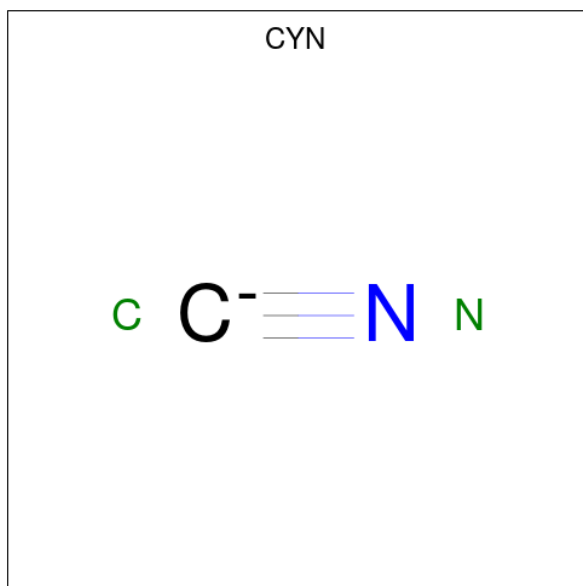
There are 5 unique types of molecules in this entry. The entry contains 17841 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	3	0
			4018	2551	713	740	14			
1	B	497	Total	C	N	O	S	0	3	0
			4018	2551	713	740	14			
1	C	497	Total	C	N	O	S	0	3	0
			4018	2551	713	740	14			
1	D	497	Total	C	N	O	S	0	3	0
			4018	2551	713	740	14			

- Molecule 2 is CYANIDE ION (CCD ID: CYN) (formula: CN).



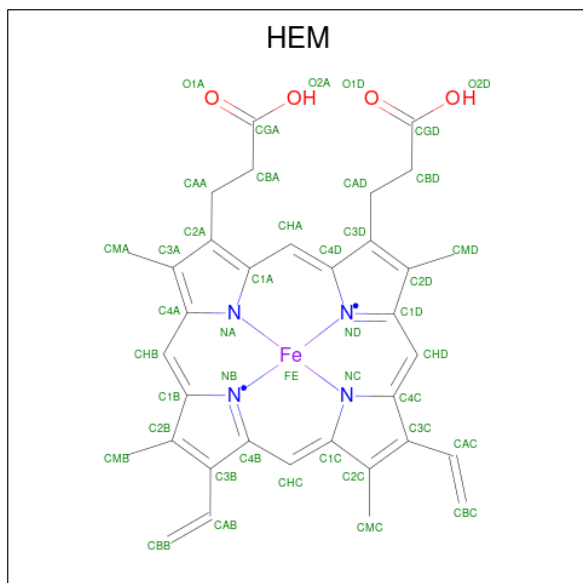
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			2	1	1		
2	B	1	Total	C	N	0	0
			2	1	1		

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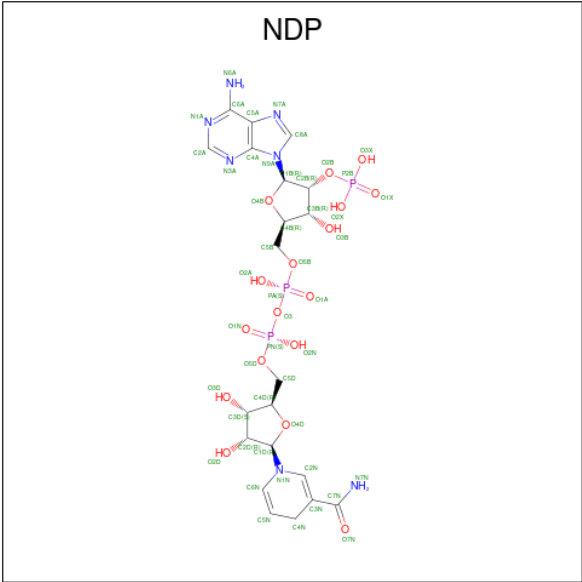
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	N	0	0
			2	1	1		
2	D	1	Total	C	N	0	0
			2	1	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 4 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

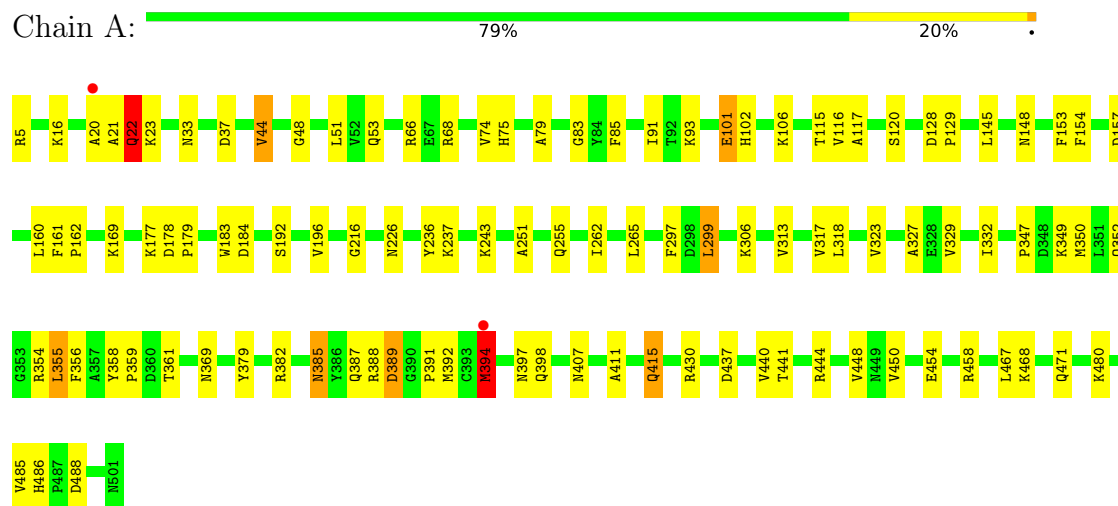
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	381	Total	O	0	0
			381	381		
5	B	380	Total	O	0	0
			380	380		
5	C	366	Total	O	0	0
			366	366		
5	D	366	Total	O	0	0
			366	366		

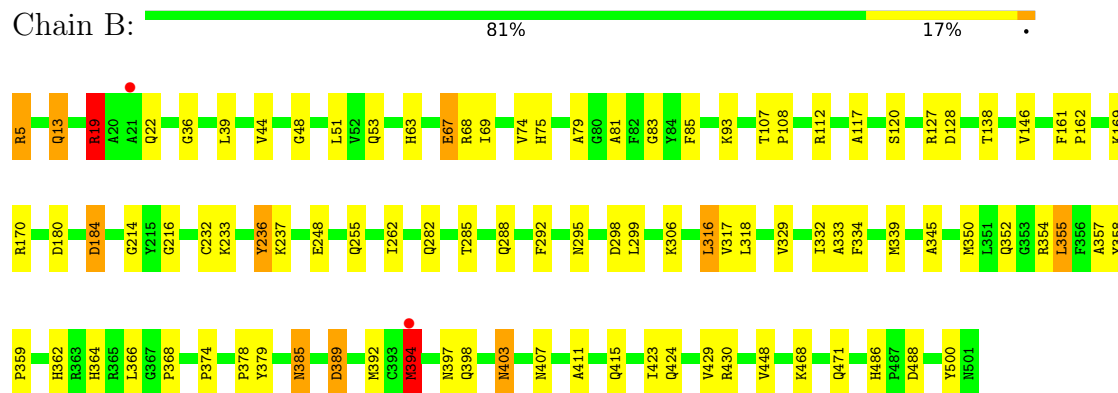
3 Residue-property plots [i](#)

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

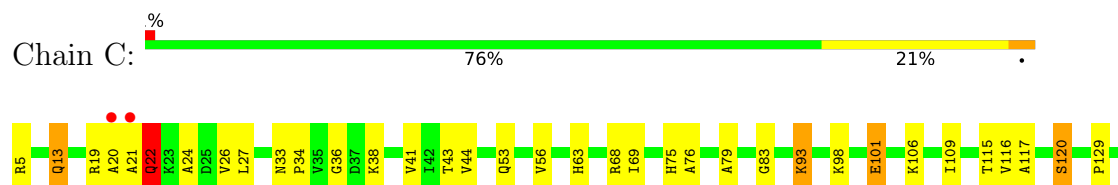
• Molecule 1: CATALASE

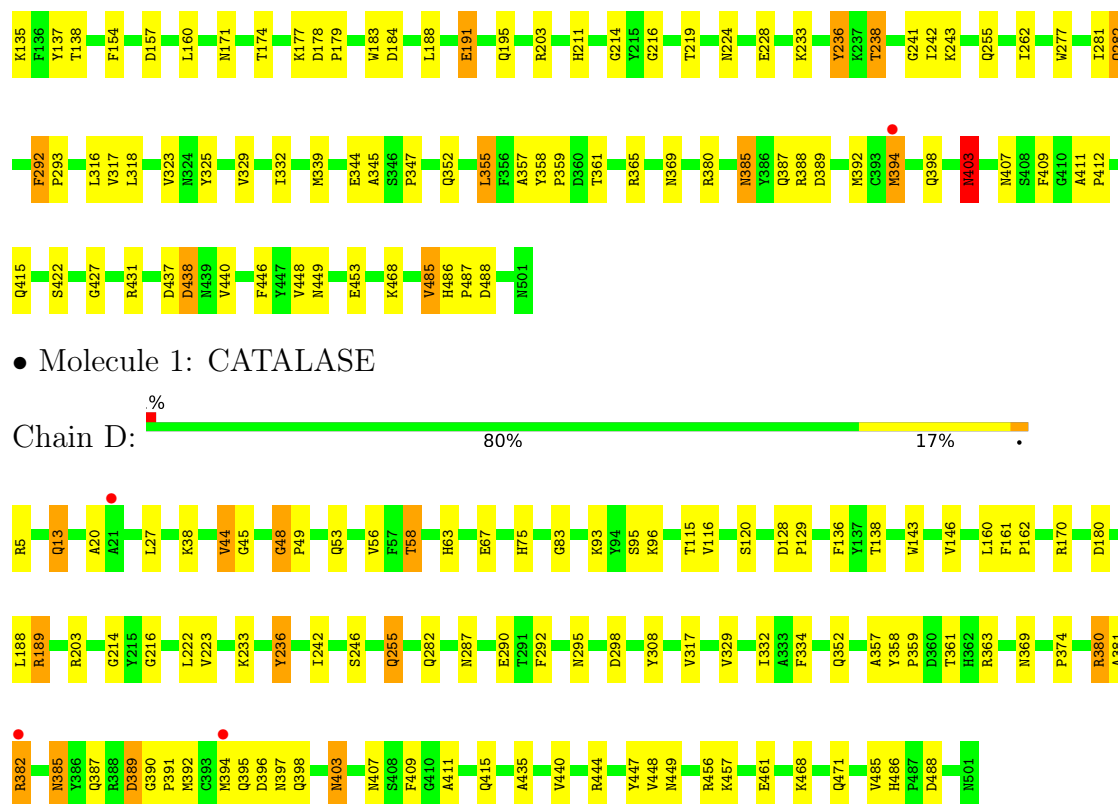


• Molecule 1: CATALASE

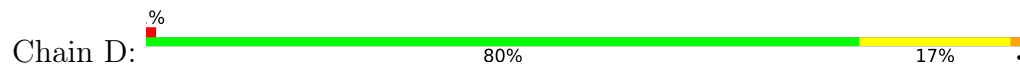


• Molecule 1: CATALASE





• Molecule 1: CATALASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.86Å 140.61Å 231.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 20.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.80) 78.2 (20.00-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.12 (at 1.80Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.178 , 0.221 0.170 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	17841	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.44	0/4137	1.00	23/5620 (0.4%)
1	B	0.42	0/4137	0.95	16/5620 (0.3%)
1	C	0.42	0/4137	0.99	27/5620 (0.5%)
1	D	0.43	0/4137	0.96	24/5620 (0.4%)
All	All	0.43	0/16548	0.97	90/22480 (0.4%)

There are no bond length outliers.

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	357	ALA	N-CA-C	8.17	120.92	111.11
1	A	323	VAL	N-CA-C	-7.67	105.21	111.81
1	A	101	GLU	N-CA-C	7.54	120.46	111.33
1	D	448	VAL	N-CA-C	7.46	117.55	110.53
1	D	216	GLY	N-CA-C	-7.39	105.50	114.66
1	C	101	GLU	N-CA-C	7.32	121.11	111.75
1	A	394	MET	N-CA-C	7.15	120.55	112.97
1	A	448	VAL	N-CA-C	7.13	117.22	110.74
1	C	357	ALA	N-CA-C	7.12	119.65	111.11
1	A	437	ASP	N-CA-C	-7.04	101.75	110.41
1	C	216	GLY	N-CA-C	-6.99	106.00	114.66
1	A	216	GLY	N-CA-C	-6.92	106.08	114.66
1	D	308	TYR	CA-C-N	6.63	126.61	119.78
1	D	308	TYR	C-N-CA	6.63	126.61	119.78
1	D	389	ASP	N-CA-C	6.53	117.66	108.00
1	C	394	MET	N-CA-C	6.43	121.13	113.28
1	B	216	GLY	N-CA-C	-6.30	106.84	114.66
1	B	415	GLN	CA-C-N	6.22	127.61	119.84
1	B	415	GLN	C-N-CA	6.22	127.61	119.84
1	C	219	THR	N-CA-C	-6.13	99.65	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	22	GLN	N-CA-C	6.01	123.60	110.80
1	A	128	ASP	CA-C-N	-5.99	114.46	120.21
1	A	128	ASP	C-N-CA	-5.99	114.46	120.21
1	A	23	LYS	N-CA-C	-5.83	102.28	110.50
1	D	357	ALA	N-CA-C	5.81	118.08	111.11
1	C	157	ASP	CA-C-N	5.80	125.66	119.28
1	C	157	ASP	C-N-CA	5.80	125.66	119.28
1	A	379	TYR	N-CA-C	5.79	119.82	112.87
1	A	68	ARG	N-CA-C	5.77	119.65	109.96
1	D	48	GLY	CA-C-N	5.76	125.73	120.03
1	D	48	GLY	C-N-CA	5.76	125.73	120.03
1	D	128	ASP	CA-C-N	-5.73	114.71	120.21
1	D	128	ASP	C-N-CA	-5.73	114.71	120.21
1	B	394	MET	N-CA-C	5.70	119.31	112.93
1	A	389	ASP	N-CA-C	5.63	118.48	109.02
1	B	292	PHE	CA-C-N	5.63	125.30	119.56
1	B	292	PHE	C-N-CA	5.63	125.30	119.56
1	C	292	PHE	CA-C-N	5.61	125.32	119.82
1	C	292	PHE	C-N-CA	5.61	125.32	119.82
1	D	56	VAL	N-CA-C	-5.60	105.05	110.42
1	B	19	ARG	N-CA-C	-5.59	106.46	113.28
1	A	440	VAL	N-CA-C	5.58	120.95	109.34
1	C	389	ASP	N-CA-C	5.57	118.38	109.02
1	C	448	VAL	N-CA-C	5.56	116.21	110.82
1	D	45	GLY	CA-C-N	5.56	125.39	119.28
1	D	45	GLY	C-N-CA	5.56	125.39	119.28
1	C	409	PHE	N-CA-C	5.45	119.24	112.59
1	C	403	ASN	N-CA-C	5.45	118.93	112.72
1	D	170	ARG	N-CA-C	5.45	118.54	110.48
1	B	184	ASP	N-CA-C	-5.39	105.49	111.36
1	C	117	ALA	N-CA-C	5.38	117.97	111.40
1	B	389	ASP	CB-CA-C	-5.37	109.40	115.79
1	B	379	TYR	N-CA-C	5.36	119.31	112.87
1	C	449	ASN	N-CA-C	5.36	119.92	112.90
1	C	453	GLU	N-CA-C	5.36	116.81	111.07
1	A	157	ASP	CA-C-N	5.34	125.01	119.56
1	A	157	ASP	C-N-CA	5.34	125.01	119.56
1	D	115	THR	N-CA-C	-5.33	101.75	109.31
1	C	191	GLU	N-CA-C	-5.31	106.06	112.54
1	B	448	VAL	N-CA-C	5.31	115.97	110.82
1	C	76	ALA	N-CA-C	5.29	116.73	111.07
1	C	120[A]	SER	N-CA-C	-5.28	102.03	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	120[B]	SER	N-CA-C	-5.28	102.03	109.96
1	B	378	PRO	N-CA-C	-5.28	105.35	112.48
1	B	117	ALA	N-CA-C	5.27	118.17	111.69
1	B	68	ARG	N-CA-C	5.24	118.77	109.96
1	A	415	GLN	CA-C-N	5.23	126.38	119.84
1	A	415	GLN	C-N-CA	5.23	126.38	119.84
1	D	292	PHE	CA-C-N	5.23	125.54	119.47
1	D	292	PHE	C-N-CA	5.23	125.54	119.47
1	A	117	ALA	N-CA-C	5.21	117.03	111.36
1	A	441	THR	N-CA-C	5.19	117.36	111.02
1	C	485	VAL	N-CA-C	-5.15	105.69	110.53
1	C	183	TRP	N-CA-C	5.14	119.27	112.89
1	D	440	VAL	N-CA-C	5.12	119.98	109.34
1	C	68	ARG	N-CA-C	5.10	118.25	110.20
1	C	184	ASP	N-CA-C	-5.10	105.64	111.14
1	A	184	ASP	N-CA-C	-5.09	105.81	111.36
1	B	67	GLU	N-CA-C	5.09	117.56	111.71
1	A	154	PHE	N-CA-C	5.08	116.81	111.28
1	A	327	ALA	N-CA-C	5.07	116.81	111.28
1	A	450	VAL	N-CA-C	5.05	115.72	110.82
1	D	189	ARG	CA-C-N	5.05	124.77	119.82
1	D	189	ARG	C-N-CA	5.05	124.77	119.82
1	D	449	ASN	N-CA-C	5.05	119.43	113.12
1	D	390	GLY	CA-C-N	5.04	125.04	119.90
1	D	390	GLY	C-N-CA	5.04	125.04	119.90
1	C	282	GLN	N-CA-C	-5.04	101.48	109.59
1	C	323	VAL	N-CA-C	-5.03	106.25	111.58
1	D	409	PHE	N-CA-C	5.01	118.93	112.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4018	0	3845	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4018	0	3845	73	0
1	C	4018	0	3845	80	0
1	D	4018	0	3845	76	0
2	A	2	0	0	4	0
2	B	2	0	0	4	0
2	C	2	0	0	4	0
2	D	2	0	0	4	0
3	A	43	0	30	6	0
3	B	43	0	30	5	0
3	C	43	0	30	4	0
3	D	43	0	30	4	0
4	A	48	0	26	0	0
4	C	48	0	26	1	0
5	A	381	0	0	8	0
5	B	380	0	0	5	0
5	C	366	0	0	13	0
5	D	366	0	0	7	0
All	All	17841	0	15552	273	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 9.

All (273) 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:392:MET:HE3	1:C:394:MET:HE1	1.27	1.15
1:A:392:MET:HE3	1:A:394:MET:HE1	1.30	1.12
1:D:382:ARG:H	1:D:382:ARG:HD3	1.13	1.10
1:A:120[B]:SER:O	1:C:120[B]:SER:O	1.78	0.99
2:A:4000:CYN:C	3:A:2000:HEM:NB	2.26	0.98
1:B:120[B]:SER:O	1:D:120[B]:SER:O	1.87	0.91
1:B:385:ASN:H	1:B:398:GLN:HE22	1.20	0.89
2:C:4002:CYN:C	3:C:2002:HEM:ND	2.38	0.86
2:B:4001:CYN:C	3:B:2001:HEM:ND	2.39	0.85
1:C:63:HIS:HE1	1:D:369:ASN:HD21	1.24	0.84
2:D:4003:CYN:C	3:D:2003:HEM:ND	2.40	0.84
2:B:4001:CYN:C	3:B:2001:HEM:NA	2.42	0.83
1:D:486:HIS:HD2	1:D:488:ASP:H	1.27	0.83
2:C:4002:CYN:C	3:C:2002:HEM:NC	2.42	0.83
1:C:385:ASN:H	1:C:398:GLN:HE22	1.23	0.82
1:B:392:MET:HE3	1:B:394:MET:HE1	1.59	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:ARG:HH21	1:B:19:ARG:HG3	1.47	0.80
1:A:369:ASN:HD21	1:B:63:HIS:HE1	1.27	0.80
2:D:4003:CYN:C	3:D:2003:HEM:NC	2.46	0.78
1:B:13:GLN:HG2	1:D:471:GLN:NE2	1.98	0.78
1:D:385:ASN:H	1:D:398:GLN:HE22	1.30	0.78
2:A:4000:CYN:C	3:A:2000:HEM:NA	2.46	0.77
2:A:4000:CYN:C	3:A:2000:HEM:NC	2.48	0.77
1:B:19:ARG:O	1:B:22:GLN:HG2	1.85	0.77
1:A:385:ASN:H	1:A:398:GLN:HE22	1.30	0.77
1:C:63:HIS:HE1	1:D:369:ASN:ND2	1.83	0.76
1:A:169:LYS:HB3	5:A:4145:HOH:O	1.86	0.76
2:D:4003:CYN:C	3:D:2003:HEM:NB	2.49	0.76
1:D:382:ARG:H	1:D:382:ARG:CD	1.97	0.75
2:C:4002:CYN:C	3:C:2002:HEM:NA	2.50	0.75
2:A:4000:CYN:C	3:A:2000:HEM:ND	2.50	0.75
1:B:13:GLN:HG2	1:D:471:GLN:HE22	1.51	0.73
1:C:369:ASN:ND2	1:D:63:HIS:HE1	1.86	0.73
1:C:34:PRO:HG3	1:D:382:ARG:HH22	1.53	0.73
2:C:4002:CYN:C	3:C:2002:HEM:NB	2.51	0.73
1:A:394:MET:HB2	1:B:394:MET:HE2	1.70	0.72
1:D:116:VAL:HG21	1:D:129:PRO:HG2	1.71	0.72
1:C:116:VAL:HG21	1:C:129:PRO:HG2	1.72	0.72
1:C:369:ASN:HD21	1:D:63:HIS:HE1	1.35	0.72
2:B:4001:CYN:C	3:B:2001:HEM:NB	2.53	0.71
1:D:392:MET:CE	1:D:394:MET:HE1	2.22	0.69
2:B:4001:CYN:C	3:B:2001:HEM:NC	2.55	0.68
5:C:4348:HOH:O	1:D:382:ARG:HG2	1.93	0.68
1:A:369:ASN:ND2	1:B:63:HIS:HE1	1.90	0.68
1:D:382:ARG:HD3	1:D:382:ARG:N	1.97	0.67
1:D:392:MET:HE3	1:D:394:MET:HE1	1.77	0.67
1:C:63:HIS:HD2	5:C:4033:HOH:O	1.80	0.65
2:D:4003:CYN:C	3:D:2003:HEM:NA	2.59	0.65
1:B:486:HIS:HD2	1:B:488:ASP:H	1.43	0.64
1:A:53:GLN:HE21	1:B:352:GLN:HE22	1.45	0.64
1:D:58:THR:HG21	5:D:4076:HOH:O	1.98	0.64
1:B:63:HIS:HD2	5:B:4015:HOH:O	1.80	0.64
1:B:407:ASN:HD21	1:B:411:ALA:HB3	1.62	0.64
1:B:19:ARG:HH21	1:B:19:ARG:CG	2.10	0.63
1:B:471:GLN:NE2	1:D:13:GLN:HG2	2.14	0.63
1:B:255:GLN:HB2	1:D:255:GLN:HB2	1.82	0.62
1:A:394:MET:HE2	1:B:394:MET:SD	2.39	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:ASP:H	1:D:397:ASN:HD21	1.48	0.61
1:A:116:VAL:HG21	1:A:129:PRO:HG2	1.82	0.61
1:B:364:HIS:HD2	5:C:4095:HOH:O	1.84	0.61
1:D:295:ASN:HB3	1:D:298:ASP:HB2	1.84	0.60
5:C:4229:HOH:O	1:D:392:MET:HE2	2.03	0.58
1:B:424:GLN:HE21	1:C:427:GLY:H	1.50	0.58
1:D:380:ARG:HB3	1:D:380:ARG:HH11	1.68	0.58
1:A:16:LYS:HE3	5:B:4326:HOH:O	2.02	0.58
1:C:329:VAL:O	1:C:332:ILE:HG22	2.04	0.57
1:A:306:LYS:HB2	5:A:4335:HOH:O	2.05	0.57
1:A:407:ASN:HD21	1:A:411:ALA:HB3	1.70	0.57
1:A:91:ILE:HG21	1:A:313:VAL:HG22	1.86	0.57
1:A:454:GLU:HB3	1:A:458:ARG:HH21	1.70	0.57
1:A:471:GLN:HE22	1:C:13:GLN:HG2	1.70	0.56
1:C:63:HIS:CE1	1:D:369:ASN:HD21	2.13	0.56
1:B:385:ASN:H	1:B:398:GLN:NE2	1.98	0.56
1:D:444:ARG:HD3	1:D:485:VAL:O	2.04	0.56
1:B:295:ASN:HB3	1:B:298:ASP:HB2	1.87	0.56
1:D:486:HIS:CD2	1:D:488:ASP:HB3	2.41	0.56
1:A:51:LEU:HD23	1:D:49:PRO:HB2	1.88	0.56
1:D:380:ARG:HH11	1:D:380:ARG:CB	2.19	0.56
1:A:444:ARG:HD3	1:A:485:VAL:O	2.07	0.55
1:C:369:ASN:HD21	1:D:63:HIS:CE1	2.21	0.55
1:A:21:ALA:O	1:A:22:GLN:HB2	2.07	0.55
1:D:161:PHE:HB3	1:D:162:PRO:HD3	1.89	0.55
1:A:33:ASN:HB3	5:B:4368:HOH:O	2.06	0.54
1:A:471:GLN:NE2	1:C:13:GLN:HG2	2.23	0.54
1:B:83:GLY:HA3	1:B:317:VAL:O	2.08	0.54
1:A:255:GLN:HB2	1:C:255:GLN:HB2	1.90	0.54
1:C:339:MET:HE1	1:C:345:ALA:HB2	1.90	0.54
1:B:389:ASP:H	1:B:397:ASN:HD21	1.56	0.54
1:B:471:GLN:HE22	1:D:13:GLN:HG2	1.71	0.54
1:A:153:PHE:CB	1:A:299:LEU:HD13	2.39	0.53
1:A:83:GLY:HA3	1:A:317:VAL:O	2.08	0.53
1:B:237:LYS:HE2	5:B:4321:HOH:O	2.08	0.53
1:A:66:ARG:HD3	1:B:368:PRO:HG3	1.91	0.53
1:C:403:ASN:C	1:C:403:ASN:HD22	2.17	0.52
1:A:385:ASN:ND2	1:A:387:GLN:H	2.08	0.52
1:B:146:VAL:HG22	1:B:334:PHE:HB3	1.91	0.52
1:C:116:VAL:CG2	1:C:129:PRO:HG2	2.40	0.52
1:A:352:GLN:HA	1:A:355:LEU:HD22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:MET:HE3	5:C:4065:HOH:O	2.09	0.52
1:B:44:VAL:O	1:B:48:GLY:HA3	2.10	0.52
1:C:486:HIS:HD2	1:C:488:ASP:H	1.58	0.52
1:A:177:LYS:HG3	5:A:4257:HOH:O	2.08	0.51
1:A:101:GLU:HG3	1:A:102:HIS:CD2	2.45	0.51
1:B:161:PHE:HB3	1:B:162:PRO:HD3	1.91	0.51
1:A:350:MET:O	1:A:354:ARG:HG3	2.10	0.51
1:D:96:LYS:HG2	1:D:223:VAL:O	2.10	0.51
1:A:329:VAL:O	1:A:332:ILE:HG22	2.11	0.51
1:A:486:HIS:HD2	1:A:488:ASP:H	1.57	0.51
1:C:233:LYS:HB2	1:C:282:GLN:HB2	1.91	0.51
1:C:344:GLU:HG2	5:C:4354:HOH:O	2.10	0.51
1:B:233:LYS:HB2	1:B:282:GLN:HB2	1.92	0.51
1:D:44:VAL:CG1	1:D:49:PRO:HD2	2.41	0.51
1:B:403:ASN:C	1:B:403:ASN:HD22	2.18	0.51
1:C:154:PHE:CE2	1:C:195:GLN:HG3	2.46	0.50
1:B:352:GLN:HA	1:B:355:LEU:HD22	1.92	0.50
1:C:19:ARG:NH2	1:C:24:ALA:HA	2.26	0.50
1:D:457:LYS:O	1:D:461:GLU:HG2	2.11	0.50
1:A:415:GLN:O	1:B:36:GLY:HA2	2.11	0.50
1:A:486:HIS:CD2	1:A:488:ASP:HB3	2.47	0.50
1:D:63:HIS:HD2	5:D:4035:HOH:O	1.94	0.50
1:D:381:ALA:HB1	1:D:382:ARG:HH11	1.77	0.50
1:D:486:HIS:CD2	1:D:488:ASP:H	2.18	0.49
1:A:153:PHE:HB3	1:A:299:LEU:HD13	1.94	0.49
1:B:430:ARG:HB3	1:C:422:SER:HB3	1.95	0.49
1:D:189:ARG:HH22	1:D:435:ALA:HB2	1.77	0.49
1:D:395:GLN:HG3	1:D:396:ASP:H	1.77	0.49
1:B:385:ASN:C	1:B:385:ASN:HD22	2.19	0.49
1:D:44:VAL:O	1:D:48:GLY:HA3	2.13	0.49
1:A:85:PHE:O	1:A:106:LYS:HA	2.13	0.49
1:B:392:MET:CE	1:B:394:MET:HE1	2.36	0.49
1:D:359:PRO:O	1:D:363:ARG:HG3	2.12	0.49
1:C:44:VAL:HG13	1:C:44:VAL:O	2.13	0.49
1:A:385:ASN:C	1:A:385:ASN:HD22	2.21	0.49
1:A:486:HIS:HD2	1:A:488:ASP:HB3	1.78	0.49
1:D:385:ASN:ND2	1:D:387:GLN:H	2.11	0.49
1:A:349:LYS:HE2	1:C:43:THR:HG21	1.94	0.49
1:B:329:VAL:O	1:B:332:ILE:HG22	2.13	0.49
1:D:407:ASN:HD21	1:D:411:ALA:HB3	1.77	0.48
1:A:237:LYS:HD2	5:A:4265:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:CYS:HA	1:B:282:GLN:O	2.13	0.48
1:D:44:VAL:HG13	1:D:49:PRO:HD2	1.96	0.48
1:D:385:ASN:HD22	1:D:387:GLN:H	1.61	0.48
1:A:299:LEU:HD12	1:A:350:MET:HG3	1.96	0.48
1:A:392:MET:HE3	1:A:394:MET:CE	2.22	0.48
1:C:98:LYS:O	1:C:101:GLU:HG2	2.13	0.48
1:A:251:ALA:O	1:C:255:GLN:HG3	2.13	0.48
1:C:238:THR:HA	1:C:277:TRP:CD1	2.48	0.48
1:C:385:ASN:H	1:C:398:GLN:NE2	2.03	0.48
1:A:361:THR:HG21	3:A:2000:HEM:HBA1	1.94	0.48
1:C:106:LYS:HE3	5:C:4304:HOH:O	2.13	0.47
1:A:389:ASP:H	1:A:397:ASN:HD21	1.61	0.47
1:C:385:ASN:C	1:C:385:ASN:HD22	2.23	0.47
1:C:79:ALA:HB2	1:C:262:ILE:HG12	1.96	0.47
1:C:233:LYS:O	1:C:281:ILE:HA	2.14	0.47
1:A:352:GLN:HE22	1:B:53:GLN:HE21	1.61	0.47
1:B:407:ASN:ND2	1:B:411:ALA:HB3	2.30	0.47
1:B:248:GLU:CD	1:B:248:GLU:H	2.22	0.47
1:C:325:TYR:HD2	5:C:4363:HOH:O	1.96	0.47
1:D:203:ARG:HE	1:D:242:ILE:HG21	1.80	0.47
1:D:380:ARG:HH11	1:D:380:ARG:CG	2.28	0.46
1:A:480:LYS:HA	5:A:4359:HOH:O	2.14	0.46
1:D:246:SER:HB2	5:D:4331:HOH:O	2.15	0.46
1:D:486:HIS:HD2	1:D:488:ASP:N	2.06	0.46
1:C:224:ASN:HD21	1:C:228:GLU:HB2	1.80	0.46
1:C:83:GLY:HA3	1:C:317:VAL:O	2.16	0.46
1:B:430:ARG:HB3	1:C:422:SER:CB	2.45	0.46
1:D:83:GLY:HA3	1:D:317:VAL:O	2.15	0.46
1:B:81:ALA:HB3	1:B:318:LEU:HD13	1.96	0.46
1:A:385:ASN:HD22	1:A:387:GLN:H	1.62	0.46
1:C:440:VAL:HG12	1:C:485:VAL:HG22	1.97	0.46
1:D:95:SER:HB2	1:D:222:LEU:HB3	1.98	0.46
1:D:403:ASN:C	1:D:403:ASN:HD22	2.22	0.46
1:A:486:HIS:CD2	1:A:488:ASP:H	2.34	0.45
1:C:388:ARG:O	1:D:67:GLU:HG2	2.16	0.45
1:C:385:ASN:ND2	1:C:387:GLN:H	2.14	0.45
1:B:429:VAL:HG12	1:B:429:VAL:O	2.16	0.45
1:C:93:LYS:HB3	5:C:4311:HOH:O	2.16	0.45
1:D:385:ASN:HD22	1:D:385:ASN:C	2.25	0.45
1:D:233:LYS:HB2	1:D:282:GLN:HB2	1.97	0.45
1:D:385:ASN:H	1:D:398:GLN:NE2	2.07	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:446:PHE:HB2	4:C:3001:NDP:O2D	2.16	0.45
1:D:394:MET:O	1:D:395:GLN:HB2	2.15	0.45
1:B:214:GLY:HA3	1:B:236:TYR:CE1	2.52	0.45
1:C:137:TYR:O	1:C:380:ARG:HD3	2.17	0.45
1:C:171:ASN:HB3	1:C:174:THR:OG1	2.17	0.45
1:C:407:ASN:HD21	1:C:411:ALA:HB3	1.82	0.44
1:A:21:ALA:O	1:A:22:GLN:CB	2.65	0.44
1:B:468:LYS:HD3	1:B:500:TYR:CD1	2.52	0.44
1:C:75:HIS:HA	1:C:115:THR:O	2.17	0.44
1:B:352:GLN:O	1:B:355:LEU:HB2	2.17	0.44
1:C:56:VAL:HG23	5:D:4091:HOH:O	2.17	0.44
1:D:398:GLN:NE2	5:D:4083:HOH:O	2.48	0.44
1:C:27:LEU:HD21	1:C:38:LYS:HD3	2.00	0.44
1:C:352:GLN:O	1:C:355:LEU:HB2	2.16	0.44
1:B:423:ILE:HG22	1:B:424:GLN:N	2.33	0.44
1:C:36:GLY:HA2	1:D:415:GLN:O	2.18	0.43
1:D:447:TYR:CZ	1:D:456:ARG:HD2	2.53	0.43
1:D:146:VAL:HG22	1:D:334:PHE:HB3	2.00	0.43
1:B:339:MET:HE1	1:B:345:ALA:HB2	1.99	0.43
1:C:203:ARG:CZ	1:C:242:ILE:HD13	2.48	0.43
1:A:352:GLN:O	1:A:355:LEU:HB2	2.18	0.43
1:B:306:LYS:HG3	5:B:4377:HOH:O	2.18	0.43
1:C:415:GLN:O	1:C:415:GLN:HG3	2.18	0.43
1:A:79:ALA:HB2	1:A:262:ILE:HG12	1.99	0.43
1:A:369:ASN:HD21	1:B:63:HIS:CE1	2.19	0.43
1:A:37:ASP:HB3	1:C:431:ARG:HD2	2.00	0.43
1:A:178:ASP:HA	1:A:179:PRO:HD2	1.93	0.43
1:B:127:ARG:O	1:B:128:ASP:HB2	2.18	0.43
1:D:389:ASP:N	1:D:397:ASN:HD21	2.14	0.43
1:D:27:LEU:HD21	1:D:38:LYS:HD3	2.00	0.43
1:A:358:TYR:HB2	1:A:359:PRO:HD3	2.00	0.42
1:C:211:HIS:HB3	1:C:243:LYS:H	1.84	0.42
1:D:329:VAL:O	1:D:332:ILE:HG22	2.19	0.42
1:C:69:ILE:HG22	1:D:391:PRO:HG3	2.01	0.42
1:A:153:PHE:HB2	1:A:299:LEU:HD13	2.02	0.42
5:A:4219:HOH:O	1:B:39:LEU:HD12	2.19	0.42
1:B:403:ASN:C	1:B:403:ASN:ND2	2.78	0.42
1:A:101:GLU:HG3	1:A:102:HIS:HD2	1.84	0.42
1:C:69:ILE:HA	5:C:4293:HOH:O	2.19	0.42
1:B:74:VAL:O	1:B:75:HIS:HB2	2.19	0.42
1:B:85:PHE:HD1	1:B:316:LEU:HD13	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:SER:O	1:A:196:VAL:HG23	2.20	0.42
1:B:5:ARG:HH22	1:D:180:ASP:CG	2.28	0.42
1:B:79:ALA:HB2	1:B:262:ILE:HG12	2.02	0.42
1:B:352:GLN:HG3	5:D:4188:HOH:O	2.19	0.42
1:A:44:VAL:O	1:A:48:GLY:HA3	2.20	0.42
1:A:251:ALA:HB2	5:A:4303:HOH:O	2.18	0.41
1:B:44:VAL:HG21	1:C:44:VAL:HG21	2.01	0.41
1:C:292:PHE:HA	1:C:293:PRO:HD3	1.86	0.41
1:C:385:ASN:HD22	1:C:387:GLN:H	1.67	0.41
1:A:407:ASN:ND2	1:A:411:ALA:HB3	2.35	0.41
1:C:365:ARG:HD2	5:C:4046:HOH:O	2.20	0.41
1:C:411:ALA:HB1	1:C:412:PRO:HD2	2.02	0.41
1:D:136:PHE:HD1	1:D:143:TRP:O	2.03	0.41
1:B:44:VAL:O	1:B:44:VAL:HG13	2.19	0.41
1:B:180:ASP:O	1:B:184:ASP:HB2	2.19	0.41
1:C:178:ASP:HA	1:C:179:PRO:HD2	1.93	0.41
1:B:51:LEU:N	1:B:51:LEU:HD12	2.35	0.41
1:C:33:ASN:HA	1:C:34:PRO:HD3	1.96	0.41
1:C:211:HIS:HD2	1:C:241:GLY:O	2.03	0.41
1:C:347:PRO:HD3	5:C:4355:HOH:O	2.20	0.41
1:B:107:THR:HA	1:B:108:PRO:HD3	1.92	0.41
1:C:358:TYR:O	1:C:361:THR:HG22	2.21	0.41
1:C:411:ALA:HB1	1:C:412:PRO:CD	2.50	0.41
1:C:437:ASP:O	1:C:438:ASP:C	2.64	0.41
1:D:358:TYR:O	1:D:361:THR:HG22	2.21	0.41
1:C:358:TYR:HB2	1:C:359:PRO:HD3	2.02	0.41
1:A:75:HIS:HA	1:A:115:THR:O	2.21	0.41
1:A:356:PHE:O	1:A:359:PRO:HD2	2.20	0.41
1:B:169:LYS:HB3	1:B:170:ARG:H	1.73	0.41
1:C:109:ILE:HA	1:C:135:LYS:O	2.21	0.41
1:C:177:LYS:HE2	5:C:4098:HOH:O	2.19	0.41
1:A:161:PHE:HB3	1:A:162:PRO:HD3	2.01	0.41
1:A:183:TRP:CD2	1:A:467:LEU:HD13	2.56	0.41
1:A:430:ARG:HB2	5:A:4164:HOH:O	2.20	0.41
1:C:214:GLY:HA3	1:C:236:TYR:CD1	2.55	0.41
1:D:203:ARG:NH2	5:D:4289:HOH:O	2.54	0.41
1:D:287:ASN:O	1:D:290:GLU:HB2	2.20	0.41
1:C:26:VAL:HG22	1:D:415:GLN:OE1	2.21	0.40
1:A:388:ARG:O	1:B:67:GLU:HG2	2.22	0.40
1:B:350:MET:O	1:B:354:ARG:HG3	2.20	0.40
1:C:355:LEU:HD23	1:D:53:GLN:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:486:HIS:HA	1:C:487:PRO:HD2	1.94	0.40
1:A:391:PRO:HG3	1:B:69:ILE:HG22	2.02	0.40
1:D:214:GLY:HA3	1:D:236:TYR:CE1	2.56	0.40
1:B:112:ARG:HD3	3:B:2001:HEM:O1D	2.21	0.40
1:C:53:GLN:HE21	1:D:352:GLN:HE22	1.68	0.40
1:D:75:HIS:CE1	1:D:116:VAL:HG22	2.57	0.40
1:A:148:ASN:CG	3:A:2000:HEM:HAC	2.47	0.40
1:A:297:PHE:CD2	1:A:347:PRO:HG2	2.57	0.40
1:B:285:THR:OG1	1:B:288:GLN:HG3	2.21	0.40
1:B:333:ALA:HB1	1:B:362:HIS:CE1	2.57	0.40
1:B:358:TYR:HB2	1:B:359:PRO:HD3	2.03	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 X-ray entries followed by that with respect to entries of similar resolution.

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	498/497 (100%)	476 (96%)	20 (4%)	2 (0%)	30	19
1	B	498/497 (100%)	476 (96%)	22 (4%)	0	100	100
1	C	498/497 (100%)	475 (95%)	19 (4%)	4 (1%)	16	6
1	D	498/497 (100%)	470 (94%)	27 (5%)	1 (0%)	43	31
All	All	1992/1988 (100%)	1897 (95%)	88 (4%)	7 (0%)	30	19

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	C	20	ALA
1	C	22	GLN
1	D	20	ALA

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Mol	Chain	Res	Type
1	A	20	ALA
1	C	21	ALA
1	C	438	ASP

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 X-ray entries followed by that with respect to entries of similar resolution.

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	430/428 (100%)	412 (96%)	18 (4%)	26	14
1	B	430/428 (100%)	416 (97%)	14 (3%)	33	21
1	C	430/428 (100%)	413 (96%)	17 (4%)	28	15
1	D	430/428 (100%)	414 (96%)	16 (4%)	30	18
All	All	1720/1712 (100%)	1655 (96%)	65 (4%)	29	17

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	22	GLN
1	A	44	VAL
1	A	74	VAL
1	A	93	LYS
1	A	145	LEU
1	A	160	LEU
1	A	226	ASN
1	A	236	TYR
1	A	243	LYS
1	A	265	LEU
1	A	299	LEU
1	A	318	LEU
1	A	355	LEU
1	A	382	ARG
1	A	385	ASN
1	A	394	MET
1	A	468	LYS

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Mol	Chain	Res	Type
1	B	5	ARG
1	B	13	GLN
1	B	19	ARG
1	B	93	LYS
1	B	138	THR
1	B	236	TYR
1	B	299	LEU
1	B	316	LEU
1	B	355	LEU
1	B	366	LEU
1	B	374	PRO
1	B	385	ASN
1	B	394	MET
1	B	403	ASN
1	C	5	ARG
1	C	13	GLN
1	C	22	GLN
1	C	41	VAL
1	C	93	LYS
1	C	138	THR
1	C	160	LEU
1	C	188	LEU
1	C	191	GLU
1	C	236	TYR
1	C	238	THR
1	C	316	LEU
1	C	318	LEU
1	C	355	LEU
1	C	385	ASN
1	C	403	ASN
1	C	468	LYS
1	D	5	ARG
1	D	13	GLN
1	D	44	VAL
1	D	58	THR
1	D	93	LYS
1	D	138	THR
1	D	160	LEU
1	D	188	LEU
1	D	236	TYR
1	D	255	GLN
1	D	374	PRO

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Mol	Chain	Res	Type
1	D	380	ARG
1	D	382	ARG
1	D	385	ASN
1	D	403	ASN
1	D	468	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	102	HIS
1	A	305	HIS
1	A	369	ASN
1	A	385	ASN
1	A	397	ASN
1	A	398	GLN
1	A	424	GLN
1	A	436	ASN
1	A	449	ASN
1	A	471	GLN
1	A	475	GLN
1	A	486	HIS
1	A	501	ASN
1	B	13	GLN
1	B	14	HIS
1	B	22	GLN
1	B	40	ASN
1	B	53	GLN
1	B	63	HIS
1	B	244	ASN
1	B	282	GLN
1	B	305	HIS
1	B	364	HIS
1	B	385	ASN
1	B	397	ASN
1	B	398	GLN
1	B	403	ASN
1	B	415	GLN
1	B	421	HIS
1	B	424	GLN
1	B	433	ASN
1	B	471	GLN

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Mol	Chain	Res	Type
1	B	475	GLN
1	B	486	HIS
1	B	501	ASN
1	C	13	GLN
1	C	14	HIS
1	C	53	GLN
1	C	63	HIS
1	C	168	GLN
1	C	211	HIS
1	C	226	ASN
1	C	305	HIS
1	C	369	ASN
1	C	385	ASN
1	C	398	GLN
1	C	403	ASN
1	C	424	GLN
1	C	436	ASN
1	C	475	GLN
1	C	486	HIS
1	C	501	ASN
1	D	18	GLN
1	D	63	HIS
1	D	168	GLN
1	D	226	ASN
1	D	255	GLN
1	D	369	ASN
1	D	385	ASN
1	D	387	GLN
1	D	397	ASN
1	D	398	GLN
1	D	403	ASN
1	D	433	ASN
1	D	471	GLN
1	D	475	GLN
1	D	486	HIS
1	D	494	GLN
1	D	501	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	B	2001	2,1	50,50,50	1.13	3 (6%)	67,82,82	0.92	2 (2%)
2	CYN	D	4003	3	1,1,1	0.31	0	-		
3	HEM	D	2003	2,1	50,50,50	1.11	2 (4%)	67,82,82	1.02	3 (4%)
4	NDP	C	3001	-	51,52,52	1.44	6 (11%)	71,80,80	1.78	13 (18%)
2	CYN	C	4002	3	1,1,1	0.22	0	-		
3	HEM	C	2002	2,1	50,50,50	1.23	2 (4%)	67,82,82	1.03	4 (5%)
4	NDP	A	3000	-	51,52,52	1.42	6 (11%)	71,80,80	1.62	8 (11%)
2	CYN	A	4000	3	1,1,1	0.20	0	-		
2	CYN	B	4001	3	1,1,1	0.22	0	-		
3	HEM	A	2000	2,1	50,50,50	1.28	3 (6%)	67,82,82	0.86	3 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	B	2001	2,1	-	5/14/54/54	-
4	NDP	C	3001	-	-	9/34/77/77	0/5/5/5
3	HEM	C	2002	2,1	-	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NDP	A	3000	-	-	6/34/77/77	0/5/5/5
3	HEM	D	2003	2,1	-	7/14/54/54	-
3	HEM	A	2000	2,1	-	8/14/54/54	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3000	NDP	C4N-C3N	-5.07	1.40	1.50
4	C	3001	NDP	C4N-C3N	-4.72	1.41	1.50
3	C	2002	HEM	FE-ND	-4.36	1.81	1.94
3	A	2000	HEM	FE-NB	-4.20	1.82	1.94
3	A	2000	HEM	FE-NC	3.76	2.07	1.95
4	A	3000	NDP	C5A-N7A	-3.53	1.32	1.39
3	A	2000	HEM	FE-ND	3.50	2.05	1.94
3	D	2003	HEM	FE-NA	3.41	2.06	1.95
3	B	2001	HEM	FE-NC	3.34	2.06	1.95
4	A	3000	NDP	C4N-C5N	-3.21	1.40	1.49
4	C	3001	NDP	C4N-C5N	-3.13	1.40	1.49
4	C	3001	NDP	C5A-N7A	-3.11	1.33	1.39
4	A	3000	NDP	C7N-C3N	2.95	1.55	1.48
4	C	3001	NDP	C7N-C3N	2.79	1.54	1.48
3	C	2002	HEM	FE-NA	2.54	2.03	1.95
4	C	3001	NDP	C6N-C5N	2.47	1.40	1.33
4	C	3001	NDP	PA-O3	2.43	1.62	1.59
3	B	2001	HEM	FE-ND	-2.32	1.87	1.94
4	A	3000	NDP	PA-O3	2.21	1.61	1.59
3	B	2001	HEM	FE-NB	2.20	2.01	1.94
4	A	3000	NDP	C6N-C5N	2.18	1.39	1.33
3	D	2003	HEM	CAC-C3C	2.01	1.52	1.47

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3001	NDP	C5A-C4A-N3A	-6.22	118.16	126.72
4	C	3001	NDP	N3A-C4A-N9A	6.07	137.49	127.17
4	A	3000	NDP	C5A-C4A-N3A	-6.01	118.44	126.72
4	A	3000	NDP	N3A-C4A-N9A	5.80	137.04	127.17
4	C	3001	NDP	N3A-C2A-N1A	-4.55	121.70	128.58
4	A	3000	NDP	C6A-C5A-C4A	4.16	122.86	117.18
4	A	3000	NDP	C6A-C5A-N7A	-3.79	124.79	132.09
4	A	3000	NDP	N3A-C2A-N1A	-3.78	122.86	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3001	NDP	C2A-N3A-C4A	3.48	120.33	111.83
4	C	3001	NDP	C6A-C5A-C4A	3.45	121.89	117.18
4	C	3001	NDP	C6A-C5A-N7A	-3.45	125.44	132.09
4	A	3000	NDP	C2A-N3A-C4A	2.93	118.99	111.83
3	D	2003	HEM	CMD-C2D-C1D	-2.87	120.54	125.03
3	C	2002	HEM	CMA-C3A-C2A	2.87	131.70	125.62
4	C	3001	NDP	C3D-C2D-C1D	2.80	106.77	101.46
4	C	3001	NDP	C2B-C1B-N9A	2.64	118.10	113.75
3	C	2002	HEM	C3B-C2B-C1B	2.59	108.36	106.41
3	D	2003	HEM	C1D-C2D-C3D	2.55	109.66	106.98
3	C	2002	HEM	CMA-C3A-C4A	-2.53	121.57	125.42
3	B	2001	HEM	C3B-C2B-C1B	2.47	108.27	106.41
3	A	2000	HEM	C3B-C2B-C1B	2.41	108.22	106.41
4	A	3000	NDP	C3D-C2D-C1D	2.39	105.99	101.46
4	C	3001	NDP	O4D-C1D-N1N	2.37	112.60	108.08
4	C	3001	NDP	O2B-P2B-O1X	-2.33	101.02	109.33
4	C	3001	NDP	C4A-N9A-C8A	2.31	108.16	105.74
4	A	3000	NDP	C2B-C1B-N9A	2.29	117.51	113.75
3	D	2003	HEM	CMA-C3A-C2A	2.29	130.47	125.62
3	C	2002	HEM	C3B-C4B-NB	2.20	111.05	109.47
4	C	3001	NDP	O4B-C1B-N9A	-2.17	103.93	108.09
3	A	2000	HEM	CMB-C2B-C1B	-2.09	121.77	125.03
3	A	2000	HEM	CHB-C1B-NB	2.07	126.93	124.37
4	C	3001	NDP	O5B-C5B-C4B	-2.07	101.93	108.99
3	B	2001	HEM	C3B-C4B-NB	2.04	110.93	109.47

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3000	NDP	C5B-O5B-PA-O1A
4	C	3001	NDP	C5D-O5D-PN-O3
4	C	3001	NDP	C5D-O5D-PN-O1N
4	A	3000	NDP	O4D-C1D-N1N-C6N
3	C	2002	HEM	C2B-C3B-CAB-CBB
4	C	3001	NDP	O4D-C1D-N1N-C6N
4	C	3001	NDP	O4B-C4B-C5B-O5B
3	A	2000	HEM	C2B-C3B-CAB-CBB
3	D	2003	HEM	C2B-C3B-CAB-CBB
4	A	3000	NDP	PA-O3-PN-O1N
4	C	3001	NDP	C5D-O5D-PN-O2N
3	A	2000	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
4	A	3000	NDP	O4B-C4B-C5B-O5B
3	D	2003	HEM	CAD-CBD-CGD-O2D
4	A	3000	NDP	C3B-C2B-O2B-P2B
4	C	3001	NDP	C3B-C2B-O2B-P2B
3	D	2003	HEM	CAD-CBD-CGD-O1D
3	A	2000	HEM	CAD-CBD-CGD-O2D
4	C	3001	NDP	PN-O3-PA-O1A
3	B	2001	HEM	CAD-CBD-CGD-O2D
3	C	2002	HEM	CAA-CBA-CGA-O1A
3	B	2001	HEM	CAD-CBD-CGD-O1D
3	C	2002	HEM	CAD-CBD-CGD-O2D
3	B	2001	HEM	C2C-C3C-CAC-CBC
3	A	2000	HEM	CAD-CBD-CGD-O1D
3	C	2002	HEM	CAD-CBD-CGD-O1D
3	A	2000	HEM	C4C-C3C-CAC-CBC
3	B	2001	HEM	C4C-C3C-CAC-CBC
3	C	2002	HEM	C4B-C3B-CAB-CBB
3	D	2003	HEM	C4B-C3B-CAB-CBB
3	D	2003	HEM	C4C-C3C-CAC-CBC
4	A	3000	NDP	PA-O3-PN-O2N
4	C	3001	NDP	PN-O3-PA-O2A
3	C	2002	HEM	CAA-CBA-CGA-O2A
3	A	2000	HEM	CAA-CBA-CGA-O1A
3	A	2000	HEM	CAA-CBA-CGA-O2A
4	C	3001	NDP	C3B-C4B-C5B-O5B
3	B	2001	HEM	CAA-CBA-CGA-O1A
3	D	2003	HEM	CAA-CBA-CGA-O1A
3	A	2000	HEM	C2C-C3C-CAC-CBC
3	D	2003	HEM	C2C-C3C-CAC-CBC

There are no ring outliers.

9 monomers are involved in 20 short contacts:

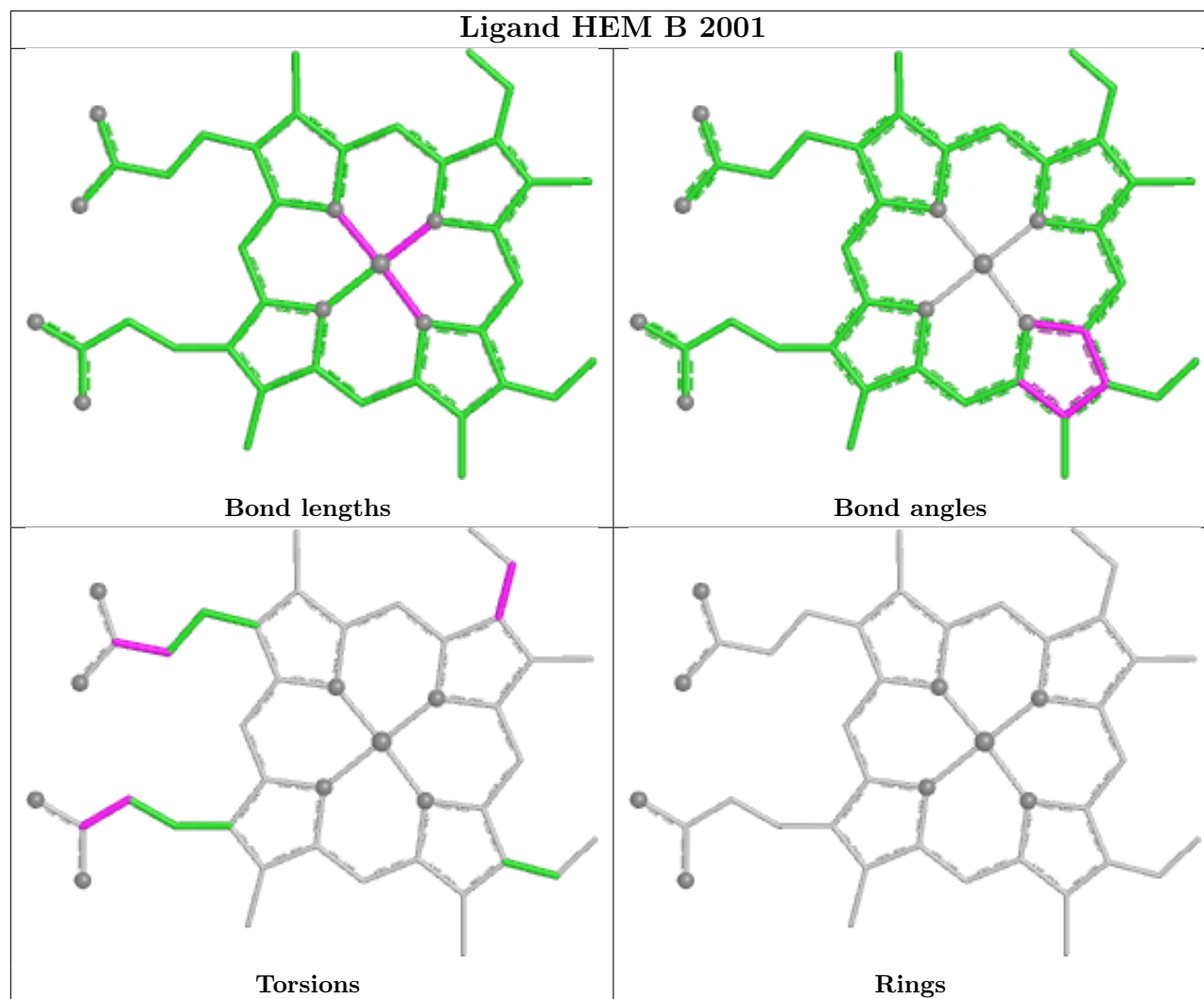
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2001	HEM	5	0
2	D	4003	CYN	4	0
3	D	2003	HEM	4	0
4	C	3001	NDP	1	0
2	C	4002	CYN	4	0
3	C	2002	HEM	4	0
2	A	4000	CYN	4	0
2	B	4001	CYN	4	0

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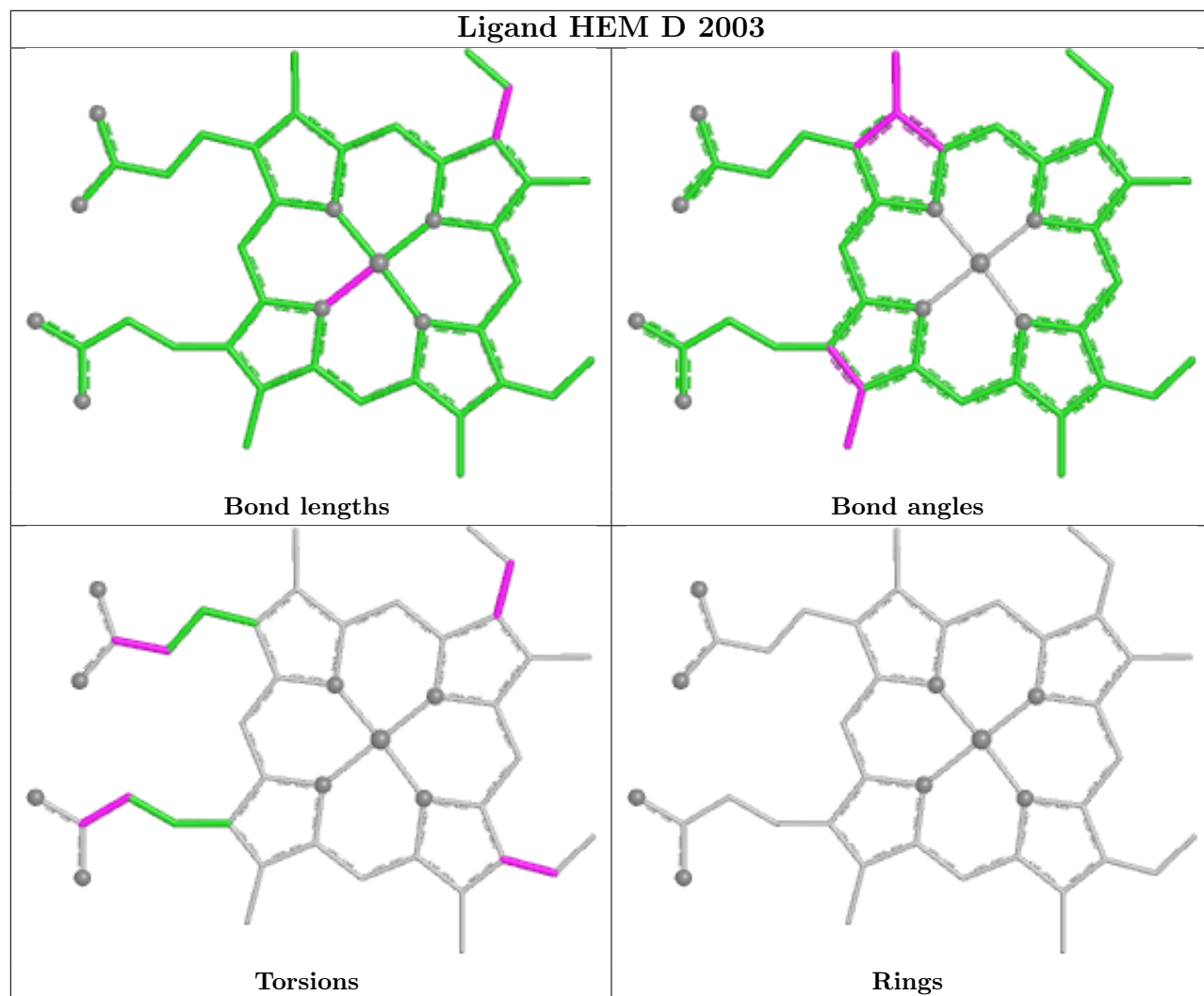
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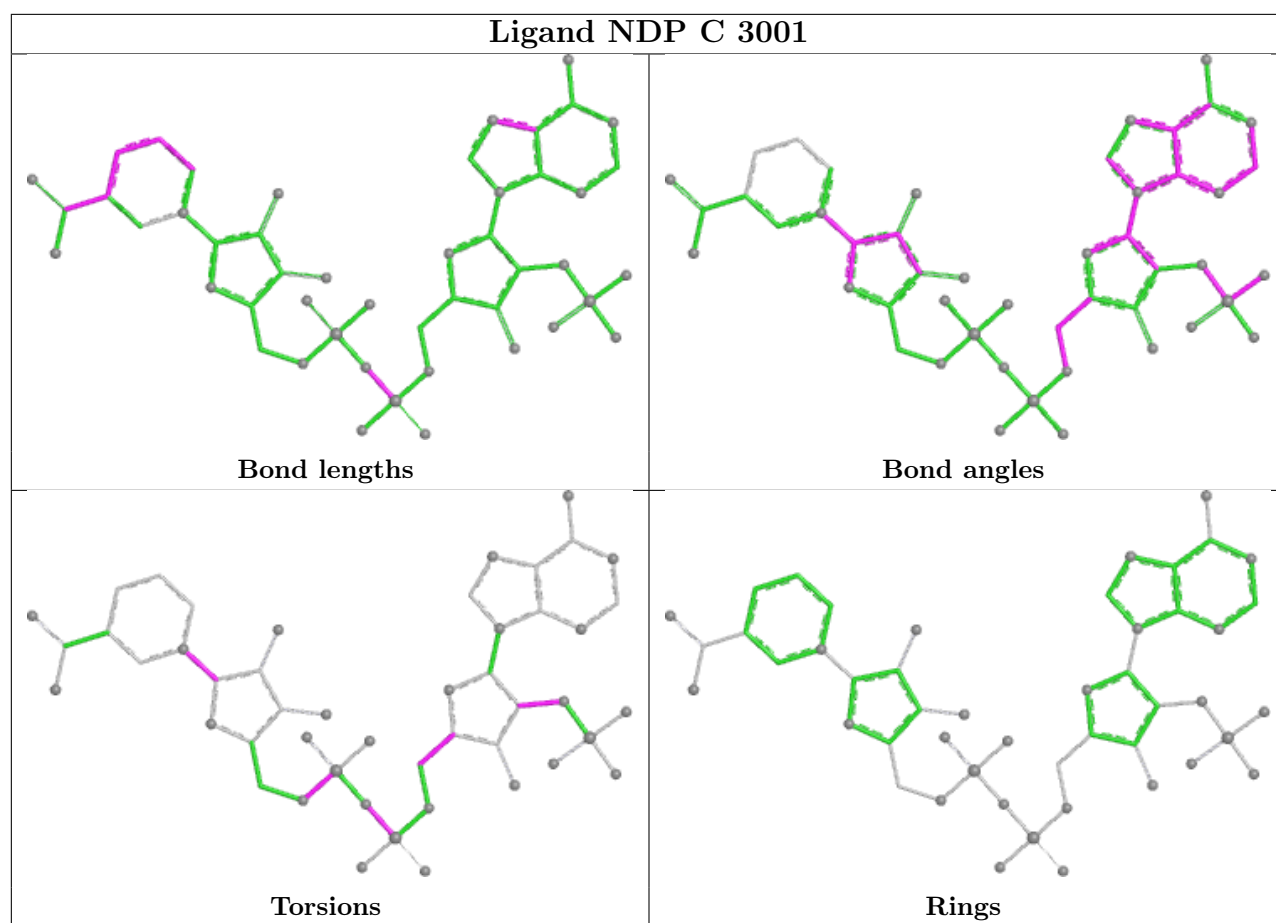
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2000	HEM	6	0

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.

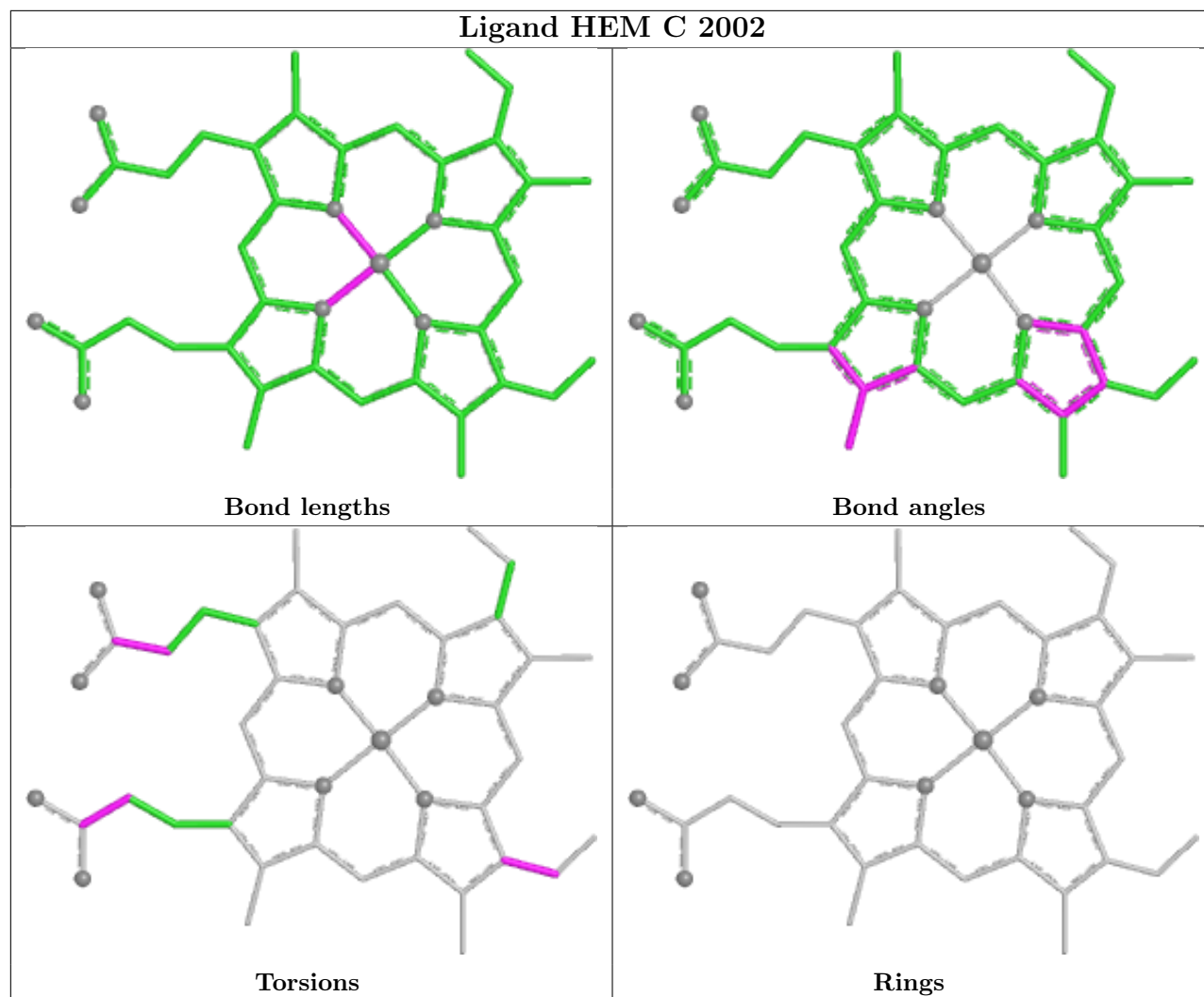


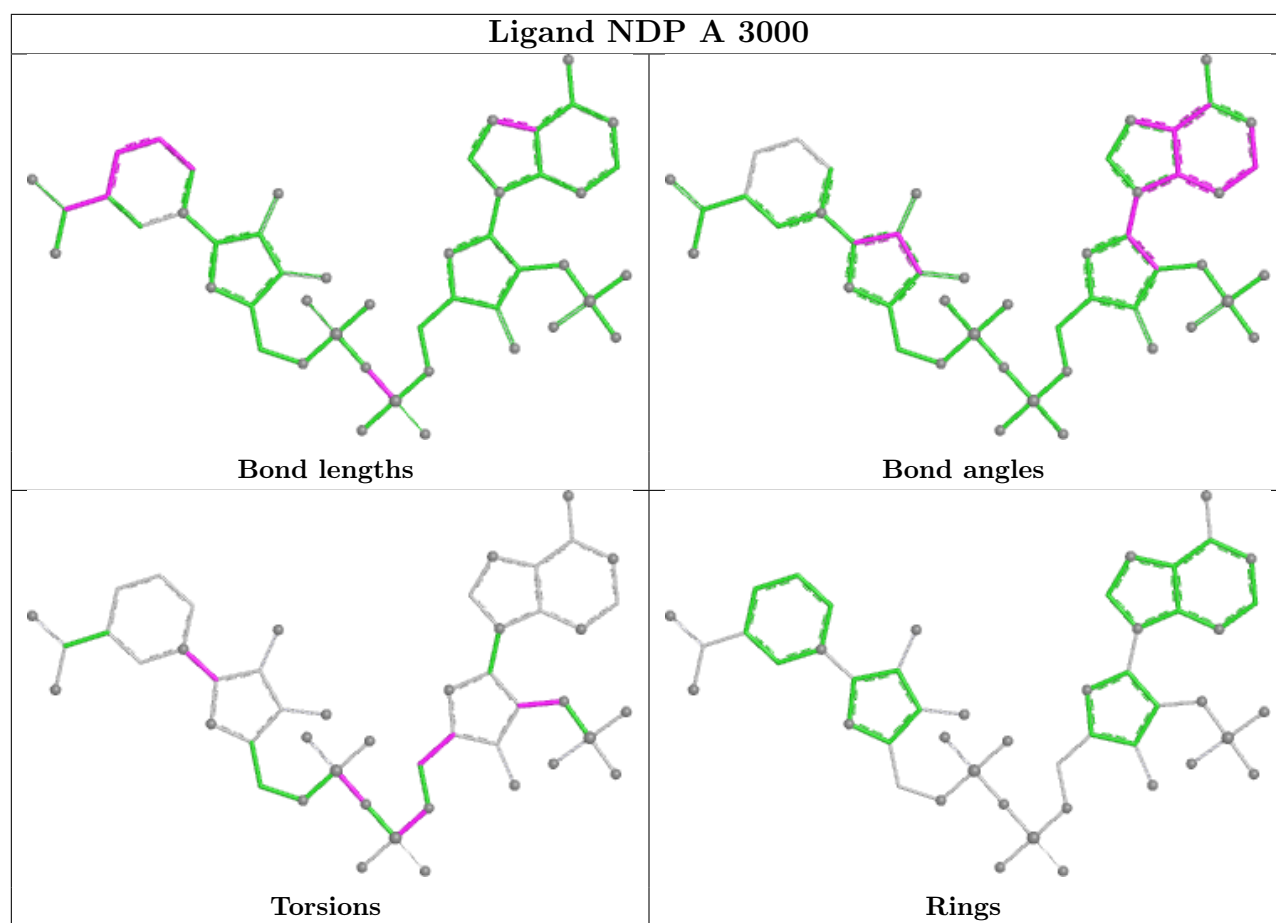
Ligand HEM D 2003

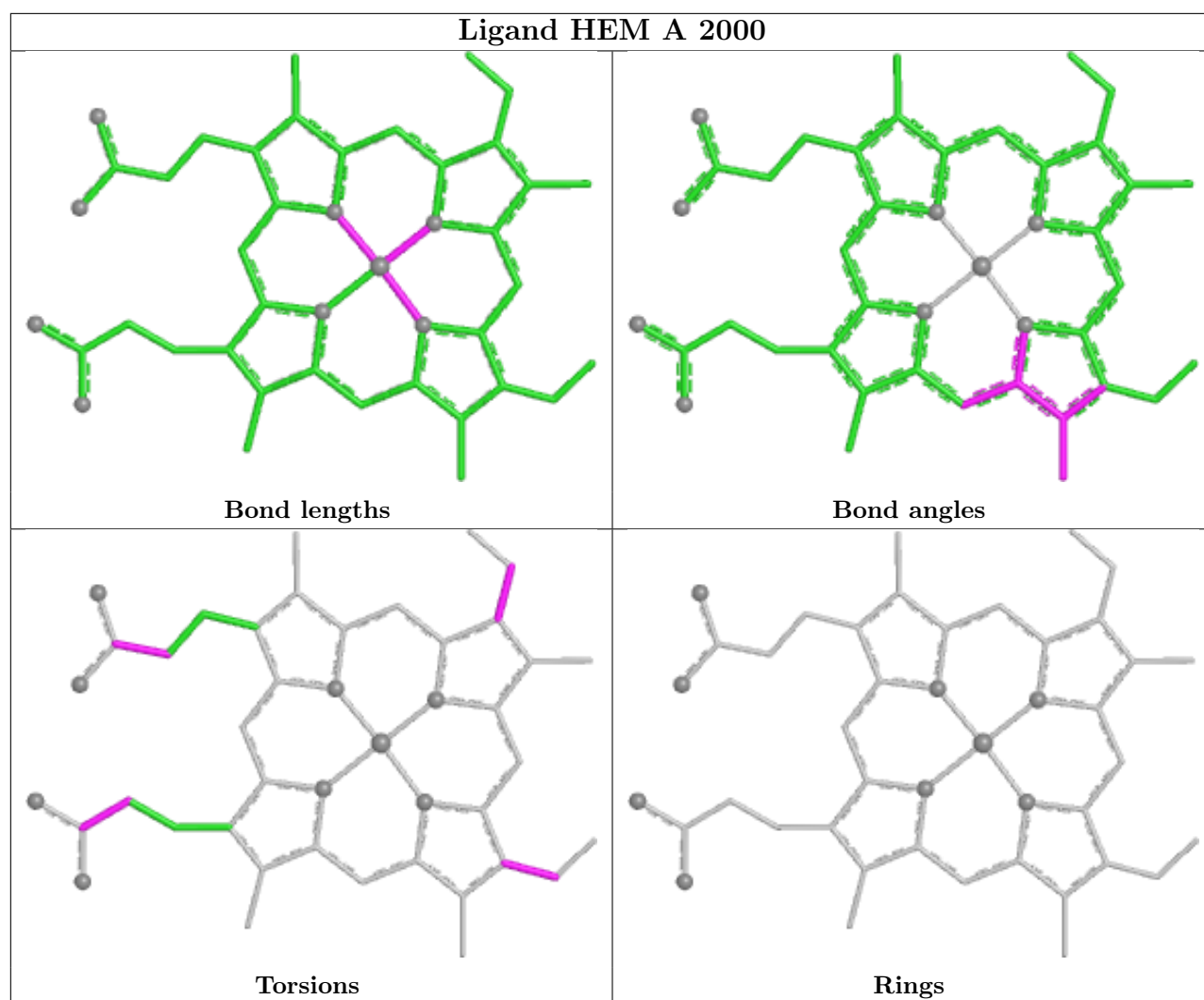




Ligand HEM C 2002







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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	497/497 (100%)	-0.39	2 (0%) 88 89	19, 42, 50, 57	3 (0%)
1	B	497/497 (100%)	-0.37	2 (0%) 88 89	19, 43, 51, 60	3 (0%)
1	C	497/497 (100%)	-0.37	3 (0%) 85 86	20, 41, 51, 56	3 (0%)
1	D	497/497 (100%)	-0.38	3 (0%) 85 86	20, 42, 49, 58	3 (0%)
All	All	1988/1988 (100%)	-0.38	10 (0%) 87 88	19, 42, 51, 60	12 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	21	ALA	4.9
1	C	20	ALA	3.4
1	D	382	ARG	3.1
1	C	394	MET	2.9
1	C	21	ALA	2.8
1	D	21	ALA	2.8
1	A	394	MET	2.6
1	D	394	MET	2.5
1	A	20	ALA	2.3
1	B	394	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

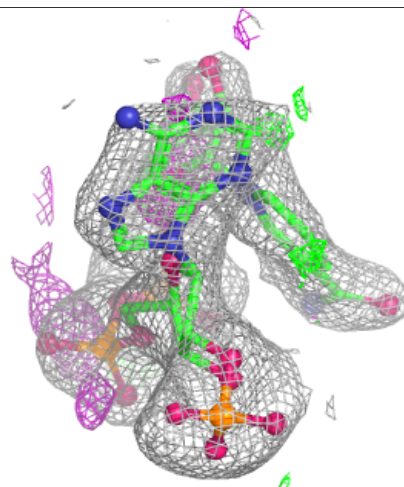
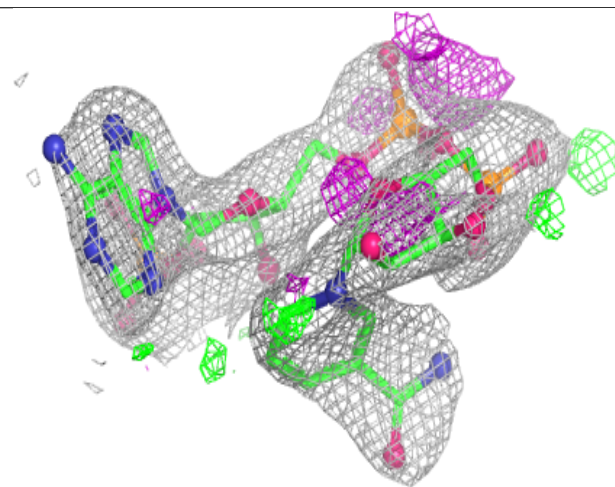
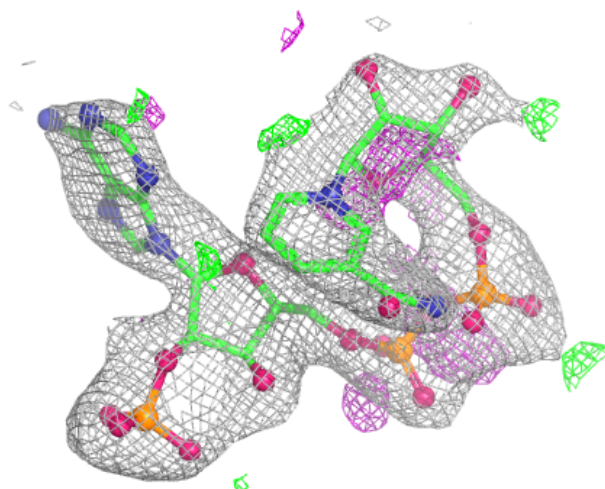
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NDP	C	3001	48/48	0.89	0.11	80,81,82,82	0
4	NDP	A	3000	48/48	0.92	0.10	62,65,66,66	0
2	CYN	D	4003	2/2	0.93	0.16	39,39,39,39	0
2	CYN	B	4001	2/2	0.95	0.17	39,39,39,40	0
2	CYN	A	4000	2/2	0.96	0.16	39,39,39,40	0
2	CYN	C	4002	2/2	0.97	0.08	39,39,39,40	0
3	HEM	D	2003	43/43	0.98	0.05	38,39,39,39	0
3	HEM	A	2000	43/43	0.99	0.05	39,39,40,40	0
3	HEM	B	2001	43/43	0.99	0.05	38,39,39,39	0
3	HEM	C	2002	43/43	0.99	0.05	38,39,39,39	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

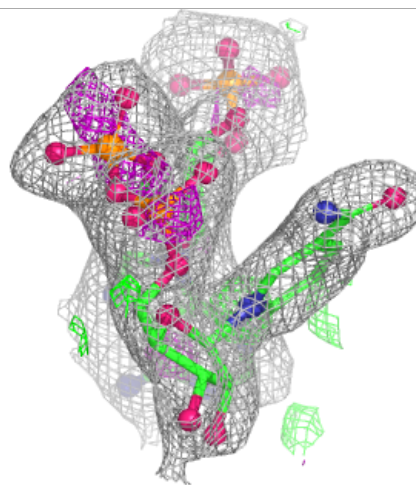
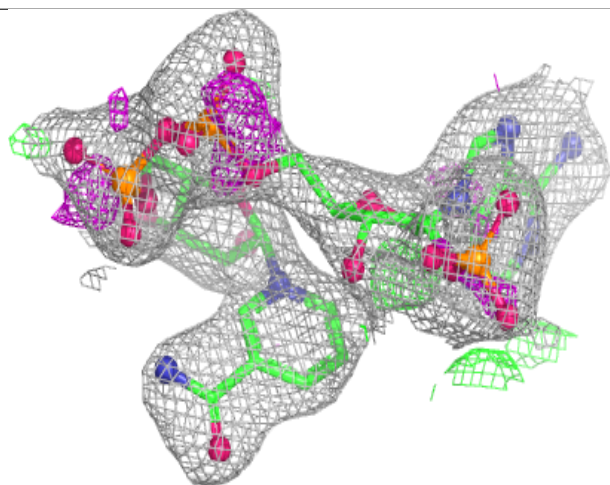
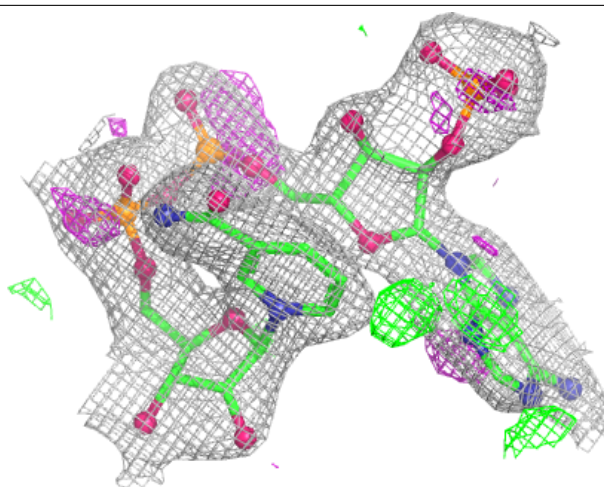
Electron density around NDP C 3001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



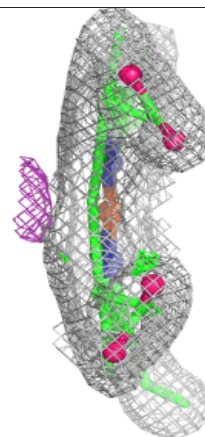
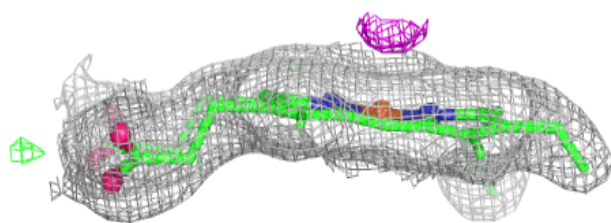
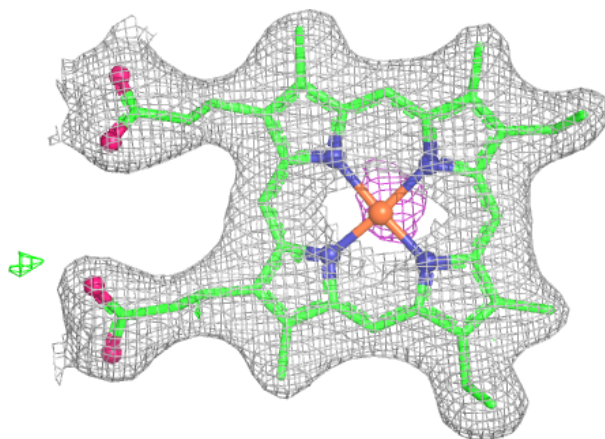
Electron density around NDP A 3000:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



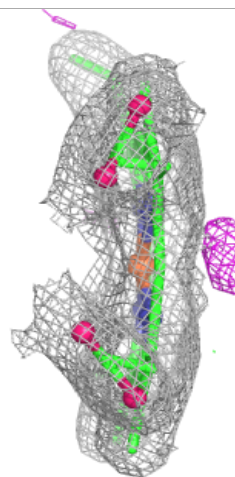
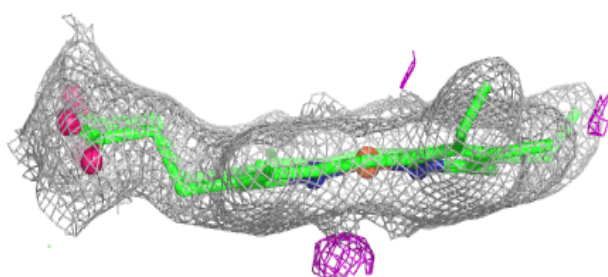
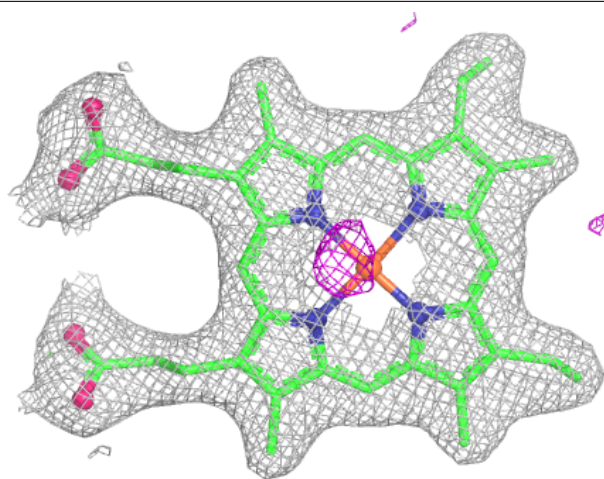
Electron density around HEM D 2003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



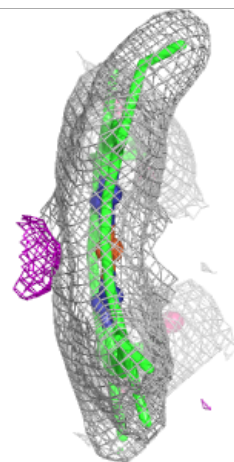
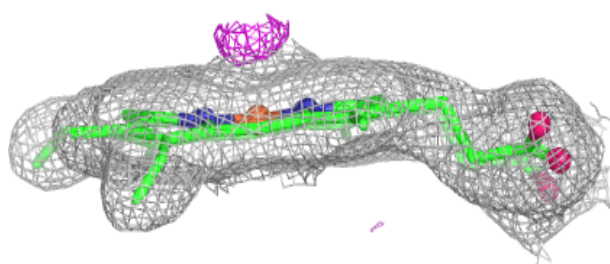
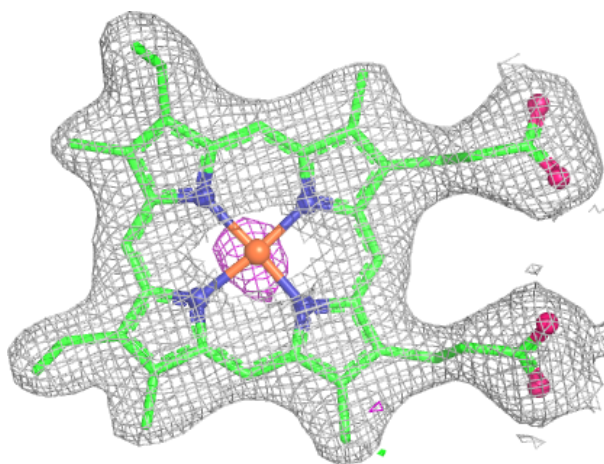
Electron density around HEM A 2000:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



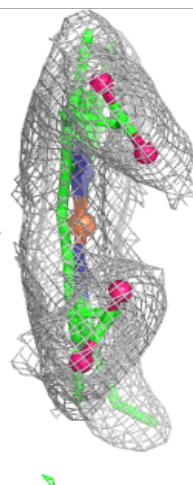
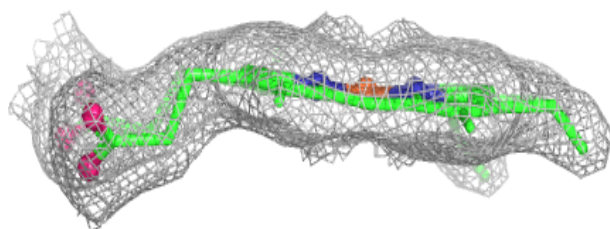
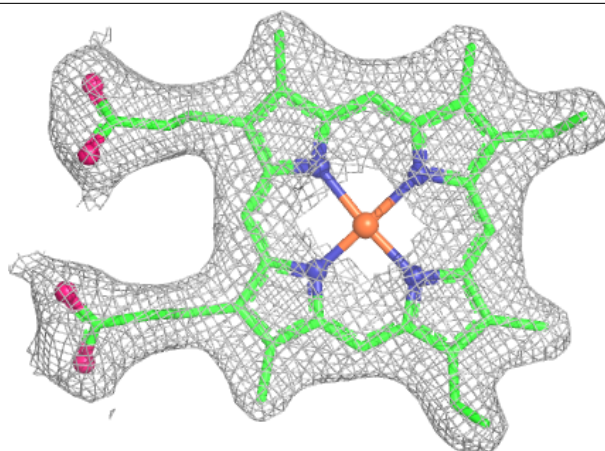
Electron density around HEM B 2001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 2002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.