



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 09:44 PM EDT

PDB ID : 1DGH / pdb_00001dgh
Title : HUMAN ERYTHROCYTE CATALASE 3-AMINO-1,2,4-TRIAZOLE COM-
PLEX
Authors : Putnam, C.D.; Arvai, A.S.; Bourne, Y.; Tainer, J.A.
Deposited on : 1999-11-24
Resolution : 2.00 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

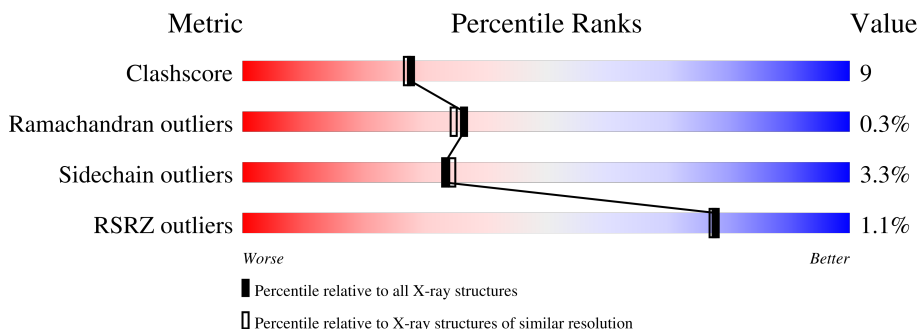
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	498	81%17%•
1	C	498	79%19%•
2	B	498	78%19%•
2	D	498	84%13%•

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17815 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 PROTEIN (CATALASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	2	0
			4012	2548	712	739	13			
1	C	498	Total	C	N	O	S	0	2	0
			4018	2551	713	741	13			

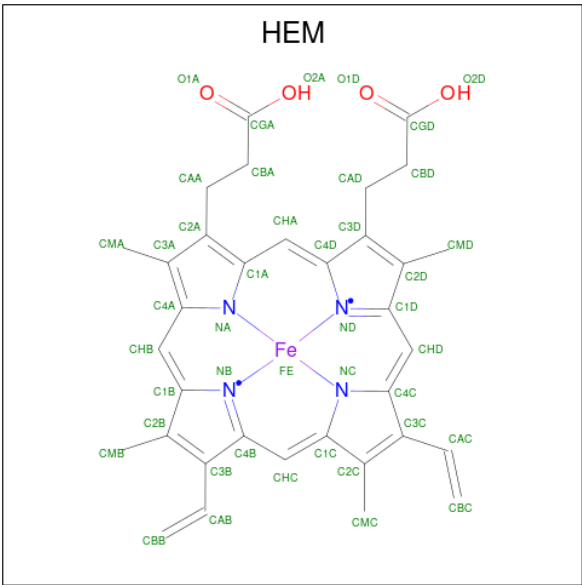
- Molecule 2 is a protein called PROTEIN (CATALASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	498	Total	C	N	O	S	0	2	0
			4024	2553	717	741	13			
2	D	498	Total	C	N	O	S	0	2	0
			4024	2553	717	741	13			

There are 2 discrepancies between the modelled and reference sequences:

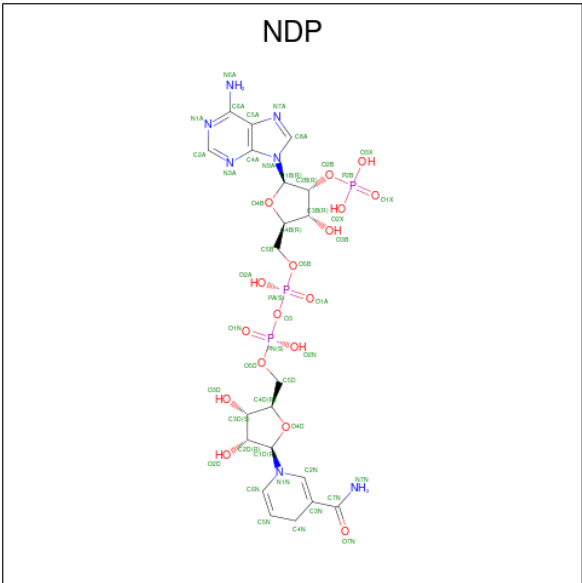
Chain	Residue	Modelled	Actual	Comment	Reference
B	75	3AH	HIS	modified residue	UNP P04040
D	75	3AH	HIS	modified residue	UNP P04040

- 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 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- 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		

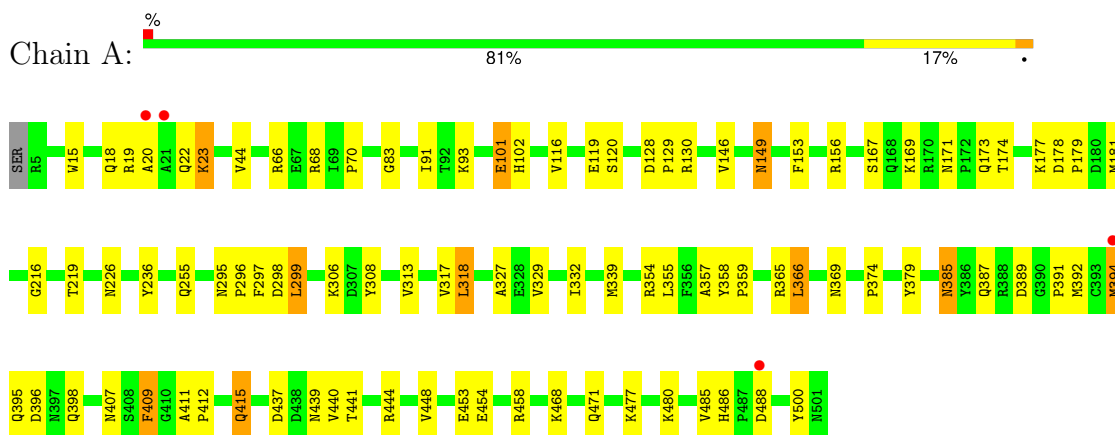
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	380	Total	O	0	0
			380	380		
5	B	357	Total	O	0	0
			357	357		
5	C	384	Total	O	0	0
			384	384		
5	D	348	Total	O	0	0
			348	348		

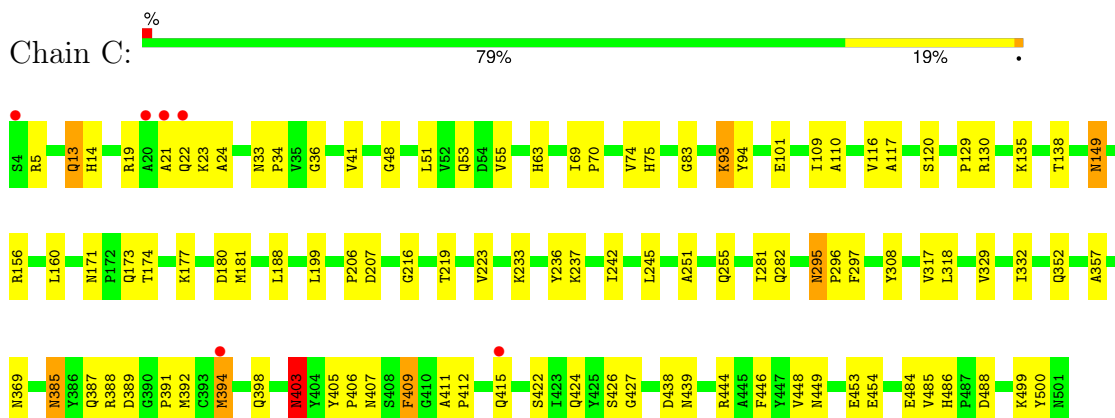
3 Residue-property plots [i](#)

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.

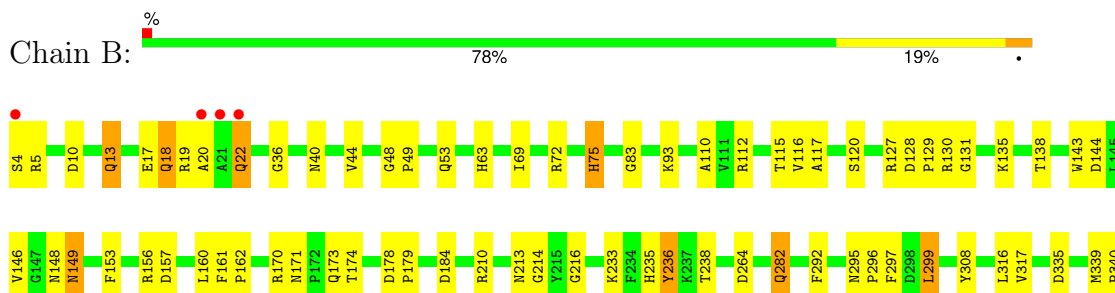
• Molecule 1: PROTEIN (CATALASE)

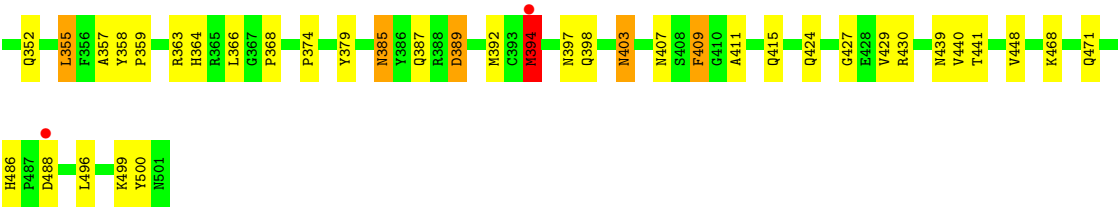


• Molecule 1: PROTEIN (CATALASE)

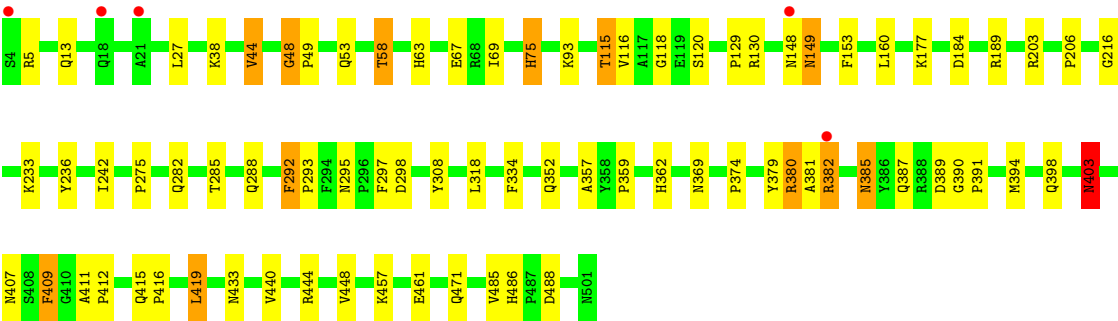
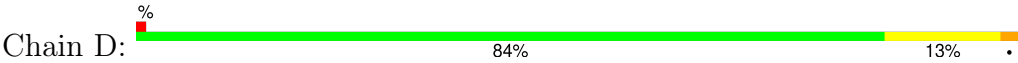


• Molecule 2: PROTEIN (CATALASE)





● Molecule 2: PROTEIN (CATALASE)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.03Å 140.64Å 231.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.00) 93.7 (20.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.74 (at 2.01Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.173 , 0.210 0.171 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	42.4	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17815	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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, 3AH, NDP

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	0.42	0/4131	0.97	21/5611 (0.4%)
1	C	0.42	0/4137	0.98	17/5619 (0.3%)
2	B	0.41	0/4125	0.97	24/5601 (0.4%)
2	D	0.42	0/4125	0.97	22/5601 (0.4%)
All	All	0.42	0/16518	0.97	84/22432 (0.4%)

There are no bond length outliers.

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	GLU	N-CA-C	8.49	121.47	111.71
2	B	357	ALA	N-CA-C	8.36	121.14	111.11
1	C	357	ALA	N-CA-C	8.23	121.29	111.33
1	C	101	GLU	N-CA-C	7.98	121.97	111.75
1	A	357	ALA	N-CA-C	7.63	120.27	111.11
2	D	448	VAL	N-CA-C	7.27	117.88	110.82
1	A	448	VAL	N-CA-C	7.25	117.85	110.82
1	C	394	MET	N-CA-C	7.16	121.67	113.15
2	D	357	ALA	N-CA-C	7.15	119.99	111.33
1	C	389	ASP	N-CA-C	6.99	118.35	108.00
2	D	48	GLY	CA-C-N	6.94	127.34	119.92
2	D	48	GLY	C-N-CA	6.94	127.34	119.92
2	B	394	MET	N-CA-C	6.84	120.22	112.97
1	C	308	TYR	CA-C-N	6.76	126.74	119.78
1	C	308	TYR	C-N-CA	6.76	126.74	119.78
2	B	117	ALA	N-CA-C	6.74	119.97	111.69
2	D	389	ASP	N-CA-C	6.73	117.97	108.00
1	A	415	GLN	CA-C-N	6.72	127.26	119.47
1	A	415	GLN	C-N-CA	6.72	127.26	119.47
1	A	216	GLY	N-CA-C	-6.61	106.47	114.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	437	ASP	N-CA-C	-6.42	102.51	110.41
2	B	216	GLY	N-CA-C	-6.42	106.70	114.66
1	C	403	ASN	N-CA-C	6.38	120.00	112.72
1	C	216	GLY	N-CA-C	-6.25	106.91	114.66
1	C	449	ASN	N-CA-C	6.21	121.08	112.45
1	A	379	TYR	N-CA-C	6.19	120.30	112.87
2	B	128	ASP	CA-C-N	-6.19	114.26	120.21
2	B	128	ASP	C-N-CA	-6.19	114.26	120.21
2	D	390	GLY	CA-C-N	5.98	126.00	119.90
2	D	390	GLY	C-N-CA	5.98	126.00	119.90
2	D	292	PHE	CA-C-N	5.96	126.39	119.47
2	D	292	PHE	C-N-CA	5.96	126.39	119.47
2	B	441	THR	N-CA-C	5.92	118.25	111.02
2	B	409	PHE	N-CA-C	5.86	120.03	112.41
2	B	448	VAL	N-CA-C	5.80	116.44	110.82
2	D	189	ARG	CA-C-N	5.77	125.48	119.82
2	D	189	ARG	C-N-CA	5.77	125.48	119.82
1	C	117	ALA	N-CA-C	5.74	117.62	111.36
2	B	146	VAL	N-CA-C	5.70	112.31	106.21
1	A	68	ARG	N-CA-C	5.69	119.19	110.20
1	A	308	TYR	CA-C-N	5.67	125.62	119.78
1	A	308	TYR	C-N-CA	5.67	125.62	119.78
2	B	184	ASP	N-CA-C	-5.62	105.24	111.36
2	D	216	GLY	N-CA-C	-5.60	107.72	114.66
2	B	292	PHE	CA-C-N	5.55	125.22	119.56
2	B	292	PHE	C-N-CA	5.55	125.22	119.56
1	C	48	GLY	CA-C-N	5.55	125.52	120.03
1	C	48	GLY	C-N-CA	5.55	125.52	120.03
1	C	282	GLN	N-CA-C	-5.52	100.70	109.59
2	D	403	ASN	N-CA-C	5.49	118.98	112.72
1	A	441	THR	N-CA-C	5.48	117.71	111.02
2	D	440	VAL	N-CA-C	5.48	120.73	109.34
1	A	440	VAL	N-CA-C	5.47	120.73	109.34
2	D	308	TYR	CA-C-N	5.42	125.36	119.78
2	D	308	TYR	C-N-CA	5.42	125.36	119.78
2	D	115	THR	N-CA-C	-5.42	101.43	109.94
2	B	157	ASP	CA-C-N	5.38	125.20	119.28
2	B	157	ASP	C-N-CA	5.38	125.20	119.28
1	A	128	ASP	CA-C-N	-5.36	115.06	120.21
1	A	128	ASP	C-N-CA	-5.36	115.06	120.21
2	D	118	GLY	N-CA-C	5.33	118.06	111.93
1	A	389	ASP	N-CA-C	5.30	117.92	109.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	409	PHE	N-CA-C	5.27	119.02	112.59
2	B	389	ASP	N-CA-C	5.27	117.87	109.02
2	D	409	PHE	N-CA-C	5.25	119.24	112.41
1	C	219	THR	N-CA-C	-5.25	100.74	109.46
1	A	453	GLU	N-CA-C	5.24	117.00	111.28
2	D	177	LYS	N-CA-C	-5.23	102.54	110.28
1	A	327	ALA	N-CA-C	5.22	117.05	111.36
1	A	177	LYS	N-CA-C	-5.21	102.68	110.23
2	D	184	ASP	N-CA-C	-5.19	105.70	111.36
1	C	448	VAL	N-CA-C	5.16	115.82	110.82
2	B	170	ARG	N-CA-C	5.14	118.50	110.32
2	B	282	GLN	N-CA-C	-5.13	101.34	109.59
2	B	415	GLN	CA-C-N	5.12	126.25	119.84
2	B	415	GLN	C-N-CA	5.12	126.25	119.84
2	B	308	TYR	CA-C-N	5.09	125.03	119.78
2	B	308	TYR	C-N-CA	5.09	125.03	119.78
2	B	379	TYR	N-CA-C	5.06	118.94	112.87
2	D	379	TYR	N-CA-C	5.06	118.94	112.87
1	C	180	ASP	N-CA-C	-5.05	105.85	111.36
1	A	219	THR	N-CA-C	-5.05	101.08	109.46
2	B	440	VAL	N-CA-C	5.04	119.81	109.34
1	A	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	4012	0	3840	72	0
1	C	4018	0	3845	93	0
2	B	4024	0	3846	93	0
2	D	4024	0	3846	80	0
3	A	43	0	30	0	0
3	B	43	0	30	1	0
3	C	43	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	43	0	30	0	0
4	A	48	0	26	0	0
4	C	48	0	26	1	0
5	A	380	0	0	6	0
5	B	357	0	0	6	0
5	C	384	0	0	11	0
5	D	348	0	0	9	0
All	All	17815	0	15549	288	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 (288) 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)
2:D:382:ARG:H	2:D:382:ARG:HD3	1.07	1.14
2:B:13:GLN:HG2	2:D:471:GLN:HE22	1.36	0.90
2:B:156:ARG:HH12	2:B:439:ASN:HD21	1.18	0.90
1:C:392:MET:HE3	1:C:394:MET:HE1	1.52	0.89
1:A:156:ARG:HH22	1:A:439:ASN:HD21	1.21	0.88
1:A:407:ASN:HD22	1:A:409:PHE:H	1.20	0.88
2:B:385:ASN:H	2:B:398:GLN:HE22	1.23	0.87
2:B:424:GLN:HE21	1:C:427:GLY:H	1.21	0.87
2:B:120[B]:SER:O	2:D:120[B]:SER:O	1.93	0.86
2:B:471:GLN:HE22	2:D:13:GLN:HE21	1.19	0.86
1:C:156:ARG:HH12	1:C:439:ASN:HD21	1.21	0.84
2:D:382:ARG:HD3	2:D:382:ARG:N	1.91	0.84
2:D:486:HIS:HD2	2:D:488:ASP:H	1.24	0.84
1:C:385:ASN:H	1:C:398:GLN:HE22	1.23	0.84
1:C:63:HIS:HE1	2:D:369:ASN:HD21	1.27	0.83
1:A:156:ARG:HH12	1:A:439:ASN:HD22	1.22	0.83
1:A:392:MET:HE3	1:A:394:MET:HE1	1.60	0.83
1:C:34:PRO:HG3	2:D:382:ARG:HH22	1.45	0.82
1:A:385:ASN:H	1:A:398:GLN:HE22	1.23	0.81
2:D:116:VAL:HG21	2:D:129:PRO:HG2	1.62	0.80
1:C:352:GLN:HE22	2:D:53:GLN:HE21	1.30	0.79
2:D:385:ASN:H	2:D:398:GLN:HE22	1.30	0.79
2:D:382:ARG:H	2:D:382:ARG:CD	1.94	0.79
1:A:369:ASN:HD21	2:B:63:HIS:HE1	1.30	0.78
1:C:369:ASN:HD21	2:D:63:HIS:HE1	1.29	0.78
1:A:156:ARG:HH12	1:A:439:ASN:ND2	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:VAL:HG21	2:B:129:PRO:HG2	1.66	0.77
2:B:424:GLN:NE2	1:C:427:GLY:H	1.83	0.77
1:A:454:GLU:HB3	1:A:458:ARG:HH21	1.48	0.77
2:D:407:ASN:HD22	2:D:409:PHE:H	1.30	0.77
1:C:394:MET:HG2	2:D:394:MET:HG3	1.66	0.76
1:C:369:ASN:ND2	2:D:63:HIS:HE1	1.83	0.76
2:B:49:PRO:HB2	1:C:51:LEU:HD23	1.66	0.76
1:C:156:ARG:HH22	1:C:439:ASN:HD22	1.33	0.74
2:B:13:GLN:HG2	2:D:471:GLN:NE2	2.01	0.74
1:A:395:GLN:HG3	1:A:396:ASP:H	1.50	0.74
5:C:3380:HOH:O	2:D:382:ARG:HG2	1.87	0.74
1:A:22:GLN:O	1:A:23:LYS:HB3	1.87	0.73
2:B:75:3AH:N2	2:B:148:ASN:HB3	2.04	0.72
1:A:171:ASN:ND2	1:A:173:GLN:H	1.87	0.72
1:A:130:ARG:H	1:A:149:ASN:ND2	1.88	0.71
1:A:116:VAL:HG21	1:A:129:PRO:HG2	1.72	0.71
2:D:58:THR:HG21	5:D:2075:HOH:O	1.90	0.71
1:C:63:HIS:HE1	2:D:369:ASN:ND2	1.88	0.70
1:C:171:ASN:ND2	1:C:173:GLN:H	1.89	0.70
1:C:407:ASN:HD22	1:C:409:PHE:H	1.40	0.70
1:C:486:HIS:HD2	1:C:488:ASP:H	1.37	0.70
2:B:156:ARG:HH22	2:B:439:ASN:HD22	1.38	0.70
2:B:171:ASN:ND2	2:B:173:GLN:H	1.89	0.70
1:C:116:VAL:HG21	1:C:129:PRO:HG2	1.74	0.69
2:B:471:GLN:HE22	2:D:13:GLN:NE2	1.91	0.68
1:A:486:HIS:HD2	1:A:488:ASP:HB3	1.60	0.67
2:B:392:MET:HE3	2:B:394:MET:HE1	1.77	0.66
1:C:149:ASN:H	1:C:149:ASN:HD22	1.43	0.66
1:C:171:ASN:HD22	1:C:174:THR:H	1.41	0.66
1:A:15:TRP:O	1:A:18:GLN:HG2	1.95	0.65
1:A:120[B]:SER:O	1:C:120[B]:SER:O	2.13	0.65
2:B:427:GLY:H	1:C:424:GLN:HE21	1.42	0.65
1:C:295:ASN:ND2	1:C:297:PHE:H	1.94	0.65
1:C:34:PRO:HG3	2:D:382:ARG:NH2	2.12	0.65
1:A:369:ASN:ND2	2:B:63:HIS:HE1	1.94	0.65
2:D:486:HIS:CD2	2:D:488:ASP:H	2.13	0.65
2:B:427:GLY:H	1:C:424:GLN:NE2	1.93	0.65
1:C:63:HIS:HD2	5:C:3032:HOH:O	1.80	0.65
2:D:444:ARG:HD3	2:D:485:VAL:O	1.96	0.65
1:C:53:GLN:HE21	2:D:352:GLN:HE22	1.44	0.64
1:A:149:ASN:H	1:A:149:ASN:HD22	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:ASN:HD22	2:B:149:ASN:H	1.44	0.64
2:D:381:ALA:HB1	2:D:382:ARG:HH11	1.63	0.64
2:D:457:LYS:O	2:D:461:GLU:HG2	1.96	0.63
2:B:424:GLN:HE21	1:C:427:GLY:N	1.95	0.63
1:C:156:ARG:HH22	1:C:439:ASN:ND2	1.97	0.62
1:A:486:HIS:CD2	1:A:488:ASP:HB3	2.34	0.62
2:D:130:ARG:H	2:D:149:ASN:ND2	1.96	0.62
2:B:153:PHE:HB3	2:B:299:LEU:HD13	1.80	0.62
1:C:369:ASN:HD21	2:D:63:HIS:CE1	2.15	0.62
2:D:380:ARG:HB3	2:D:380:ARG:HH11	1.65	0.62
2:D:486:HIS:CD2	2:D:488:ASP:HB3	2.35	0.61
1:A:394:MET:SD	2:B:394:MET:HE2	2.39	0.61
1:A:471:GLN:NE2	1:C:13:GLN:HG2	2.16	0.61
1:A:171:ASN:HD22	1:A:173:GLN:H	1.49	0.60
2:B:171:ASN:HD22	2:B:174:THR:H	1.47	0.60
1:C:392:MET:HB3	1:C:394:MET:HE1	1.82	0.60
2:B:407:ASN:HD22	2:B:409:PHE:H	1.50	0.60
1:C:352:GLN:NE2	2:D:53:GLN:HE21	1.99	0.60
2:D:75:3AH:HN32	2:D:153:PHE:HE2	1.50	0.60
1:A:471:GLN:HE22	1:C:13:GLN:HG2	1.66	0.59
2:B:171:ASN:HD22	2:B:173:GLN:H	1.49	0.59
2:B:156:ARG:HH22	2:B:439:ASN:ND2	2.00	0.59
1:A:480:LYS:HA	5:A:3350:HOH:O	2.03	0.58
1:C:486:HIS:CD2	1:C:488:ASP:H	2.20	0.58
2:D:380:ARG:HH11	2:D:380:ARG:CB	2.17	0.58
2:B:17:GLU:C	2:B:19:ARG:H	2.10	0.58
1:C:130:ARG:H	1:C:149:ASN:ND2	2.03	0.57
1:C:149:ASN:HD22	1:C:149:ASN:N	2.02	0.57
2:D:75:3AH:N2	2:D:148:ASN:HB3	2.20	0.57
2:B:149:ASN:HD22	2:B:149:ASN:N	2.01	0.57
2:B:130:ARG:H	2:B:149:ASN:ND2	2.03	0.57
1:C:329:VAL:O	1:C:332:ILE:HG22	2.05	0.57
2:B:295:ASN:HD22	2:B:296:PRO:HD2	1.69	0.56
2:D:75:3AH:HN31	2:D:148:ASN:ND2	2.03	0.56
2:B:153:PHE:CB	2:B:299:LEU:HD13	2.35	0.56
1:A:169:LYS:HB3	5:A:3146:HOH:O	2.06	0.56
2:B:63:HIS:HD2	5:B:2013:HOH:O	1.88	0.56
2:B:496:LEU:O	2:B:499:LYS:HG2	2.06	0.56
1:C:392:MET:HE3	1:C:394:MET:CE	2.31	0.55
1:C:171:ASN:ND2	1:C:174:THR:H	2.03	0.55
1:C:237:LYS:HE2	5:C:3322:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:ASN:HD22	1:C:173:GLN:H	1.55	0.55
2:B:486:HIS:HD2	2:B:488:ASP:H	1.54	0.55
2:B:156:ARG:HH12	2:B:439:ASN:ND2	1.99	0.54
1:C:63:HIS:CE1	2:D:369:ASN:HD21	2.16	0.54
2:B:389:ASP:H	2:B:397:ASN:HD21	1.54	0.54
1:A:156:ARG:NH2	1:A:439:ASN:HD21	1.99	0.53
2:B:385:ASN:C	2:B:385:ASN:HD22	2.17	0.53
1:C:83:GLY:HA3	1:C:317:VAL:O	2.08	0.53
2:D:149:ASN:HD22	2:D:149:ASN:H	1.56	0.53
2:B:53:GLN:HB2	5:C:3018:HOH:O	2.07	0.53
2:D:44:VAL:CG1	2:D:49:PRO:HD2	2.38	0.53
1:C:295:ASN:C	1:C:295:ASN:HD22	2.17	0.52
2:D:295:ASN:ND2	2:D:297:PHE:H	2.07	0.52
2:D:385:ASN:HD22	2:D:385:ASN:C	2.18	0.52
2:B:385:ASN:ND2	2:B:387:GLN:H	2.08	0.51
2:D:380:ARG:HH11	2:D:380:ARG:CG	2.23	0.51
1:A:339:MET:HE2	5:A:3330:HOH:O	2.09	0.51
2:B:127:ARG:NH1	5:B:2274:HOH:O	2.38	0.51
1:A:295:ASN:HD22	1:A:296:PRO:HD2	1.75	0.51
2:D:295:ASN:HB3	2:D:298:ASP:HB2	1.92	0.51
1:C:385:ASN:C	1:C:385:ASN:HD22	2.19	0.51
2:B:352:GLN:HA	2:B:355:LEU:HD22	1.93	0.50
2:D:63:HIS:HD2	5:D:2038:HOH:O	1.92	0.50
1:A:394:MET:HE2	2:B:394:MET:HB2	1.93	0.50
2:B:19:ARG:HB2	2:B:22:GLN:NE2	2.26	0.50
2:D:385:ASN:ND2	2:D:387:GLN:H	2.09	0.50
2:D:44:VAL:O	2:D:48:GLY:HA3	2.10	0.50
2:D:416:PRO:O	2:D:419:LEU:HB2	2.11	0.50
2:B:161:PHE:HB3	2:B:162:PRO:HD3	1.93	0.50
1:C:484:GLU:HG3	5:C:3349:HOH:O	2.12	0.50
2:D:419:LEU:HD12	5:D:2224:HOH:O	2.11	0.50
2:D:486:HIS:HD2	2:D:488:ASP:N	2.01	0.50
2:B:156:ARG:NH1	2:B:439:ASN:HD21	1.99	0.50
2:D:203:ARG:NH1	2:D:242:ILE:HD13	2.27	0.49
2:D:381:ALA:HB1	2:D:382:ARG:NH1	2.27	0.49
2:B:171:ASN:ND2	2:B:174:THR:H	2.09	0.49
1:C:454:GLU:CD	1:C:454:GLU:H	2.19	0.49
1:A:171:ASN:HD22	1:A:174:THR:H	1.60	0.49
2:B:44:VAL:O	2:B:48:GLY:HA3	2.12	0.49
2:D:285:THR:OG1	2:D:288:GLN:HG3	2.12	0.49
2:D:44:VAL:HG13	2:D:49:PRO:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ASN:ND2	1:A:387:GLN:H	2.11	0.49
1:C:21:ALA:O	1:C:23:LYS:N	2.42	0.49
2:B:210:ARG:HD3	2:B:264:ASP:OD2	2.12	0.49
2:D:130:ARG:O	2:D:148:ASN:HB2	2.13	0.49
2:B:364:HIS:HD2	5:C:3095:HOH:O	1.95	0.48
1:C:55:VAL:HG22	5:D:2088:HOH:O	2.12	0.48
2:D:149:ASN:HD22	2:D:149:ASN:N	2.09	0.48
2:D:75:3AH:HA	2:D:115:THR:O	2.12	0.48
2:D:352:GLN:HG3	5:D:2021:HOH:O	2.12	0.48
2:B:430:ARG:HB3	1:C:422:SER:HB3	1.95	0.48
2:D:116:VAL:CG2	2:D:129:PRO:HG2	2.40	0.48
1:C:177:LYS:HE2	5:C:3097:HOH:O	2.13	0.48
1:C:110:ALA:HB3	1:C:135:LYS:HB3	1.96	0.48
2:B:18:GLN:NE2	5:B:2021:HOH:O	2.44	0.48
2:B:83:GLY:HA3	2:B:317:VAL:O	2.13	0.48
2:B:392:MET:CE	2:B:394:MET:HE1	2.43	0.48
1:A:477:LYS:HZ3	1:A:480:LYS:HE3	1.79	0.47
1:A:295:ASN:ND2	1:A:297:PHE:H	2.12	0.47
1:A:385:ASN:C	1:A:385:ASN:HD22	2.22	0.47
1:C:36:GLY:HA2	2:D:415:GLN:O	2.14	0.47
1:A:415:GLN:O	2:B:36:GLY:HA2	2.14	0.47
2:B:75:3AH:HA	2:B:115:THR:O	2.14	0.47
1:C:14:HIS:HD2	5:C:3298:HOH:O	1.96	0.47
2:D:233:LYS:HB2	2:D:282:GLN:HB2	1.96	0.47
2:B:468:LYS:HD3	2:B:500:TYR:CD1	2.50	0.47
2:B:72:ARG:HG3	2:B:72:ARG:HH11	1.80	0.47
2:B:403:ASN:HD21	1:C:181:MET:HE3	1.80	0.47
1:C:156:ARG:HH12	1:C:439:ASN:ND2	2.01	0.47
1:A:407:ASN:HD21	1:A:411:ALA:H	1.62	0.47
1:A:329:VAL:O	1:A:332:ILE:HG22	2.16	0.46
1:A:411:ALA:HB1	1:A:412:PRO:HD2	1.97	0.46
1:C:223:VAL:HG11	5:C:3374:HOH:O	2.14	0.46
1:A:119:GLU:HB2	1:C:120[B]:SER:O	2.15	0.46
1:C:403:ASN:C	1:C:403:ASN:HD22	2.22	0.46
1:C:295:ASN:HD22	1:C:296:PRO:N	2.14	0.46
1:C:411:ALA:HB1	1:C:412:PRO:HD2	1.98	0.46
2:B:295:ASN:ND2	2:B:297:PHE:H	2.14	0.46
1:A:91:ILE:HG21	1:A:313:VAL:HG22	1.96	0.46
1:A:394:MET:HG2	2:B:394:MET:HG2	1.97	0.46
2:B:295:ASN:HD22	2:B:296:PRO:CD	2.28	0.46
2:B:352:GLN:O	2:B:355:LEU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:407:ASN:HD21	2:B:411:ALA:H	1.64	0.46
1:A:394:MET:HE2	2:B:394:MET:SD	2.57	0.45
1:A:19:ARG:HD2	5:A:3355:HOH:O	2.14	0.45
2:B:143:TRP:HB2	2:B:340:PRO:HD3	1.97	0.45
1:C:388:ARG:O	2:D:67:GLU:HG2	2.17	0.45
1:A:295:ASN:HB3	1:A:298:ASP:HB2	1.98	0.45
1:A:385:ASN:HD22	1:A:387:GLN:H	1.64	0.45
2:D:275:PRO:HG2	2:D:318:LEU:HB2	1.99	0.45
1:A:407:ASN:HD22	1:A:409:PHE:N	2.02	0.45
1:C:19:ARG:NH2	1:C:24:ALA:HA	2.31	0.45
2:B:4:SER:HB2	2:B:10:ASP:OD2	2.16	0.45
1:A:468:LYS:HD3	1:A:500:TYR:HB3	1.99	0.45
1:C:109:ILE:HA	1:C:135:LYS:O	2.17	0.44
1:A:444:ARG:HD3	1:A:485:VAL:O	2.17	0.44
2:B:149:ASN:H	2:B:149:ASN:ND2	2.13	0.44
2:B:427:GLY:N	1:C:424:GLN:HE21	2.12	0.44
1:C:75:HIS:CE1	1:C:116:VAL:HG22	2.52	0.44
1:C:446:PHE:HB2	4:C:3001:NDP:O2D	2.16	0.44
2:D:27:LEU:HD21	2:D:38:LYS:HD3	1.98	0.44
2:D:359:PRO:HG2	5:D:2084:HOH:O	2.17	0.44
1:C:93:LYS:HE3	1:C:94:TYR:CZ	2.53	0.44
1:C:129:PRO:HD3	1:C:199:LEU:HD13	1.98	0.44
2:B:144:ASP:HB2	2:B:335:ASP:O	2.17	0.44
2:B:235:HIS:NE2	2:B:282:GLN:NE2	2.65	0.44
1:A:101:GLU:HG3	1:A:102:HIS:HD2	1.83	0.44
1:A:306:LYS:HB2	5:A:3327:HOH:O	2.17	0.44
1:C:19:ARG:HH22	1:C:24:ALA:HA	1.82	0.44
1:C:233:LYS:O	1:C:281:ILE:HA	2.17	0.44
1:A:101:GLU:HG3	1:A:102:HIS:CD2	2.53	0.44
1:C:207:ASP:HA	1:C:245:LEU:HG	1.99	0.44
1:A:171:ASN:ND2	1:A:174:THR:H	2.15	0.43
1:A:369:ASN:HD21	2:B:63:HIS:CE1	2.21	0.43
2:D:206:PRO:HG3	5:D:2201:HOH:O	2.17	0.43
1:A:66:ARG:HD3	2:B:368:PRO:HG3	2.00	0.43
2:B:358:TYR:HB2	2:B:359:PRO:HD3	1.99	0.43
1:C:171:ASN:HB3	1:C:174:THR:OG1	2.19	0.43
2:D:203:ARG:NH2	5:D:2282:HOH:O	2.52	0.43
2:D:292:PHE:HA	2:D:293:PRO:HD3	1.85	0.43
1:A:411:ALA:HB1	1:A:412:PRO:CD	2.48	0.43
2:B:116:VAL:CG2	2:B:129:PRO:HG2	2.43	0.43
1:A:255:GLN:HG3	1:C:251:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:75:3AH:N2	2:D:148:ASN:CB	2.81	0.43
1:C:156:ARG:NH1	1:C:439:ASN:HD21	2.03	0.43
2:B:20:ALA:O	2:B:22:GLN:N	2.50	0.43
1:C:69:ILE:HG22	2:D:391:PRO:HG3	2.01	0.43
1:C:454:GLU:CD	1:C:454:GLU:N	2.76	0.43
2:D:407:ASN:HD21	2:D:411:ALA:H	1.66	0.43
1:C:405:TYR:CD1	1:C:406:PRO:HA	2.53	0.42
2:D:403:ASN:C	2:D:403:ASN:HD22	2.26	0.42
1:A:391:PRO:HG3	2:B:69:ILE:HG22	2.00	0.42
2:B:171:ASN:HD22	2:B:173:GLN:N	2.16	0.42
1:A:153:PHE:CB	1:A:299:LEU:HD13	2.49	0.42
2:B:112:ARG:HD3	3:B:2001:HEM:O1D	2.18	0.42
1:C:74:VAL:O	1:C:75:HIS:HB2	2.19	0.42
1:C:444:ARG:HD3	1:C:485:VAL:O	2.18	0.42
1:A:149:ASN:HD22	1:A:149:ASN:N	2.09	0.42
2:B:233:LYS:HB2	2:B:282:GLN:HB2	2.00	0.42
1:A:178:ASP:HA	1:A:179:PRO:HD2	1.92	0.42
2:D:411:ALA:HB1	2:D:412:PRO:CD	2.50	0.42
1:A:153:PHE:HB2	1:A:299:LEU:HD13	2.02	0.42
1:A:365:ARG:HG2	1:A:366:LEU:HD13	2.01	0.42
2:B:110:ALA:HB3	2:B:135:LYS:HB3	2.02	0.42
1:A:318:LEU:HD12	1:A:318:LEU:HA	1.84	0.42
2:B:178:ASP:HA	2:B:179:PRO:HD2	1.97	0.42
2:B:17:GLU:C	2:B:19:ARG:N	2.77	0.41
2:B:214:GLY:HA3	2:B:236:TYR:CE1	2.55	0.41
1:C:295:ASN:ND2	1:C:295:ASN:C	2.76	0.41
1:C:499:LYS:HE3	1:C:500:TYR:HE1	1.85	0.41
1:A:395:GLN:HG3	1:A:396:ASP:N	2.28	0.41
2:D:411:ALA:HB1	2:D:412:PRO:HD2	2.03	0.41
1:C:352:GLN:HG3	5:C:3291:HOH:O	2.20	0.41
1:C:391:PRO:HG3	2:D:69:ILE:HG22	2.03	0.41
1:A:70:PRO:HD3	1:C:70:PRO:HG3	2.02	0.41
2:B:179:PRO:HG2	5:B:2092:HOH:O	2.21	0.41
2:D:53:GLN:NE2	5:D:2265:HOH:O	2.52	0.41
1:A:146:VAL:HB	1:A:354:ARG:HH22	1.86	0.41
2:B:385:ASN:HD22	2:B:387:GLN:H	1.69	0.41
5:B:2156:HOH:O	1:C:422:SER:HA	2.20	0.41
1:C:392:MET:HE1	2:D:369:ASN:O	2.21	0.41
2:B:213:ASN:OD1	2:B:238:THR:HG22	2.21	0.41
2:D:334:PHE:O	2:D:362:HIS:HE1	2.04	0.41
1:A:83:GLY:HA3	1:A:317:VAL:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:3AH:N2	2:B:148:ASN:CB	2.80	0.40
2:D:385:ASN:HD22	2:D:387:GLN:H	1.69	0.40
1:A:255:GLN:HB2	1:C:255:GLN:HB2	2.02	0.40
1:A:295:ASN:HD22	1:A:296:PRO:CD	2.34	0.40
2:B:339:MET:HE2	5:B:2111:HOH:O	2.20	0.40
2:B:429:VAL:O	2:B:429:VAL:HG12	2.22	0.40
1:C:394:MET:HG2	2:D:394:MET:CG	2.43	0.40
1:A:179:PRO:HG2	5:A:3253:HOH:O	2.20	0.40
1:A:358:TYR:HB2	1:A:359:PRO:HD3	2.03	0.40
2:B:75:3AH:HN1	2:B:131:GLY:HA2	1.87	0.40
1:C:385:ASN:ND2	1:C:387:GLN:H	2.18	0.40
1:A:167:SER:HA	1:A:181:MET:HE2	2.04	0.40
2:B:40:ASN:ND2	2:D:433:ASN:HA	2.37	0.40
2:B:359:PRO:O	2:B:363:ARG:HG3	2.22	0.40
1:C:33:ASN:HA	1:C:34:PRO:HD3	1.95	0.40
1:C:206:PRO:HG3	5:C:3163:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	497/498 (100%)	476 (96%)	19 (4%)	2 (0%)	30	27
1	C	498/498 (100%)	470 (94%)	26 (5%)	2 (0%)	30	27
2	B	497/498 (100%)	471 (95%)	24 (5%)	2 (0%)	30	27
2	D	497/498 (100%)	475 (96%)	22 (4%)	0	100	100
All	All	1989/1992 (100%)	1892 (95%)	91 (5%)	6 (0%)	36	35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	22	GLN
2	B	22	GLN
1	C	438	ASP
1	A	20	ALA
1	A	23	LYS
2	B	18	GLN

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	429/429 (100%)	417 (97%)	12 (3%)	38	41
1	C	430/429 (100%)	413 (96%)	17 (4%)	28	27
2	B	429/428 (100%)	414 (96%)	15 (4%)	32	32
2	D	429/428 (100%)	416 (97%)	13 (3%)	36	38
All	All	1717/1714 (100%)	1660 (97%)	57 (3%)	33	34

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	VAL
1	A	93	LYS
1	A	149	ASN
1	A	226	ASN
1	A	236	TYR
1	A	299	LEU
1	A	318	LEU
1	A	355	LEU
1	A	366	LEU
1	A	374	PRO
1	A	385	ASN
1	A	394	MET
2	B	5	ARG
2	B	13	GLN
2	B	93	LYS
2	B	138	THR

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Mol	Chain	Res	Type
2	B	149	ASN
2	B	160	LEU
2	B	236	TYR
2	B	299	LEU
2	B	316	LEU
2	B	355	LEU
2	B	366	LEU
2	B	374	PRO
2	B	385	ASN
2	B	394	MET
2	B	403	ASN
1	C	5	ARG
1	C	13	GLN
1	C	41	VAL
1	C	93	LYS
1	C	138	THR
1	C	149	ASN
1	C	160	LEU
1	C	188	LEU
1	C	236	TYR
1	C	242	ILE
1	C	295	ASN
1	C	318	LEU
1	C	385	ASN
1	C	403	ASN
1	C	415	GLN
1	C	426	SER
1	C	453	GLU
2	D	5	ARG
2	D	44	VAL
2	D	58	THR
2	D	93	LYS
2	D	149	ASN
2	D	160	LEU
2	D	236	TYR
2	D	374	PRO
2	D	380	ARG
2	D	382	ARG
2	D	385	ASN
2	D	403	ASN
2	D	419	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	102	HIS
1	A	149	ASN
1	A	168	GLN
1	A	171	ASN
1	A	282	GLN
1	A	295	ASN
1	A	338	ASN
1	A	369	ASN
1	A	385	ASN
1	A	398	GLN
1	A	407	ASN
1	A	421	HIS
1	A	433	ASN
1	A	439	ASN
1	A	449	ASN
1	A	471	GLN
1	A	475	GLN
1	A	486	HIS
1	A	501	ASN
2	B	13	GLN
2	B	18	GLN
2	B	40	ASN
2	B	63	HIS
2	B	149	ASN
2	B	168	GLN
2	B	171	ASN
2	B	226	ASN
2	B	282	GLN
2	B	287	ASN
2	B	295	ASN
2	B	338	ASN
2	B	364	HIS
2	B	385	ASN
2	B	397	ASN
2	B	398	GLN
2	B	403	ASN
2	B	407	ASN
2	B	421	HIS
2	B	424	GLN
2	B	433	ASN
2	B	439	ASN

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Mol	Chain	Res	Type
2	B	475	GLN
2	B	486	HIS
2	B	501	ASN
1	C	14	HIS
1	C	40	ASN
1	C	53	GLN
1	C	63	HIS
1	C	149	ASN
1	C	168	GLN
1	C	171	ASN
1	C	226	ASN
1	C	255	GLN
1	C	282	GLN
1	C	295	ASN
1	C	369	ASN
1	C	385	ASN
1	C	395	GLN
1	C	398	GLN
1	C	403	ASN
1	C	407	ASN
1	C	421	HIS
1	C	424	GLN
1	C	439	ASN
1	C	449	ASN
1	C	471	GLN
1	C	475	GLN
1	C	486	HIS
1	C	501	ASN
2	D	11	GLN
2	D	13	GLN
2	D	40	ASN
2	D	53	GLN
2	D	63	HIS
2	D	148	ASN
2	D	149	ASN
2	D	168	GLN
2	D	226	ASN
2	D	244	ASN
2	D	255	GLN
2	D	295	ASN
2	D	338	ASN
2	D	369	ASN

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Mol	Chain	Res	Type
2	D	385	ASN
2	D	398	GLN
2	D	403	ASN
2	D	407	ASN
2	D	421	HIS
2	D	471	GLN
2	D	475	GLN
2	D	486	HIS
2	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 ⓘ

2 non-standard protein/DNA/RNA residues 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	3AH	D	75	2	15,17,18	2.21	3 (20%)	12,23,25	1.78	5 (41%)
2	3AH	B	75	2	15,17,18	2.06	3 (20%)	12,23,25	1.80	5 (41%)

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	3AH	D	75	2	-	0/9/10/12	0/2/2/2
2	3AH	B	75	2	-	2/9/10/12	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	75	3AH	C3-N4	-6.24	1.31	1.37
2	B	75	3AH	C3-N4	-5.09	1.32	1.37
2	B	75	3AH	C5-N1	4.57	1.38	1.34
2	D	75	3AH	C5-N1	4.48	1.38	1.34
2	B	75	3AH	C3-N2	-2.49	1.29	1.33
2	D	75	3AH	C3-N2	-2.27	1.29	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	75	3AH	NE2-CE1-ND1	-3.12	108.44	112.12
2	D	75	3AH	NE2-CE1-ND1	-2.87	108.74	112.12
2	D	75	3AH	C5-N1-N2	-2.75	105.82	111.23
2	B	75	3AH	N3A-C3-N4	-2.54	117.68	121.29
2	B	75	3AH	CD2-NE2-CE1	2.44	108.84	106.24
2	D	75	3AH	N3A-C3-N4	-2.41	117.86	121.29
2	B	75	3AH	C5-N1-N2	-2.39	106.53	111.23
2	D	75	3AH	CD2-NE2-CE1	2.20	108.59	106.24
2	B	75	3AH	CE1-ND1-CG	2.18	109.30	105.80
2	D	75	3AH	CE1-ND1-CG	2.15	109.25	105.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	75	3AH	N1-C5-NE2-CE1
2	B	75	3AH	N1-C5-NE2-CD2

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	75	3AH	5	0
2	B	75	3AH	4	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

6 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
4	NDP	C	3001	-	51,52,52	1.38	6 (11%)	71,80,80	1.65	9 (12%)
3	HEM	A	2000	1	50,50,50	1.04	1 (2%)	67,82,82	0.91	0
3	HEM	D	2003	2	50,50,50	1.03	1 (2%)	67,82,82	0.87	1 (1%)
4	NDP	A	3000	-	51,52,52	1.35	6 (11%)	71,80,80	1.62	13 (18%)
3	HEM	C	2002	1	50,50,50	0.95	0	67,82,82	0.92	2 (2%)
3	HEM	B	2001	2	50,50,50	1.02	1 (2%)	67,82,82	0.92	2 (2%)

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
4	NDP	C	3001	-	-	3/34/77/77	0/5/5/5
3	HEM	A	2000	1	-	4/14/54/54	-
3	HEM	D	2003	2	-	6/14/54/54	-
4	NDP	A	3000	-	-	3/34/77/77	0/5/5/5
3	HEM	C	2002	1	-	8/14/54/54	-
3	HEM	B	2001	2	-	6/14/54/54	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3000	NDP	C4N-C3N	-4.80	1.40	1.50
4	C	3001	NDP	C4N-C3N	-4.79	1.40	1.50
4	A	3000	NDP	C5A-N7A	-3.28	1.33	1.39
4	A	3000	NDP	C4N-C5N	-3.25	1.40	1.49
4	C	3001	NDP	C4N-C5N	-3.23	1.40	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3001	NDP	C5A-N7A	-3.12	1.33	1.39
3	D	2003	HEM	FE-NA	2.93	2.04	1.95
4	A	3000	NDP	C7N-C3N	2.77	1.54	1.48
3	B	2001	HEM	FE-NC	2.62	2.03	1.95
3	A	2000	HEM	FE-NC	2.42	2.03	1.95
4	C	3001	NDP	C7N-C3N	2.36	1.53	1.48
4	C	3001	NDP	C6N-C5N	2.34	1.40	1.33
4	A	3000	NDP	C6N-C5N	2.27	1.40	1.33
4	C	3001	NDP	P2B-O2B	2.26	1.63	1.59
4	A	3000	NDP	C4A-N9A	-2.16	1.33	1.37

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3001	NDP	C5A-C4A-N3A	-6.00	118.45	126.72
4	A	3000	NDP	C5A-C4A-N3A	-5.35	119.35	126.72
4	C	3001	NDP	N3A-C4A-N9A	5.31	136.20	127.17
4	A	3000	NDP	N3A-C4A-N9A	5.09	135.82	127.17
4	C	3001	NDP	N3A-C2A-N1A	-4.45	121.85	128.58
4	A	3000	NDP	N3A-C2A-N1A	-4.37	121.97	128.58
4	C	3001	NDP	C2B-C1B-N9A	3.48	119.48	113.75
4	C	3001	NDP	C2A-N3A-C4A	3.38	120.09	111.83
4	A	3000	NDP	C6A-C5A-C4A	3.30	121.68	117.18
4	A	3000	NDP	C4A-N9A-C8A	3.22	109.12	105.74
4	C	3001	NDP	C6A-C5A-C4A	3.18	121.52	117.18
4	A	3000	NDP	C2A-N3A-C4A	3.01	119.18	111.83
4	A	3000	NDP	N9A-C8A-N7A	-3.00	109.68	113.94
4	C	3001	NDP	C6A-C5A-N7A	-2.95	126.41	132.09
4	A	3000	NDP	C6A-C5A-N7A	-2.61	127.06	132.09
3	C	2002	HEM	C3B-C4B-NB	2.61	111.34	109.47
3	B	2001	HEM	C3B-C4B-NB	2.51	111.27	109.47
3	D	2003	HEM	CMA-C3A-C2A	2.49	130.90	125.62
4	C	3001	NDP	O2B-P2B-O1X	-2.42	100.70	109.33
4	A	3000	NDP	C4A-N9A-C1B	-2.31	121.24	126.63
4	A	3000	NDP	O2B-P2B-O1X	-2.25	101.33	109.33
4	C	3001	NDP	C3N-C2N-N1N	-2.23	119.93	123.20
4	A	3000	NDP	O4B-C1B-N9A	2.21	112.33	108.09
3	B	2001	HEM	C3B-C2B-C1B	2.20	108.06	106.41
4	A	3000	NDP	C2A-N1A-C6A	2.14	122.25	118.73
4	A	3000	NDP	C3N-C2N-N1N	-2.06	120.18	123.20
3	C	2002	HEM	CMA-C3A-C2A	2.04	129.96	125.62

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2002	HEM	C2B-C3B-CAB-CBB
3	B	2001	HEM	C4C-C3C-CAC-CBC
4	A	3000	NDP	O4D-C1D-N1N-C6N
3	B	2001	HEM	C2C-C3C-CAC-CBC
3	C	2002	HEM	C2C-C3C-CAC-CBC
3	D	2003	HEM	C2C-C3C-CAC-CBC
4	C	3001	NDP	O4D-C1D-N1N-C6N
3	C	2002	HEM	C4C-C3C-CAC-CBC
4	A	3000	NDP	O4B-C4B-C5B-O5B
3	D	2003	HEM	CAD-CBD-CGD-O2D
3	D	2003	HEM	CAD-CBD-CGD-O1D
3	B	2001	HEM	CAD-CBD-CGD-O2D
3	C	2002	HEM	CAD-CBD-CGD-O2D
3	A	2000	HEM	CAD-CBD-CGD-O2D
3	B	2001	HEM	CAD-CBD-CGD-O1D
3	C	2002	HEM	CAD-CBD-CGD-O1D
3	A	2000	HEM	CAD-CBD-CGD-O1D
3	C	2002	HEM	C4B-C3B-CAB-CBB
3	D	2003	HEM	C4C-C3C-CAC-CBC
3	C	2002	HEM	CAA-CBA-CGA-O1A
3	A	2000	HEM	CAA-CBA-CGA-O2A
3	A	2000	HEM	CAA-CBA-CGA-O1A
3	B	2001	HEM	CAA-CBA-CGA-O1A
3	D	2003	HEM	CAA-CBA-CGA-O1A
3	C	2002	HEM	CAA-CBA-CGA-O2A
4	C	3001	NDP	C2B-C1B-N9A-C8A
3	B	2001	HEM	CAA-CBA-CGA-O2A
3	D	2003	HEM	CAA-CBA-CGA-O2A
4	A	3000	NDP	PA-O3-PN-O2N
4	C	3001	NDP	PA-O3-PN-O1N

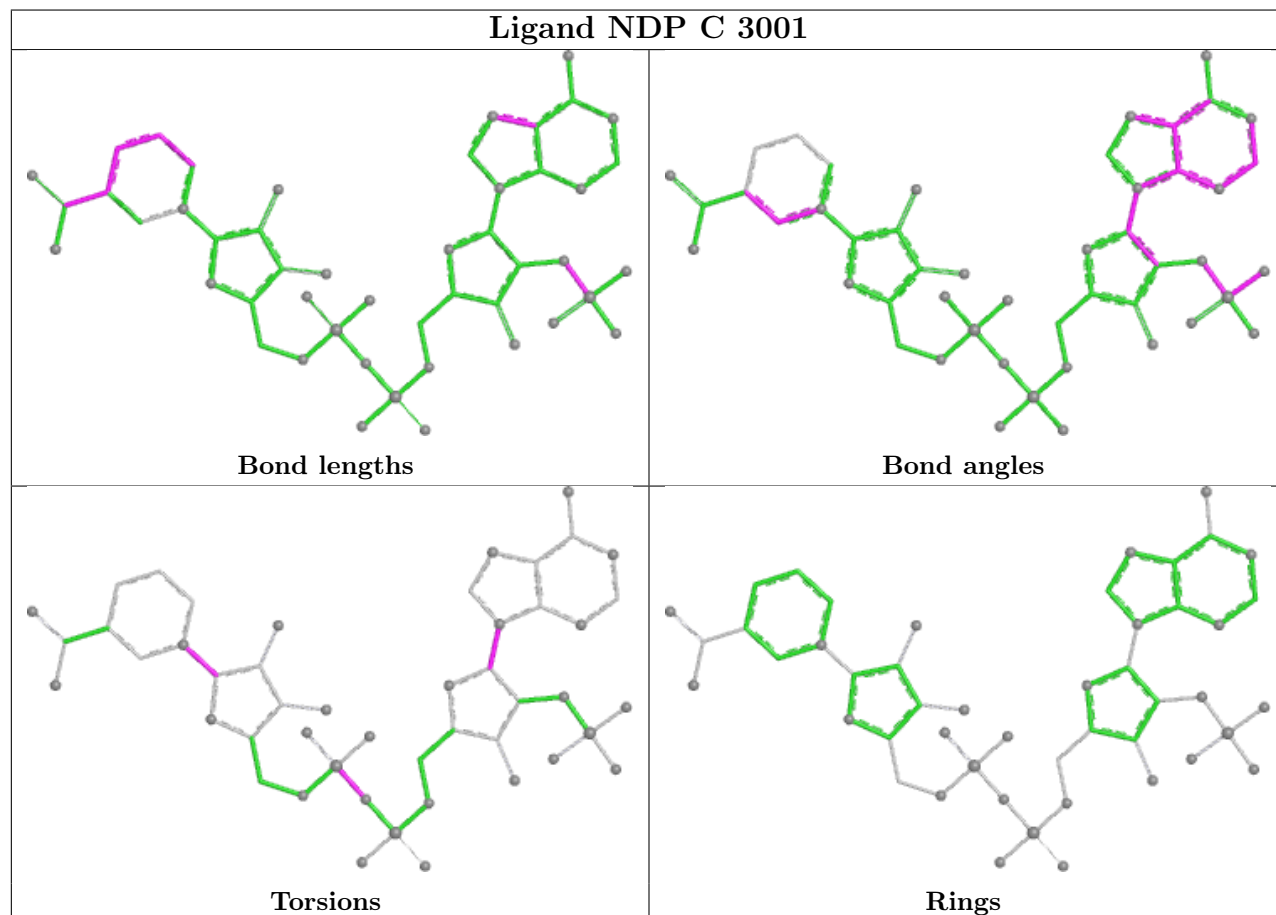
There are no ring outliers.

2 monomers are involved in 2 short contacts:

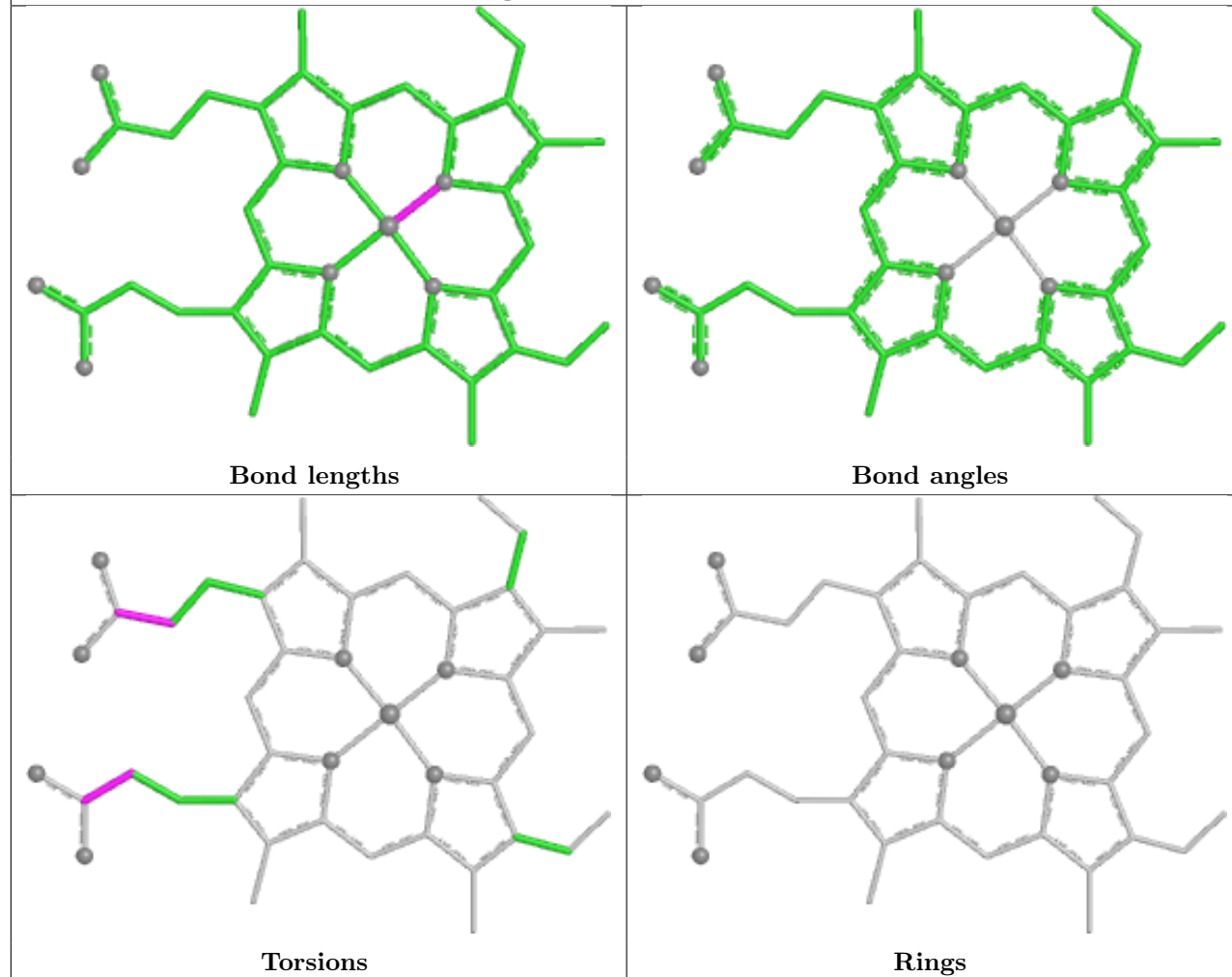
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	3001	NDP	1	0
3	B	2001	HEM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

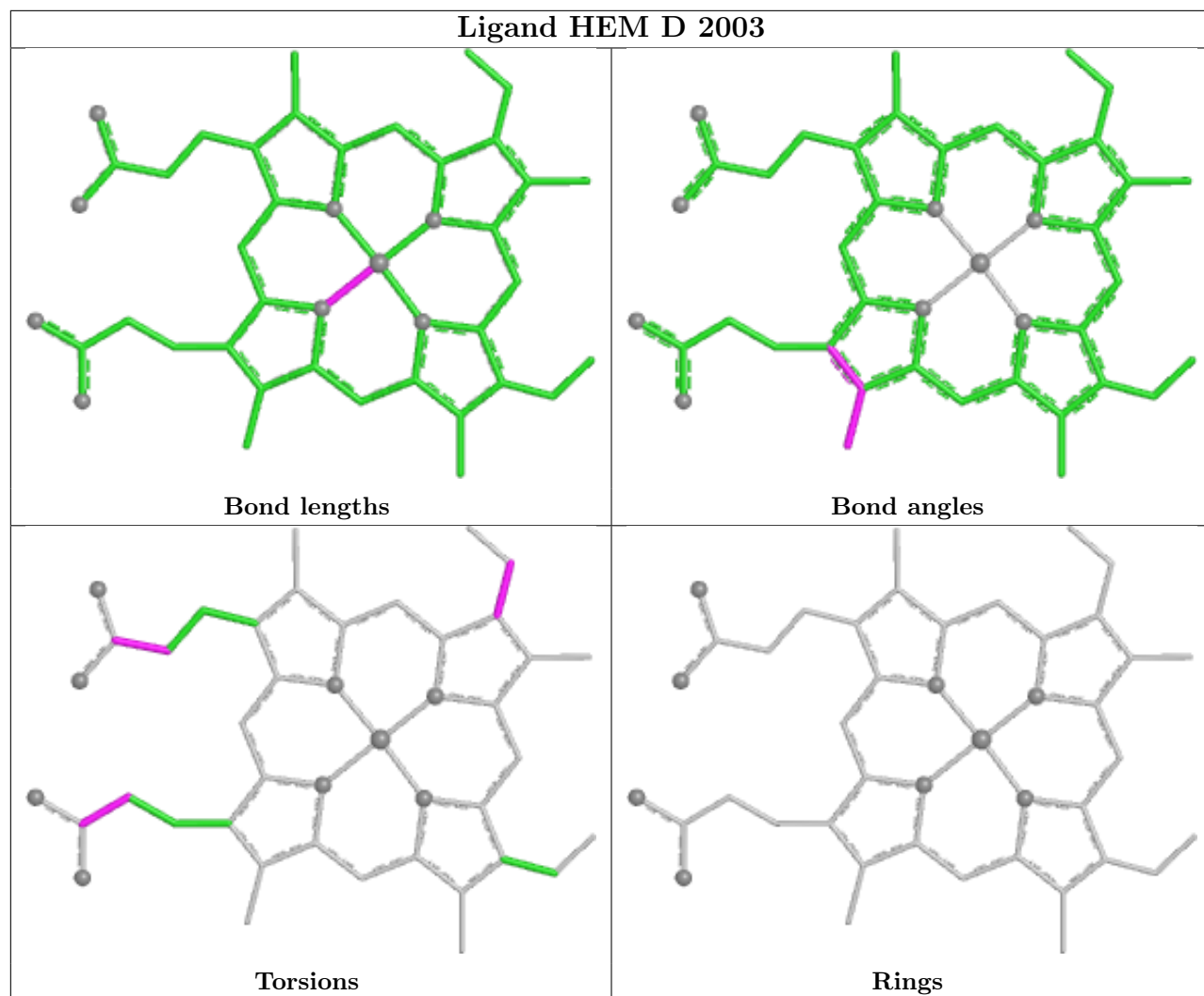
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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

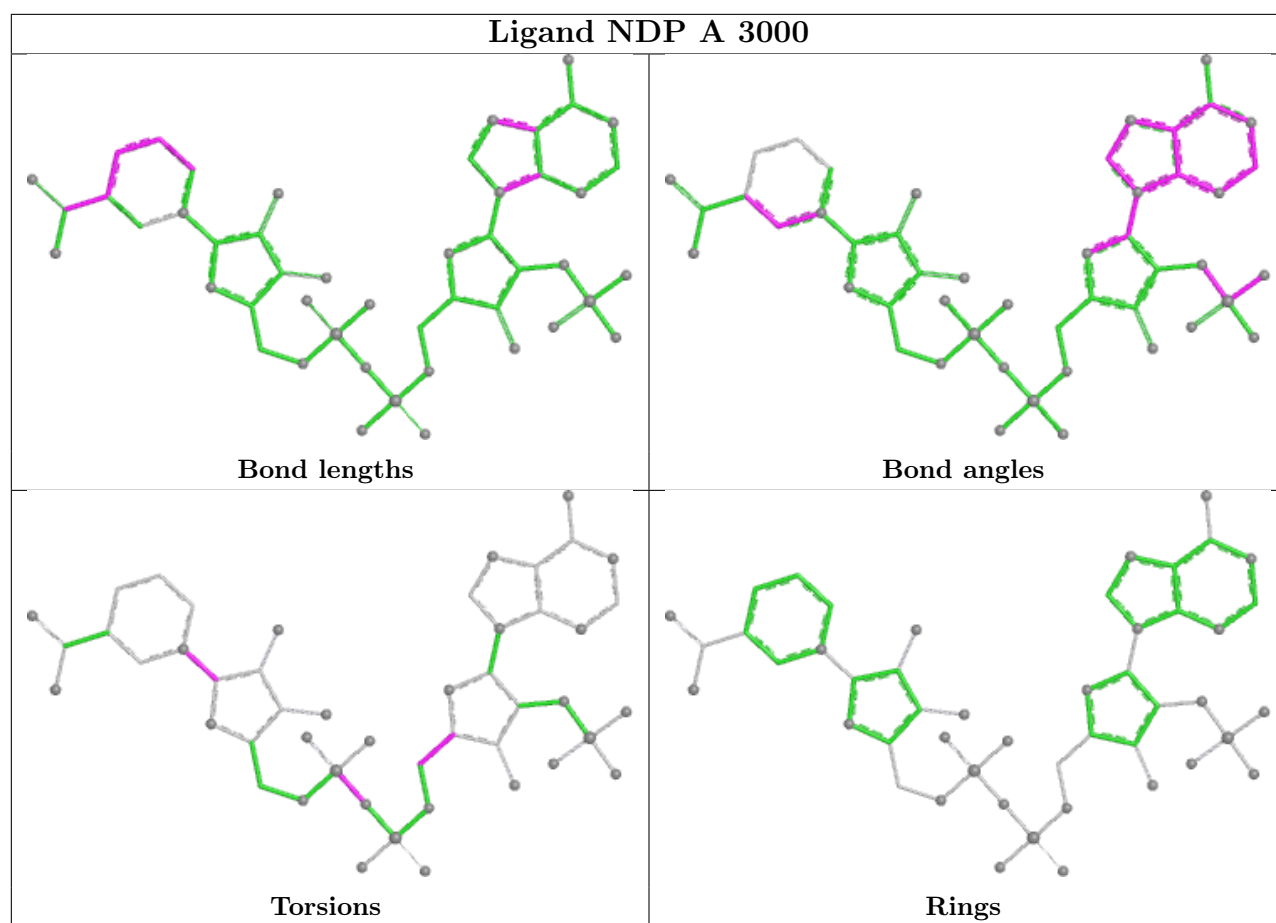


Ligand HEM A 2000

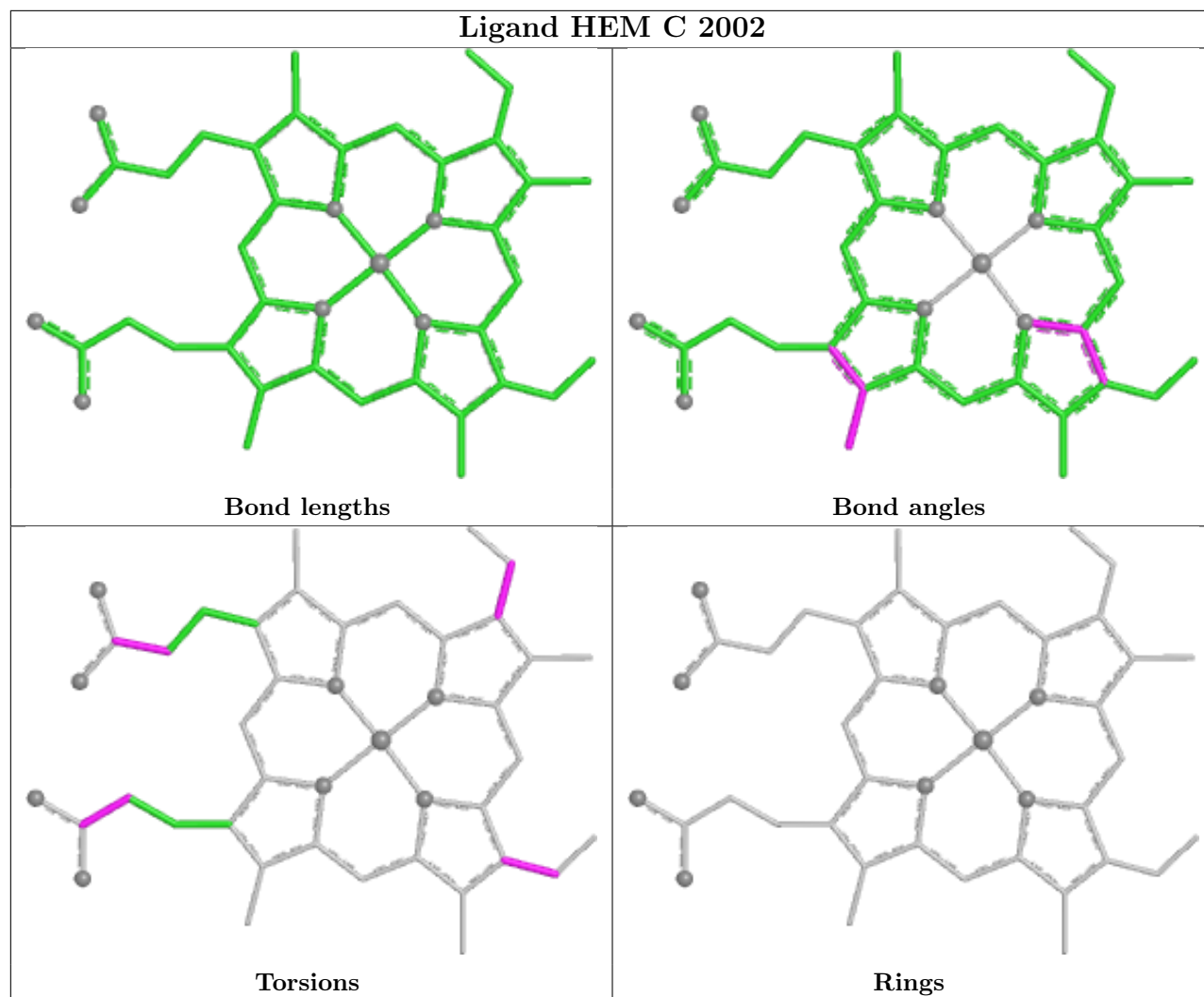


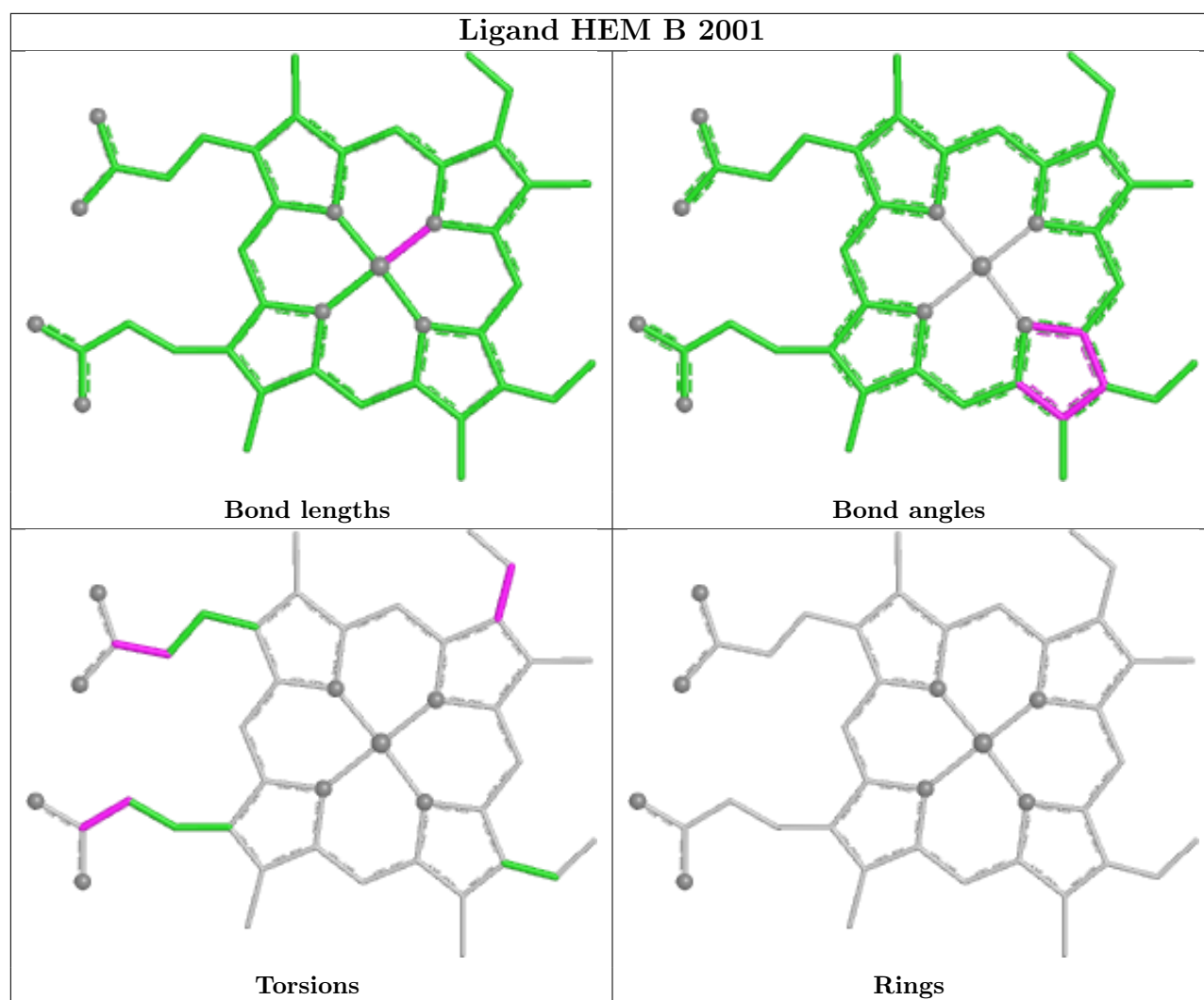
Ligand HEM D 2003





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

6.1 Protein, DNA and RNA chains

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	497/498 (99%)	-0.42	4 (0%) 82 82	18, 38, 48, 57	2 (0%)
1	C	498/498 (100%)	-0.38	6 (1%) 76 76	18, 38, 50, 60	2 (0%)
2	B	497/498 (99%)	-0.37	6 (1%) 76 76	17, 39, 50, 58	2 (0%)
2	D	497/498 (99%)	-0.37	5 (1%) 79 79	18, 39, 47, 58	2 (0%)
All	All	1989/1992 (99%)	-0.38	21 (1%) 78 77	17, 39, 49, 60	8 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	21	ALA	5.7
1	C	22	GLN	5.6
2	B	22	GLN	5.5
2	D	21	ALA	4.3
1	C	4	SER	4.3
2	D	4	SER	3.9
2	B	4	SER	3.6
2	D	382	ARG	3.1
1	A	488	ASP	3.0
1	C	21	ALA	2.8
2	B	394	MET	2.7
1	C	394	MET	2.7
1	A	20	ALA	2.6
2	B	488	ASP	2.5
1	C	415	GLN	2.4
2	B	20	ALA	2.4
1	C	20	ALA	2.3
2	D	148	ASN	2.2
2	D	18	GLN	2.1
1	A	21	ALA	2.1
1	A	394	MET	2.0

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

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(Å ²)	Q<0.9
2	3AH	B	75	16/17	0.90	0.13	35,39,51,52	0
2	3AH	D	75	16/17	0.90	0.12	35,39,50,51	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

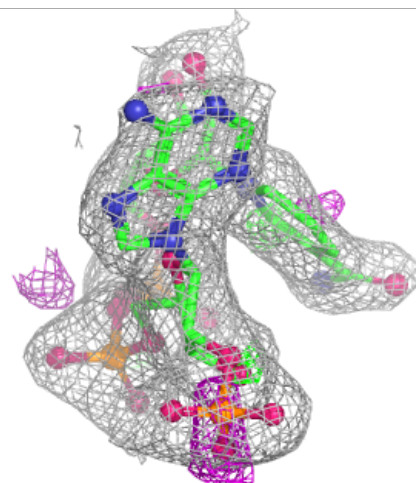
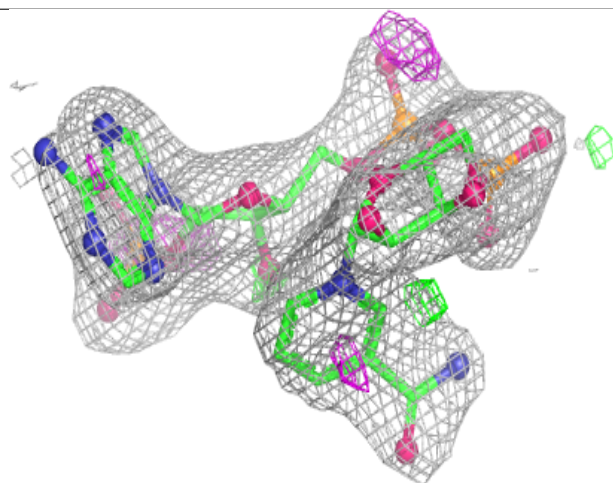
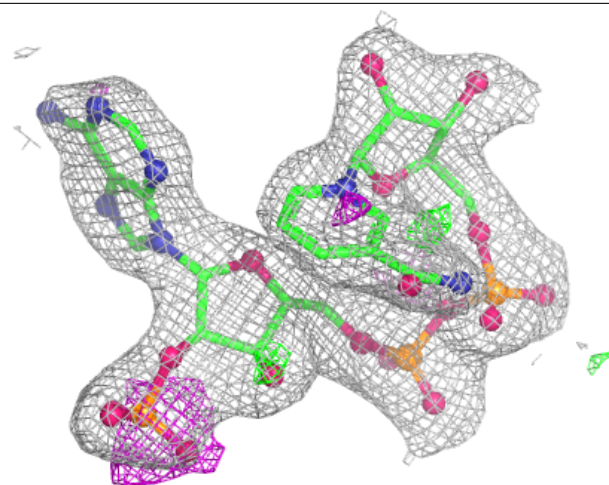
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NDP	C	3001	48/48	0.91	0.09	55,59,63,63	0
4	NDP	A	3000	48/48	0.94	0.08	48,51,57,57	0
3	HEM	C	2002	43/43	0.98	0.05	33,34,35,35	0
3	HEM	A	2000	43/43	0.98	0.05	33,33,34,34	0
3	HEM	B	2001	43/43	0.98	0.06	33,34,35,35	0
3	HEM	D	2003	43/43	0.99	0.05	33,34,35,35	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.

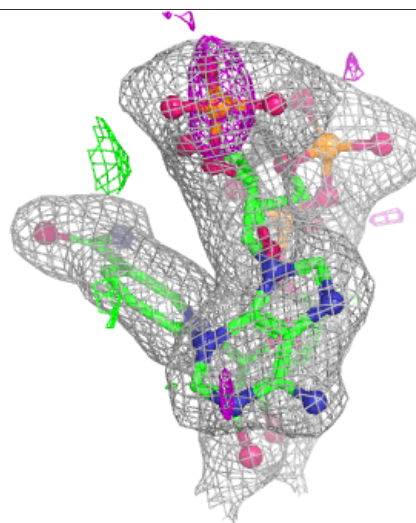
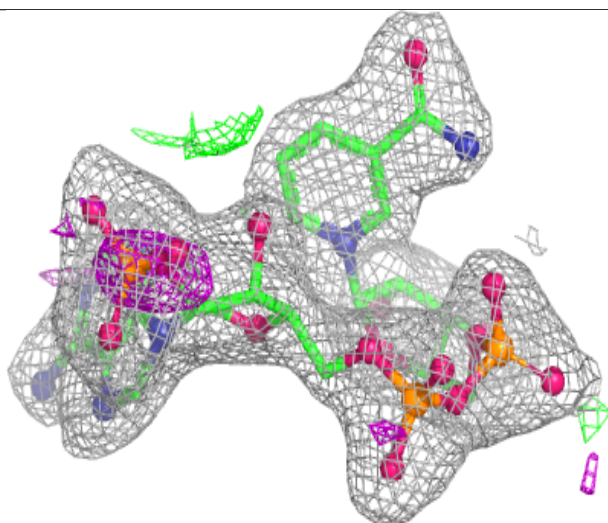
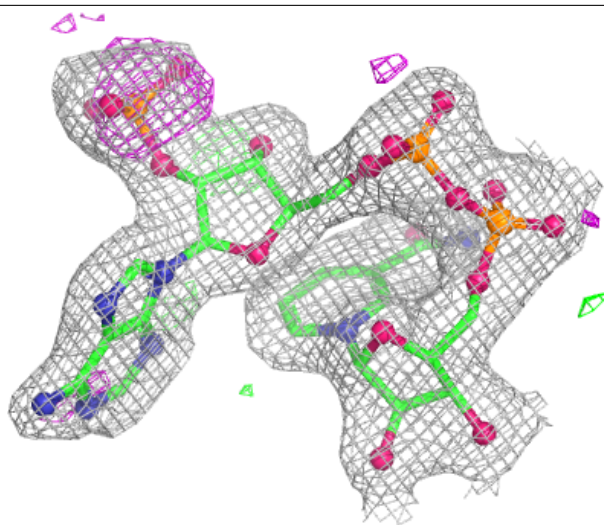
Electron density around NDP C 3001:

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



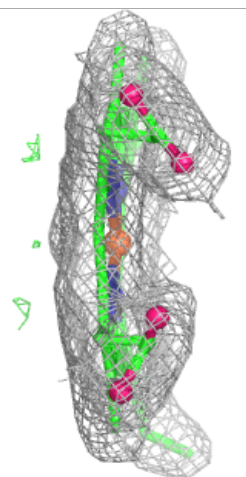
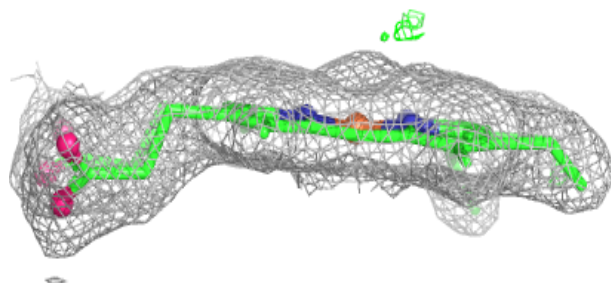
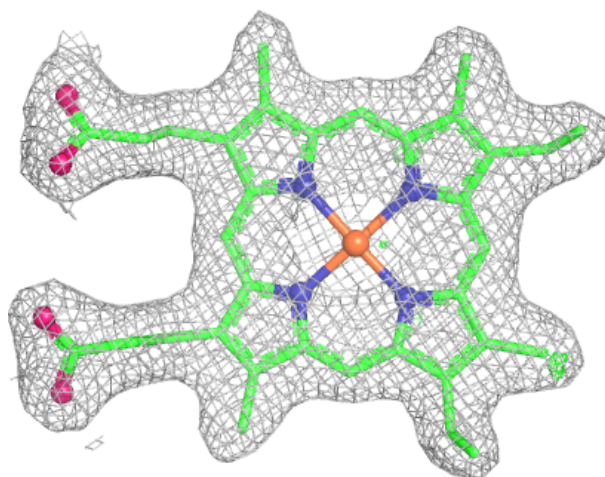
Electron density around NDP A 3000:

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



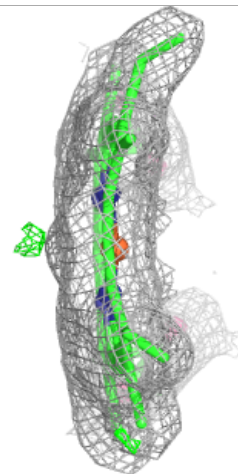
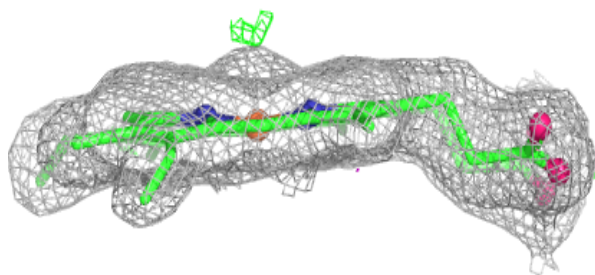
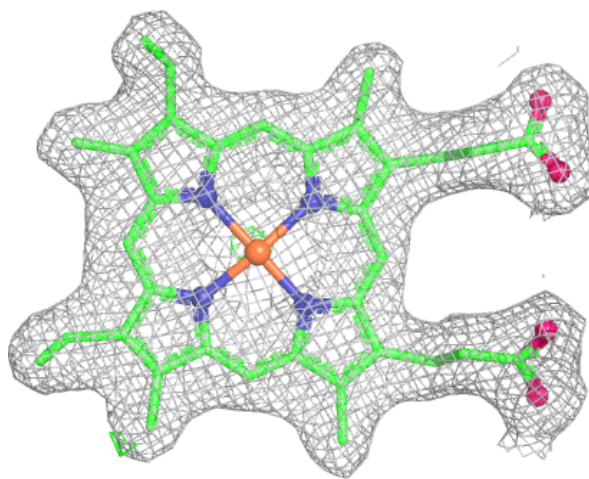
Electron density around HEM C 2002:

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



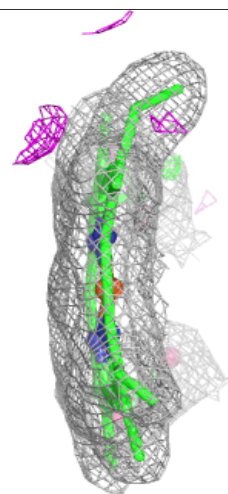
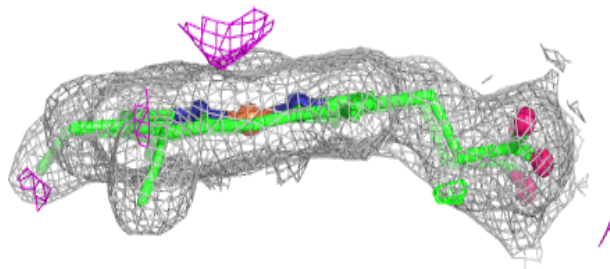
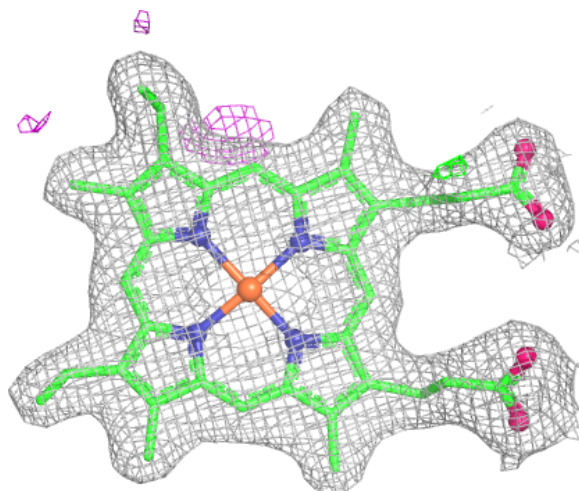
Electron density around HEM A 2000:

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



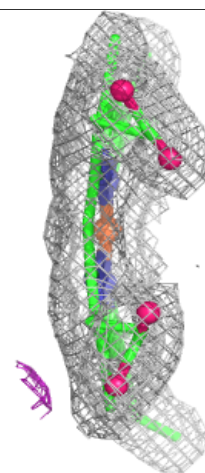
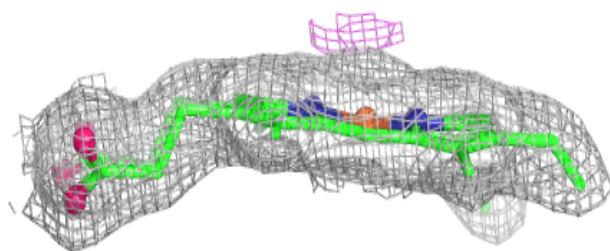
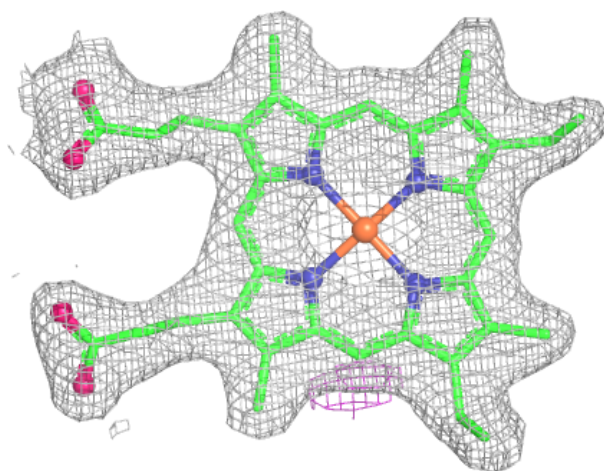
Electron density around HEM B 2001:

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



Electron density around HEM 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.