



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:16 AM UTC

PDB ID : 1P81 / pdb_00001p81
Title : Crystal structure of the D181E variant of catalase HP11 from E. coli
Authors : Chelikani, P.; Carpena, X.; Fita, I.; Loewen, P.C.
Deposited on : 2003-05-06
Resolution : 1.81 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

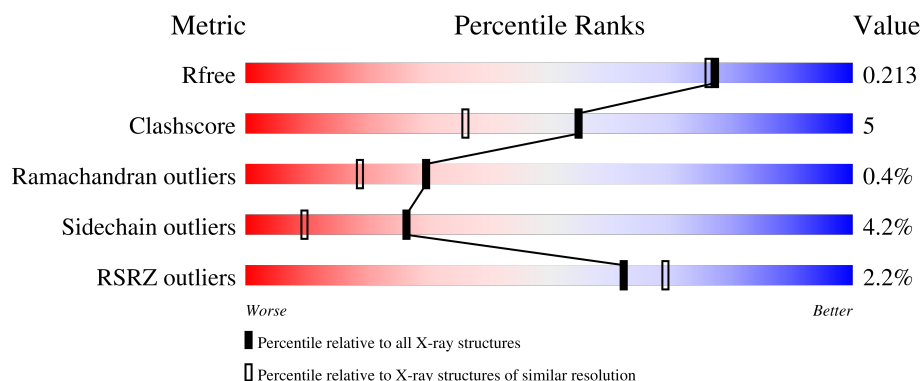
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

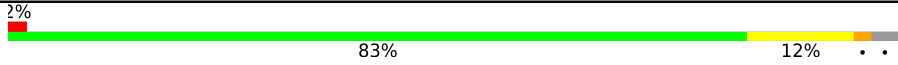
The reported resolution of this entry is 1.81 Å.

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))
R_{free}	180053	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	753	
1	B	753	
1	C	753	
1	D	753	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26236 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.

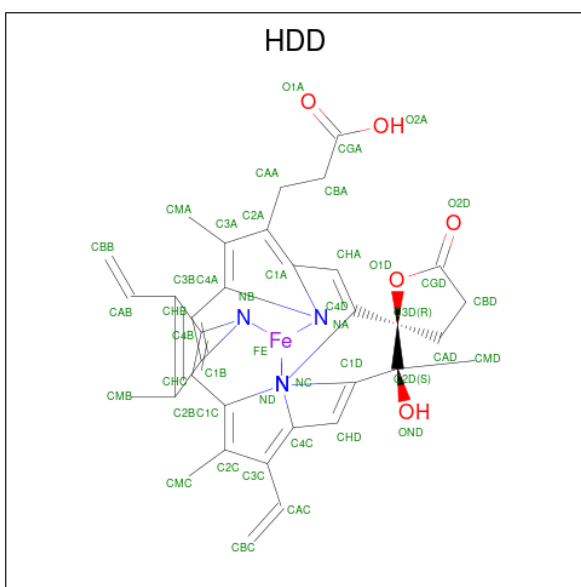
- Molecule 1 is a protein called Catalase HP11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5747	3648	1005	1082	12			
1	B	727	Total	C	N	O	S	0	0	0
			5747	3648	1005	1082	12			
1	C	727	Total	C	N	O	S	0	0	0
			5747	3648	1005	1082	12			
1	D	727	Total	C	N	O	S	0	0	0
			5747	3648	1005	1082	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	GLU	ASP	engineered mutation	UNP P21179
B	181	GLU	ASP	engineered mutation	UNP P21179
C	181	GLU	ASP	engineered mutation	UNP P21179
D	181	GLU	ASP	engineered mutation	UNP P21179

- Molecule 2 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (CCD ID: HDD) (formula: C₃₄H₃₂FeN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 44	C 34	Fe 1	N 4	O 5	0	0
2	B	1	Total 44	C 34	Fe 1	N 4	O 5	0	0
2	C	1	Total 44	C 34	Fe 1	N 4	O 5	0	0
2	D	1	Total 44	C 34	Fe 1	N 4	O 5	0	0

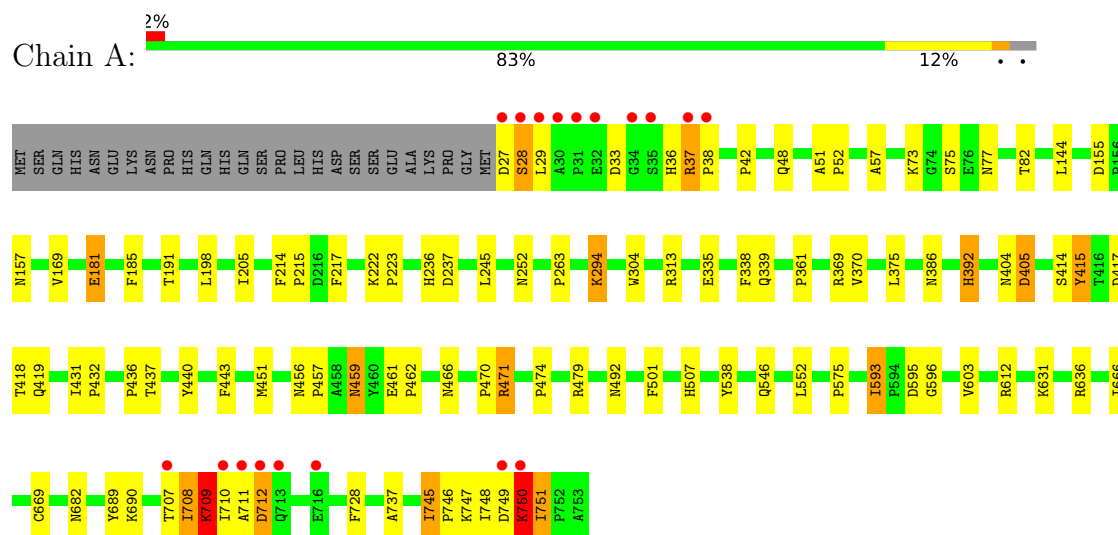
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	815	Total O 815 815	0	0
3	B	702	Total O 702 702	0	0
3	C	768	Total O 768 768	0	0
3	D	787	Total O 787 787	0	0

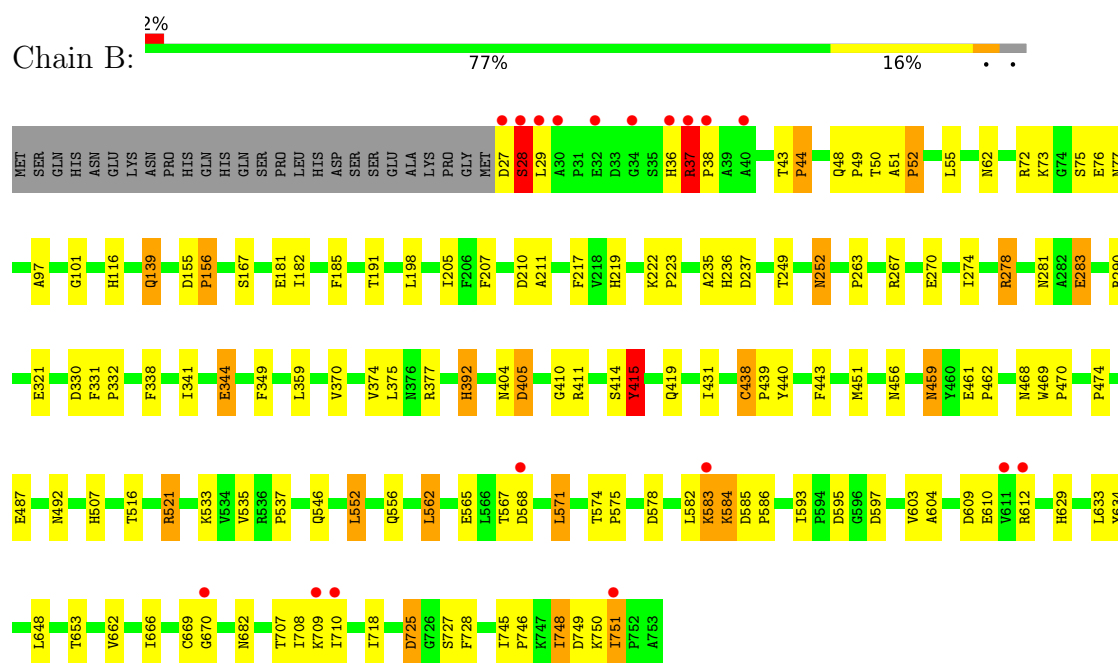
3 Residue-property plots [i](#)

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

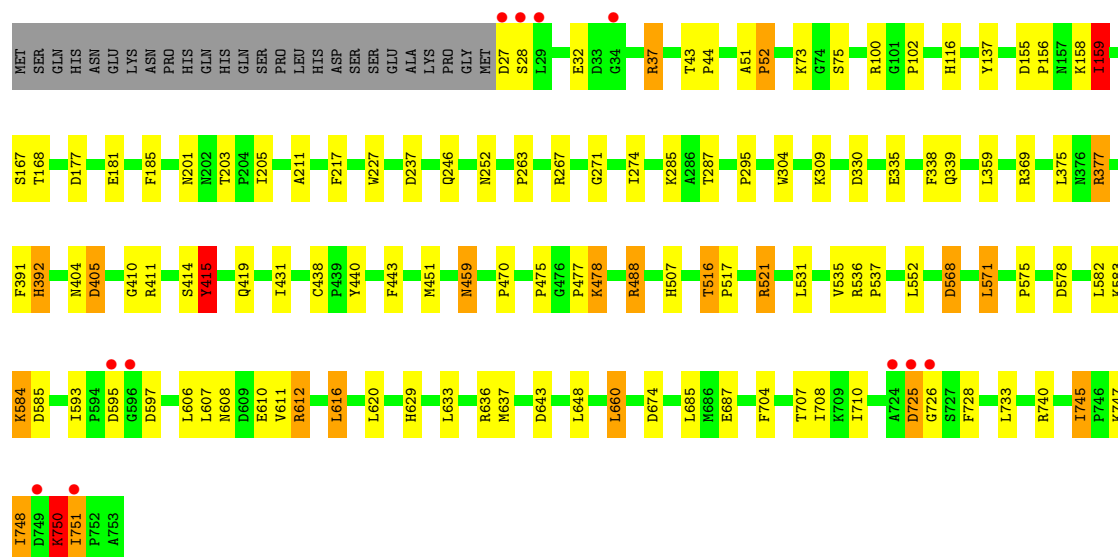
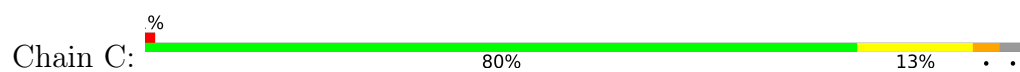
• Molecule 1: Catalase HP1I



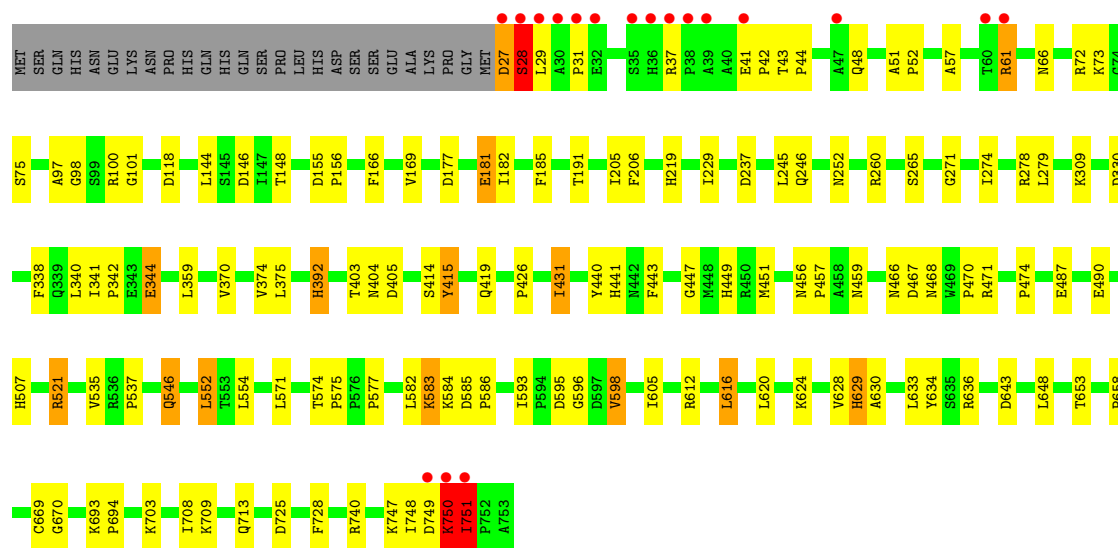
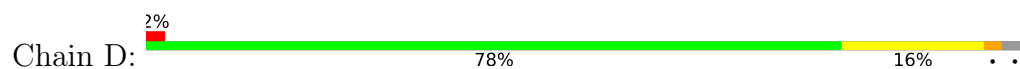
• Molecule 1: Catalase HP1I



• Molecule 1: Catalase HP1I



• Molecule 1: Catalase HP11



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.38Å 132.86Å 122.04Å 90.00° 109.50° 90.00°	Depositor
Resolution (Å)	29.90 – 1.81 29.90 – 1.81	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.90-1.81) 98.8 (29.90-1.81)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 1.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.172 , 0.216 0.176 , 0.213	Depositor DCC
R_{free} test set	12587 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	13.9	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26236	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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: HDD

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	0.71	0/5903	1.57	63/8025 (0.8%)
1	B	0.69	0/5903	1.58	73/8025 (0.9%)
1	C	0.70	0/5903	1.54	67/8025 (0.8%)
1	D	0.71	0/5903	1.60	78/8025 (1.0%)
All	All	0.70	0/23612	1.57	281/32100 (0.9%)

There are no bond length outliers.

All (281) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	612	ARG	CD-NE-CZ	29.59	165.83	124.40
1	D	449	HIS	CA-CB-CG	13.08	126.88	113.80
1	A	728	PHE	CA-CB-CG	10.47	124.27	113.80
1	B	283	GLU	CB-CG-CD	9.94	129.49	112.60
1	B	595	ASP	CA-CB-CG	9.90	122.50	112.60
1	A	575	PRO	N-CA-CB	9.40	108.46	103.19
1	C	674	ASP	CA-CB-CG	9.40	122.00	112.60
1	A	751	ILE	N-CA-CB	9.33	120.52	110.17
1	D	27	ASP	CA-CB-CG	9.20	121.80	112.60
1	D	338	PHE	CA-CB-CG	9.18	122.98	113.80
1	D	575	PRO	N-CA-CB	9.18	108.33	103.19
1	B	44	PRO	N-CA-CB	8.90	108.17	103.19
1	B	185	PHE	CA-CB-CG	8.88	122.68	113.80
1	C	725	ASP	CA-CB-CG	-8.83	103.77	112.60
1	C	419	GLN	CB-CG-CD	-8.80	97.64	112.60
1	B	43	THR	CA-C-N	8.77	126.06	119.66
1	B	43	THR	C-N-CA	8.77	126.06	119.66
1	C	728	PHE	CA-CB-CG	8.77	122.57	113.80
1	C	568	ASP	CA-CB-CG	-8.76	103.84	112.60
1	A	419	GLN	CB-CG-CD	-8.62	97.94	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	419	GLN	CB-CG-CD	-8.57	98.03	112.60
1	B	728	PHE	CA-CB-CG	8.53	122.33	113.80
1	C	597	ASP	CA-CB-CG	8.34	120.94	112.60
1	B	597	ASP	CA-CB-CG	8.19	120.79	112.60
1	C	536	ARG	CA-C-O	8.19	124.61	119.29
1	B	270	GLU	CA-C-N	8.18	127.21	121.65
1	B	270	GLU	C-N-CA	8.18	127.21	121.65
1	C	751	ILE	CA-C-O	8.16	123.97	119.15
1	C	575	PRO	N-CA-CB	8.14	107.45	103.22
1	D	419	GLN	CB-CG-CD	-8.08	98.86	112.60
1	C	43	THR	CA-C-N	8.04	125.53	119.66
1	C	43	THR	C-N-CA	8.04	125.53	119.66
1	A	479	ARG	CD-NE-CZ	7.92	135.49	124.40
1	C	726	GLY	N-CA-C	-7.86	94.54	113.18
1	B	338	PHE	CA-CB-CG	7.78	121.58	113.80
1	C	28	SER	N-CA-C	-7.75	101.76	112.30
1	B	575	PRO	N-CA-CB	7.75	107.53	103.19
1	D	61	ARG	NE-CZ-NH2	7.64	126.08	119.20
1	B	574	THR	CA-C-N	7.45	125.10	119.66
1	B	574	THR	C-N-CA	7.45	125.10	119.66
1	A	595	ASP	CA-CB-CG	7.44	120.04	112.60
1	D	44	PRO	N-CA-CB	7.29	107.27	103.19
1	D	61	ARG	NE-CZ-NH1	-7.28	114.22	121.50
1	D	612	ARG	NE-CZ-NH2	7.23	125.71	119.20
1	B	392	HIS	ND1-CE1-NE2	-7.17	101.23	108.40
1	D	474	PRO	N-CA-CB	7.11	106.91	103.22
1	D	728	PHE	CA-CB-CG	7.11	120.91	113.80
1	B	155	ASP	CA-CB-CG	7.02	119.62	112.60
1	C	338	PHE	CA-CB-CG	6.99	120.79	113.80
1	A	546	GLN	OE1-CD-NE2	-6.97	115.63	122.60
1	D	344	GLU	CA-CB-CG	6.92	127.94	114.10
1	B	492	ASN	CA-CB-CG	-6.91	105.69	112.60
1	D	574	THR	CA-C-N	6.90	124.70	119.66
1	D	574	THR	C-N-CA	6.90	124.70	119.66
1	A	181	GLU	CB-CG-CD	6.88	124.30	112.60
1	C	44	PRO	N-CA-CB	6.87	107.03	103.19
1	D	431	ILE	N-CA-C	-6.86	102.23	108.95
1	A	414	SER	N-CA-C	6.83	118.81	111.36
1	C	44	PRO	CA-C-O	6.75	125.76	120.90
1	A	501	PHE	CA-CB-CG	6.74	120.54	113.80
1	A	42	PRO	N-CA-CB	6.71	109.14	103.17
1	C	745	ILE	N-CA-CB	6.70	115.01	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	PHE	CA-CB-CG	6.68	120.48	113.80
1	B	474	PRO	N-CA-CB	6.68	106.93	103.19
1	C	237	ASP	N-CA-C	6.67	119.11	111.11
1	D	521	ARG	NE-CZ-NH2	6.64	125.18	119.20
1	D	237	ASP	N-CA-C	6.61	119.04	111.11
1	B	263	PRO	N-CA-CB	6.58	109.08	103.35
1	B	546	GLN	OE1-CD-NE2	-6.56	116.04	122.60
1	C	750	LYS	CA-C-N	-6.54	117.88	122.59
1	C	750	LYS	C-N-CA	-6.54	117.88	122.59
1	C	287	THR	CA-C-O	-6.52	113.08	120.32
1	D	271	GLY	O-C-N	-6.40	118.37	123.49
1	A	157	ASN	CA-CB-CG	-6.39	106.21	112.60
1	C	725	ASP	N-CA-CB	6.39	121.28	110.49
1	C	392	HIS	ND1-CE1-NE2	-6.38	102.02	108.40
1	B	419	GLN	CG-CD-NE2	6.38	125.97	116.40
1	B	341	ILE	CA-C-O	6.38	123.26	119.94
1	C	391	PHE	CA-CB-CG	6.32	120.12	113.80
1	D	100	ARG	CG-CD-NE	6.28	125.82	112.00
1	D	229	ILE	N-CA-C	-6.27	104.05	109.19
1	D	155	ASP	CA-CB-CG	6.25	118.85	112.60
1	A	236	HIS	CA-CB-CG	6.25	120.05	113.80
1	B	648	LEU	CA-C-N	6.24	126.45	119.90
1	B	648	LEU	C-N-CA	6.24	126.45	119.90
1	A	750	LYS	N-CA-C	-6.22	105.82	113.41
1	C	431	ILE	N-CA-C	-6.21	102.86	108.95
1	C	185	PHE	CA-CB-CG	6.20	120.00	113.80
1	A	471	ARG	NE-CZ-NH2	6.20	124.78	119.20
1	D	546	GLN	OE1-CD-NE2	-6.16	116.44	122.60
1	C	392	HIS	ND1-CG-CD2	-6.10	100.00	106.10
1	B	521	ARG	NE-CZ-NH1	6.09	127.59	121.50
1	B	431	ILE	N-CA-C	-6.04	103.03	108.95
1	B	28	SER	N-CA-CB	6.01	120.65	110.49
1	B	405	ASP	CA-CB-CG	6.00	118.61	112.60
1	D	43	THR	CA-C-N	6.00	124.04	119.66
1	D	43	THR	C-N-CA	6.00	124.04	119.66
1	D	414	SER	N-CA-C	5.99	117.89	111.36
1	C	263	PRO	N-CA-CB	5.98	108.55	103.35
1	C	158	LYS	CA-C-N	-5.97	115.79	123.19
1	C	158	LYS	C-N-CA	-5.97	115.79	123.19
1	A	708	ILE	CA-C-N	5.96	132.91	121.54
1	A	708	ILE	C-N-CA	5.96	132.91	121.54
1	D	629	HIS	CA-CB-CG	-5.94	107.86	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	37	ARG	CA-C-N	5.93	125.69	119.76
1	D	37	ARG	C-N-CA	5.93	125.69	119.76
1	B	392	HIS	ND1-CG-CD2	-5.93	100.17	106.10
1	B	182	ILE	N-CA-C	-5.92	103.52	110.21
1	D	246	GLN	CA-C-N	5.92	125.59	119.56
1	D	246	GLN	C-N-CA	5.92	125.59	119.56
1	D	521	ARG	CD-NE-CZ	-5.91	116.12	124.40
1	D	595	ASP	CA-CB-CG	5.91	118.51	112.60
1	D	467	ASP	CA-C-O	5.91	128.39	121.54
1	D	658	PRO	N-CA-CB	5.90	108.94	103.39
1	B	415	TYR	CA-CB-CG	5.90	124.52	113.90
1	B	37	ARG	CA-C-N	5.89	125.65	119.76
1	B	37	ARG	C-N-CA	5.89	125.65	119.76
1	D	265	SER	N-CA-CB	-5.89	102.61	111.56
1	C	304	TRP	N-CA-C	5.89	118.18	111.11
1	D	61	ARG	CD-NE-CZ	5.88	132.63	124.40
1	C	377	ARG	NE-CZ-NH1	-5.88	115.62	121.50
1	C	595	ASP	CA-CB-CG	5.87	118.47	112.60
1	D	593	ILE	CB-CA-C	-5.86	104.44	111.18
1	A	474	PRO	O-C-N	-5.86	118.62	121.31
1	C	177	ASP	N-CA-C	5.85	117.46	111.14
1	D	643	ASP	CA-CB-CG	5.85	118.45	112.60
1	D	709	LYS	CA-CB-CG	5.83	125.76	114.10
1	C	414	SER	N-CA-C	5.83	117.31	111.07
1	D	403	THR	N-CA-CB	5.81	120.41	111.22
1	D	419	GLN	CG-CD-NE2	5.81	125.11	116.40
1	D	206	PHE	CA-CB-CG	-5.80	108.00	113.80
1	A	405	ASP	CA-C-N	5.78	125.40	119.56
1	A	405	ASP	C-N-CA	5.78	125.40	119.56
1	B	278	ARG	CD-NE-CZ	5.76	132.47	124.40
1	C	217	PHE	CA-CB-CG	-5.76	108.04	113.80
1	B	167	SER	N-CA-CB	-5.74	102.63	111.46
1	B	414	SER	N-CA-C	5.73	117.61	111.36
1	A	471	ARG	N-CA-C	5.71	119.36	110.17
1	C	295	PRO	N-CA-CB	5.70	107.86	103.30
1	C	271	GLY	O-C-N	-5.64	118.40	123.37
1	A	747	LYS	N-CA-C	5.64	119.88	112.89
1	B	419	GLN	CA-CB-CG	-5.64	102.83	114.10
1	D	185	PHE	CA-CB-CG	5.62	119.42	113.80
1	D	457	PRO	N-CA-CB	5.61	109.45	103.39
1	C	116	HIS	CA-CB-CG	-5.60	108.20	113.80
1	C	636	ARG	NE-CZ-NH2	5.60	124.24	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	392	HIS	CB-CG-CD2	5.60	138.48	131.20
1	D	585	ASP	CA-C-N	5.59	125.27	119.56
1	D	585	ASP	C-N-CA	5.59	125.27	119.56
1	A	712	ASP	CA-CB-CG	5.59	118.19	112.60
1	C	203	THR	O-C-N	-5.59	117.91	121.88
1	A	155	ASP	CA-CB-CG	5.56	118.16	112.60
1	D	166	PHE	CA-C-O	-5.55	114.73	121.28
1	C	159	ILE	CB-CA-C	5.54	119.08	110.83
1	C	168	THR	N-CA-C	-5.53	101.25	109.94
1	B	492	ASN	CA-C-O	-5.52	114.92	121.66
1	A	419	GLN	N-CA-CB	5.51	119.36	110.42
1	B	392	HIS	CA-C-N	5.51	125.13	119.56
1	B	392	HIS	C-N-CA	5.51	125.13	119.56
1	C	246	GLN	CA-C-N	5.51	125.86	119.47
1	C	246	GLN	C-N-CA	5.51	125.86	119.47
1	D	596	GLY	N-CA-C	5.51	117.81	111.36
1	D	260	ARG	NH1-CZ-NH2	5.51	126.46	119.30
1	D	392	HIS	CA-C-N	5.51	125.12	119.56
1	D	392	HIS	C-N-CA	5.51	125.12	119.56
1	B	438	CYS	CA-C-N	5.50	125.42	119.76
1	B	438	CYS	C-N-CA	5.50	125.42	119.76
1	A	712	ASP	CA-C-O	5.47	124.71	118.47
1	D	392	HIS	ND1-CE1-NE2	-5.46	102.94	108.40
1	A	57	ALA	CA-C-N	5.46	125.08	119.56
1	A	57	ALA	C-N-CA	5.46	125.08	119.56
1	D	156	PRO	N-CA-CB	5.46	108.94	103.48
1	A	237	ASP	N-CA-C	5.46	117.66	111.11
1	A	33	ASP	N-CA-C	5.46	119.56	113.01
1	C	339	GLN	N-CA-C	-5.45	99.84	108.73
1	B	72	ARG	N-CA-CB	5.45	117.97	109.85
1	A	392	HIS	ND1-CE1-NE2	-5.44	102.96	108.40
1	B	237	ASP	N-CA-C	5.43	117.63	111.11
1	C	636	ARG	NE-CZ-NH1	-5.43	116.07	121.50
1	D	177	ASP	N-CA-C	5.43	118.02	111.40
1	B	748	ILE	CA-C-N	5.42	127.81	120.38
1	B	748	ILE	C-N-CA	5.42	127.81	120.38
1	A	304	TRP	N-CA-C	5.39	117.58	111.11
1	A	77	ASN	OD1-CG-ND2	5.39	127.99	122.60
1	D	98	GLY	N-CA-C	-5.37	104.98	112.18
1	B	290	ARG	N-CA-CB	5.37	119.69	110.68
1	B	456	ASN	CA-CB-CG	5.35	117.95	112.60
1	A	492	ASN	CA-C-O	-5.34	115.41	121.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	182	ILE	N-CA-C	-5.33	104.18	110.21
1	A	745	ILE	CA-C-N	5.32	125.39	119.32
1	A	745	ILE	C-N-CA	5.32	125.39	119.32
1	D	342	PRO	N-CA-CB	5.32	107.97	103.35
1	B	567	THR	CA-C-N	5.31	129.64	121.19
1	B	567	THR	C-N-CA	5.31	129.64	121.19
1	B	593	ILE	CA-C-N	5.31	126.48	119.84
1	B	593	ILE	C-N-CA	5.31	126.48	119.84
1	A	48	GLN	O-C-N	5.31	125.53	121.65
1	A	437	THR	N-CA-C	-5.31	106.85	113.38
1	C	392	HIS	CA-C-N	5.31	124.92	119.56
1	C	392	HIS	C-N-CA	5.31	124.92	119.56
1	B	52	PRO	N-CA-CB	5.31	107.92	103.25
1	B	236	HIS	CA-CB-CG	5.31	119.11	113.80
1	A	507	HIS	CA-C-N	5.30	124.75	119.24
1	A	507	HIS	C-N-CA	5.30	124.75	119.24
1	C	167	SER	N-CA-CB	-5.30	103.30	111.46
1	B	217	PHE	CA-CB-CG	-5.30	108.50	113.80
1	C	740	ARG	CD-NE-CZ	5.29	131.81	124.40
1	C	748	ILE	N-CA-C	5.28	117.69	111.09
1	D	751	ILE	CA-C-O	5.28	127.02	119.95
1	A	185	PHE	CA-CB-CG	5.28	119.08	113.80
1	D	471	ARG	N-CA-C	5.28	118.34	109.95
1	A	431	ILE	CA-C-N	5.27	126.43	119.84
1	A	431	ILE	C-N-CA	5.27	126.43	119.84
1	B	349	PHE	CA-C-N	-5.27	113.90	122.65
1	B	349	PHE	C-N-CA	-5.27	113.90	122.65
1	D	57	ALA	CA-C-N	5.27	125.08	119.28
1	D	57	ALA	C-N-CA	5.27	125.08	119.28
1	D	636	ARG	CA-C-O	-5.26	115.82	121.45
1	B	586	PRO	N-CA-CB	5.25	108.73	103.48
1	D	431	ILE	CA-C-N	5.25	126.40	119.84
1	D	431	ILE	C-N-CA	5.25	126.40	119.84
1	C	438	CYS	CA-C-N	5.24	125.16	119.76
1	C	438	CYS	C-N-CA	5.24	125.16	119.76
1	D	740	ARG	NE-CZ-NH1	5.24	126.74	121.50
1	C	102	PRO	N-CA-CB	5.24	108.21	103.34
1	B	609	ASP	CA-CB-CG	5.23	117.83	112.60
1	B	585	ASP	CA-C-N	5.23	124.89	119.56
1	B	585	ASP	C-N-CA	5.23	124.89	119.56
1	D	586	PRO	N-CA-CB	5.23	108.71	103.48
1	C	405	ASP	CA-C-N	5.22	125.30	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	405	ASP	C-N-CA	5.22	125.30	119.87
1	C	246	GLN	OE1-CD-NE2	-5.21	117.39	122.60
1	A	631	LYS	N-CA-CB	5.20	118.93	110.77
1	D	447	GLY	N-CA-C	-5.18	106.21	112.48
1	B	156	PRO	N-CA-CB	5.18	108.66	103.48
1	A	339	GLN	N-CA-C	-5.17	100.31	108.73
1	A	37	ARG	CA-C-N	5.16	125.41	119.83
1	A	37	ARG	C-N-CA	5.16	125.41	119.83
1	C	415	TYR	CA-CB-CG	5.16	123.19	113.90
1	C	52	PRO	N-CA-CB	5.16	107.84	103.19
1	D	521	ARG	CG-CD-NE	5.16	123.36	112.00
1	C	392	HIS	CA-CB-CG	5.16	118.96	113.80
1	A	82	THR	N-CA-C	-5.15	103.24	110.35
1	A	263	PRO	N-CA-CB	5.15	108.12	103.33
1	B	139	GLN	OE1-CD-NE2	5.15	127.75	122.60
1	D	72	ARG	N-CA-CB	5.15	117.52	109.85
1	A	466	ASN	N-CA-C	-5.14	105.30	112.30
1	A	593	ILE	CA-C-N	5.14	125.43	119.93
1	A	593	ILE	C-N-CA	5.14	125.43	119.93
1	A	386	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	D	42	PRO	N-CA-CB	5.13	107.80	103.19
1	A	217	PHE	CA-CB-CG	-5.12	108.67	113.80
1	A	361	PRO	N-CA-CB	5.12	107.76	103.25
1	C	516	THR	CA-C-N	5.12	124.73	119.05
1	C	516	THR	C-N-CA	5.12	124.73	119.05
1	C	608	ASN	CA-C-O	-5.11	115.57	121.49
1	B	419	GLN	CG-CD-OE1	-5.10	110.60	120.80
1	B	377	ARG	CA-CB-CG	-5.10	103.90	114.10
1	B	392	HIS	CG-ND1-CE1	5.10	117.97	109.30
1	C	475	PRO	N-CA-CB	5.10	107.79	103.35
1	A	636	ARG	CA-C-O	-5.08	116.02	121.45
1	D	612	ARG	CG-CD-NE	5.06	123.12	112.00
1	A	456	ASN	CA-C-N	5.05	124.84	119.28
1	A	456	ASN	C-N-CA	5.05	124.84	119.28
1	A	77	ASN	CA-CB-CG	-5.04	107.56	112.60
1	D	374	VAL	CA-C-O	-5.04	115.14	120.39
1	D	725	ASP	CA-CB-CG	5.04	117.64	112.60
1	C	585	ASP	CA-C-N	5.04	124.70	119.56
1	C	585	ASP	C-N-CA	5.04	124.70	119.56
1	B	516	THR	CA-C-N	5.04	124.64	119.05
1	B	516	THR	C-N-CA	5.04	124.64	119.05
1	A	392	HIS	ND1-CG-CD2	-5.03	101.07	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	749	ASP	CA-CB-CG	-5.03	107.57	112.60
1	B	210	ASP	CA-CB-CG	5.03	117.63	112.60
1	B	374	VAL	CA-C-O	-5.03	115.16	120.39
1	D	155	ASP	CA-C-N	5.02	124.68	119.56
1	D	155	ASP	C-N-CA	5.02	124.68	119.56
1	A	436	PRO	CB-CA-C	-5.02	104.81	111.23
1	B	62	ASN	CA-CB-CG	5.01	117.61	112.60
1	D	456	ASN	CA-C-N	5.00	124.78	119.28
1	D	456	ASN	C-N-CA	5.00	124.78	119.28

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	5747	0	5580	45	0
1	B	5747	0	5580	72	0
1	C	5747	0	5580	56	0
1	D	5747	0	5580	56	0
2	A	44	0	31	5	0
2	B	44	0	31	4	0
2	C	44	0	31	6	0
2	D	44	0	31	2	0
3	A	815	0	0	5	1
3	B	702	0	0	6	1
3	C	768	0	0	8	0
3	D	787	0	0	7	0
All	All	26236	0	22444	220	1

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 5.

All (220) 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:B:392:HIS:ND1	1:B:415:TYR:HB2	1.38	1.39
1:A:392:HIS:ND1	1:A:415:TYR:HB2	1.40	1.35
1:C:392:HIS:ND1	1:C:415:TYR:HB2	1.42	1.32
1:D:392:HIS:ND1	1:D:415:TYR:HB2	1.39	1.31
1:A:451:MET:HE2	1:C:451:MET:HE2	1.32	1.07
1:B:451:MET:HE2	1:D:451:MET:HE2	1.36	1.03
1:C:392:HIS:ND1	1:C:415:TYR:CB	2.33	0.89
1:A:392:HIS:ND1	1:A:415:TYR:CB	2.34	0.86
1:B:392:HIS:ND1	1:B:415:TYR:CB	2.34	0.85
1:D:392:HIS:ND1	1:D:415:TYR:CB	2.35	0.80
1:D:750:LYS:HD3	1:D:751:ILE:H	1.48	0.77
1:B:583:LYS:H	1:B:583:LYS:NZ	1.82	0.77
1:C:392:HIS:CG	1:C:415:TYR:HB2	2.22	0.75
1:B:710:ILE:HD13	1:B:718:ILE:HG13	1.69	0.74
1:C:748:ILE:O	1:C:751:ILE:HG22	1.89	0.73
2:A:760:HDD:HMC1	2:A:760:HDD:HBC1	1.73	0.69
1:B:583:LYS:H	1:B:583:LYS:HZ3	1.40	0.69
1:C:267:ARG:HG3	3:C:3862:HOH:O	1.94	0.67
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.24	0.67
1:A:181:GLU:HG2	3:A:4194:HOH:O	1.94	0.67
1:D:27:ASP:O	1:D:28:SER:HB2	1.94	0.66
1:A:392:HIS:CG	1:A:415:TYR:HB2	2.29	0.66
1:A:28:SER:HB2	1:D:245:LEU:HD13	1.78	0.65
1:B:267:ARG:HG3	3:B:2872:HOH:O	1.95	0.65
1:B:533:LYS:HE2	3:B:4201:HOH:O	1.96	0.65
1:B:51:ALA:HB1	1:B:52:PRO:HD2	1.79	0.64
1:B:521:ARG:NH2	1:B:745:ILE:HD13	2.13	0.63
1:B:583:LYS:O	1:B:584:LYS:HB3	1.98	0.63
1:D:392:HIS:CG	1:D:415:TYR:HB2	2.28	0.62
1:A:690:LYS:HG3	1:A:751:ILE:HD11	1.80	0.62
1:D:552:LEU:HD11	1:D:571:LEU:HD23	1.81	0.62
1:A:709:LYS:HA	1:A:709:LYS:HE3	1.81	0.62
1:C:552:LEU:HD21	1:C:571:LEU:HD12	1.83	0.61
1:D:546:GLN:HG3	3:D:3688:HOH:O	2.00	0.61
1:A:245:LEU:HD13	1:D:29:LEU:HD13	1.84	0.60
1:B:552:LEU:HD22	1:B:556:GLN:HG3	1.82	0.60
1:B:612:ARG:HD3	1:B:670:GLY:HA2	1.82	0.60
2:B:760:HDD:HMC1	2:B:760:HDD:HBC1	1.83	0.60
1:C:745:ILE:HD13	3:C:3866:HOH:O	2.00	0.60
1:C:274:ILE:HD12	2:C:760:HDD:HMB1	1.84	0.59
1:C:583:LYS:O	1:C:584:LYS:HB3	2.02	0.59
1:C:521:ARG:HG2	3:C:3866:HOH:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:748:ILE:O	1:B:751:ILE:HG22	2.03	0.59
1:B:281:ASN:OD1	1:B:283:GLU:HG3	2.03	0.59
2:A:760:HDD:HMB1	2:A:760:HDD:HBB1	1.85	0.58
1:A:748:ILE:O	1:A:751:ILE:HG13	2.03	0.58
1:C:477:PRO:HB2	1:C:478:LYS:HD3	1.86	0.58
1:A:750:LYS:O	1:A:750:LYS:HE3	2.04	0.57
1:D:431:ILE:HD11	3:D:4022:HOH:O	2.04	0.57
1:B:37:ARG:HD2	3:B:3832:HOH:O	2.04	0.57
1:D:51:ALA:HB1	1:D:52:PRO:HD2	1.88	0.56
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.20	0.56
1:D:629:HIS:HD2	3:D:2510:HOH:O	1.88	0.56
1:A:51:ALA:HB1	1:A:52:PRO:HD2	1.88	0.55
1:B:359:LEU:H	1:B:507:HIS:HD2	1.52	0.55
1:D:750:LYS:HD3	1:D:751:ILE:N	2.20	0.55
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.89	0.55
1:C:578:ASP:HB2	1:C:582:LEU:O	2.07	0.55
1:D:583:LYS:NZ	1:D:583:LYS:HB2	2.22	0.55
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.89	0.54
1:D:535:VAL:O	1:D:537:PRO:HD3	2.06	0.54
1:A:36:HIS:CD2	1:A:36:HIS:H	2.26	0.54
1:B:392:HIS:CG	1:B:415:TYR:HB2	2.34	0.53
1:C:535:VAL:O	1:C:537:PRO:HD3	2.08	0.53
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.90	0.53
1:B:521:ARG:NH2	1:B:745:ILE:HG21	2.24	0.53
1:B:535:VAL:O	1:B:537:PRO:HD3	2.09	0.53
1:A:27:ASP:O	1:A:28:SER:C	2.51	0.53
1:B:634:TYR:O	1:B:653:THR:HA	2.08	0.53
1:A:708:ILE:O	1:A:710:ILE:HG22	2.09	0.52
1:C:610:GLU:OE1	1:C:643:ASP:HA	2.09	0.52
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.92	0.52
1:D:274:ILE:HD12	2:D:760:HDD:HMB1	1.92	0.52
1:D:278:ARG:HH12	1:D:487:GLU:CD	2.17	0.52
1:C:443:PHE:CZ	1:C:470:PRO:HD2	2.45	0.52
1:B:603:VAL:HG11	1:B:666:ILE:HD12	1.92	0.51
1:C:704:PHE:O	1:C:707:THR:HG22	2.11	0.51
1:D:61:ARG:HH11	1:D:66:ASN:HA	1.76	0.51
1:A:443:PHE:CZ	1:A:470:PRO:HD2	2.45	0.51
2:C:760:HDD:HMB1	2:C:760:HDD:HBB1	1.93	0.51
1:C:359:LEU:H	1:C:507:HIS:HD2	1.59	0.51
1:D:443:PHE:CZ	1:D:470:PRO:HD2	2.46	0.51
2:B:760:HDD:HBB1	2:B:760:HDD:HMB1	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:748:ILE:O	1:D:751:ILE:HG22	2.12	0.50
1:A:751:ILE:O	1:A:751:ILE:HD12	2.12	0.50
1:B:708:ILE:HG13	1:B:710:ILE:HD12	1.93	0.50
1:A:682:ASN:HB3	1:A:707:THR:HG21	1.94	0.50
3:A:3472:HOH:O	1:C:27:ASP:HB3	2.10	0.50
1:A:457:PRO:HG2	1:C:37:ARG:HH21	1.77	0.50
1:A:144:LEU:HD11	1:A:370:VAL:HG13	1.94	0.50
1:A:750:LYS:HE3	1:A:750:LYS:C	2.36	0.50
1:D:577:PRO:HG2	3:D:4041:HOH:O	2.11	0.50
1:B:578:ASP:HB3	1:B:582:LEU:O	2.11	0.49
1:A:538:TYR:CE2	1:D:31:PRO:HG3	2.47	0.49
1:B:629:HIS:HD2	3:B:1690:HOH:O	1.95	0.49
1:C:629:HIS:HD2	3:C:2098:HOH:O	1.95	0.49
1:A:689:TYR:OH	1:A:710:ILE:HG21	2.13	0.49
1:C:745:ILE:O	1:C:748:ILE:HG12	2.12	0.49
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.96	0.49
1:C:607:LEU:HD22	1:C:611:VAL:HG21	1.95	0.49
2:C:760:HDD:HBC1	2:C:760:HDD:HMC3	1.95	0.48
1:D:341:ILE:HG13	3:D:3967:HOH:O	2.14	0.48
1:D:616:LEU:HD22	1:D:620:LEU:HG	1.95	0.48
1:B:76:GLU:O	1:B:77:ASN:HB2	2.14	0.48
1:A:603:VAL:HG11	1:A:666:ILE:HD12	1.96	0.48
1:D:61:ARG:NH1	1:D:66:ASN:HA	2.29	0.48
1:C:747:LYS:HE2	3:C:3968:HOH:O	2.13	0.47
1:B:50:THR:HG21	1:C:227:TRP:CZ3	2.49	0.47
1:B:222:LYS:HB3	1:B:223:PRO:HD2	1.96	0.47
1:B:443:PHE:CZ	1:B:470:PRO:HD2	2.48	0.47
2:A:760:HDD:HBC1	2:A:760:HDD:CMC	2.42	0.47
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.96	0.47
1:A:457:PRO:HG2	1:C:37:ARG:NH2	2.29	0.47
1:B:745:ILE:O	1:B:748:ILE:HG12	2.15	0.47
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.30	0.47
1:D:144:LEU:HD11	1:D:370:VAL:HG13	1.96	0.47
1:A:745:ILE:N	1:A:746:PRO:HD2	2.30	0.47
1:B:274:ILE:HD12	2:B:760:HDD:HMB1	1.96	0.47
3:A:1180:HOH:O	1:C:52:PRO:HG3	2.15	0.46
1:B:29:LEU:HG	3:B:3519:HOH:O	2.14	0.46
1:A:612:ARG:HE	1:A:669:CYS:HB3	1.79	0.46
3:B:1590:HOH:O	1:D:52:PRO:HG3	2.16	0.46
1:B:359:LEU:H	1:B:507:HIS:CD2	2.31	0.46
1:B:604:ALA:HB2	1:B:662:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:PRO:HG2	1:B:55:LEU:HD12	1.97	0.46
1:C:201:ASN:CG	2:C:760:HDD:HMB2	2.41	0.46
1:C:612:ARG:CZ	1:C:612:ARG:HB2	2.45	0.46
1:A:471:ARG:CZ	1:C:27:ASP:HA	2.46	0.45
1:C:211:ALA:CB	1:C:410:GLY:HA3	2.46	0.45
1:A:294:LYS:NZ	3:A:2181:HOH:O	2.49	0.45
2:A:760:HDD:HMC1	2:A:760:HDD:CBC	2.44	0.45
1:D:359:LEU:H	1:D:507:HIS:HD2	1.64	0.45
1:A:708:ILE:O	1:A:709:LYS:C	2.59	0.45
1:B:562:LEU:HA	1:C:637:MET:HB2	1.99	0.45
1:B:725:ASP:OD2	1:B:727:SER:N	2.49	0.45
1:D:583:LYS:HB2	1:D:583:LYS:HZ2	1.80	0.45
1:A:612:ARG:NH2	3:A:4124:HOH:O	2.49	0.45
1:B:521:ARG:HH21	1:B:745:ILE:HD13	1.78	0.45
1:C:359:LEU:H	1:C:507:HIS:CD2	2.35	0.45
2:C:760:HDD:HBC1	2:C:760:HDD:CMC	2.47	0.45
1:B:461:GLU:HA	1:B:462:PRO:C	2.42	0.45
1:D:634:TYR:O	1:D:653:THR:HA	2.17	0.45
1:C:51:ALA:HB1	1:C:52:PRO:HD2	1.98	0.44
1:C:309:LYS:HB3	1:C:660:LEU:HD21	1.98	0.44
1:D:521:ARG:HH11	1:D:521:ARG:HD3	1.56	0.44
1:D:146:ASP:HB2	3:D:3343:HOH:O	2.18	0.44
1:B:468:ASN:HD22	1:D:27:ASP:N	2.14	0.44
2:D:760:HDD:HMB1	2:D:760:HDD:HBB1	1.98	0.44
1:B:411:ARG:HG2	2:B:760:HDD:C2C	2.47	0.44
1:B:404:ASN:O	1:B:405:ASP:C	2.61	0.44
1:D:598:VAL:HG13	1:D:628:VAL:CG2	2.48	0.44
1:A:38:PRO:HG2	1:A:51:ALA:HB2	1.99	0.44
1:C:359:LEU:HD12	1:C:359:LEU:C	2.43	0.44
1:D:624:LYS:HD3	1:D:624:LYS:C	2.43	0.44
1:C:73:LYS:HD2	3:C:3629:HOH:O	2.17	0.43
1:C:616:LEU:O	1:C:620:LEU:HG	2.18	0.43
1:C:660:LEU:HD13	1:C:687:GLU:CD	2.43	0.43
1:D:404:ASN:O	1:D:405:ASP:C	2.60	0.43
1:D:669:CYS:SG	1:D:670:GLY:N	2.89	0.43
1:A:418:THR:HG21	2:A:760:HDD:HBD2	2.00	0.43
1:A:404:ASN:O	1:A:405:ASP:C	2.59	0.43
1:B:459:ASN:H	1:B:459:ASN:HD22	1.67	0.43
1:D:583:LYS:O	1:D:584:LYS:HB3	2.19	0.43
1:B:278:ARG:HH22	1:B:487:GLU:CD	2.27	0.43
1:B:48:GLN:HB3	1:B:49:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:552:LEU:C	1:C:552:LEU:HD13	2.44	0.43
1:D:552:LEU:HD11	1:D:571:LEU:CD2	2.49	0.43
1:A:603:VAL:HG11	1:A:666:ILE:CD1	2.49	0.43
1:C:404:ASN:O	1:C:405:ASP:C	2.60	0.43
1:B:29:LEU:HD12	1:D:468:ASN:HB2	2.00	0.42
1:D:605:ILE:HD12	1:D:630:ALA:HB1	2.00	0.42
1:A:335:GLU:OE1	1:A:369:ARG:HD3	2.19	0.42
1:C:516:THR:HB	1:C:517:PRO:CD	2.49	0.42
1:B:438:CYS:HB2	1:B:439:PRO:HD2	2.00	0.42
1:B:521:ARG:HH21	1:B:521:ARG:HD2	1.60	0.42
1:B:745:ILE:HB	1:B:746:PRO:HD3	2.01	0.42
1:A:461:GLU:HA	1:A:462:PRO:C	2.43	0.42
1:B:344:GLU:H	1:B:344:GLU:CD	2.27	0.42
1:B:669:CYS:SG	1:B:670:GLY:N	2.90	0.42
1:C:155:ASP:HA	1:C:156:PRO:HD2	1.86	0.42
1:D:278:ARG:HH21	1:D:278:ARG:HD2	1.74	0.42
1:B:521:ARG:HH21	1:B:745:ILE:HG21	1.85	0.42
1:B:207:PHE:O	1:B:249:THR:HA	2.20	0.42
1:A:313:ARG:NH1	1:D:309:LYS:HD2	2.35	0.41
1:A:417:ASP:OD2	1:D:118:ASP:OD1	2.38	0.41
1:B:44:PRO:HB3	1:B:629:HIS:CD2	2.56	0.41
1:B:359:LEU:HD12	1:B:359:LEU:C	2.45	0.41
1:B:252:ASN:HD22	1:B:252:ASN:HA	1.61	0.41
1:A:214:PHE:HB3	1:A:215:PRO:HD3	2.02	0.41
1:A:169:VAL:HB	1:A:181:GLU:OE2	2.20	0.41
1:B:211:ALA:CB	1:B:410:GLY:HA3	2.51	0.41
1:C:411:ARG:HG2	2:C:760:HDD:C2C	2.51	0.41
1:C:750:LYS:HA	1:C:750:LYS:HD3	1.86	0.41
1:D:703:LYS:HE2	3:D:3690:HOH:O	2.19	0.41
1:B:139:GLN:HG2	1:B:156:PRO:O	2.20	0.41
1:C:516:THR:HB	1:C:517:PRO:HD2	2.03	0.41
1:C:37:ARG:NH1	3:C:2821:HOH:O	2.54	0.41
1:A:222:LYS:HB3	1:A:223:PRO:HD2	2.02	0.41
1:B:36:HIS:H	1:B:36:HIS:HD1	1.67	0.41
1:B:37:ARG:HA	1:B:38:PRO:HD3	1.88	0.41
1:B:97:ALA:O	1:B:101:GLY:HA3	2.20	0.41
1:B:469:TRP:HA	1:B:470:PRO:C	2.45	0.41
1:C:100:ARG:HH11	1:C:100:ARG:HD3	1.78	0.41
1:C:751:ILE:HD12	3:C:3317:HOH:O	2.20	0.41
1:D:97:ALA:O	1:D:101:GLY:HA3	2.21	0.41
1:D:169:VAL:HB	1:D:181:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:693:LYS:HA	1:D:694:PRO:HD3	1.86	0.41
1:A:37:ARG:HA	1:A:38:PRO:HD3	1.89	0.41
1:A:596:GLY:HA3	1:A:737:ALA:O	2.21	0.41
1:C:488:ARG:HE	1:C:488:ARG:HB2	1.59	0.40
1:B:37:ARG:NH1	1:D:466:ASN:OD1	2.54	0.40
1:B:116:HIS:CD2	1:D:426:PRO:HB2	2.57	0.40
1:B:235:ALA:HB1	1:B:533:LYS:HD3	2.03	0.40
1:B:331:PHE:HA	1:B:332:PRO:HD3	1.89	0.40
1:B:211:ALA:HB3	1:B:410:GLY:HA3	2.02	0.40
1:D:148:THR:HB	1:D:279:LEU:HB3	2.03	0.40
1:B:73:LYS:HD3	1:D:441:HIS:CD2	2.56	0.40
1:C:32:GLU:OE1	1:C:32:GLU:HA	2.21	0.40
1:D:552:LEU:HD22	1:D:552:LEU:HA	1.85	0.40
1:C:335:GLU:OE2	1:C:369:ARG:NH2	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1050:HOH:O	3:B:3904:HOH:O[2_747]	1.45	0.75

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	725/753 (96%)	699 (96%)	22 (3%)	4 (1%)	21	11
1	B	725/753 (96%)	699 (96%)	22 (3%)	4 (1%)	21	11
1	C	725/753 (96%)	703 (97%)	21 (3%)	1 (0%)	48	38
1	D	725/753 (96%)	700 (97%)	21 (3%)	4 (1%)	21	11
All	All	2900/3012 (96%)	2801 (97%)	86 (3%)	13 (0%)	30	19

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	709	LYS
1	B	28	SER
1	D	28	SER
1	D	750	LYS
1	D	751	ILE
1	B	725	ASP
1	A	75	SER
1	A	711	ALA
1	C	75	SER
1	B	75	SER
1	B	584	LYS
1	D	75	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	612/636 (96%)	595 (97%)	17 (3%)	38	21
1	B	612/636 (96%)	585 (96%)	27 (4%)	25	9
1	C	612/636 (96%)	583 (95%)	29 (5%)	23	7
1	D	612/636 (96%)	583 (95%)	29 (5%)	23	7
All	All	2448/2544 (96%)	2346 (96%)	102 (4%)	26	10

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	73	LYS
1	A	191	THR
1	A	198	LEU
1	A	205	ILE
1	A	252	ASN
1	A	294	LYS

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Mol	Chain	Res	Type
1	A	375	LEU
1	A	415	TYR
1	A	432	PRO
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	593	ILE
1	A	709	LYS
1	A	712	ASP
1	A	750	LYS
1	B	27	ASP
1	B	28	SER
1	B	37	ARG
1	B	181	GLU
1	B	191	THR
1	B	198	LEU
1	B	205	ILE
1	B	252	ASN
1	B	321	GLU
1	B	344	GLU
1	B	370	VAL
1	B	375	LEU
1	B	415	TYR
1	B	440	TYR
1	B	459	ASN
1	B	552	LEU
1	B	562	LEU
1	B	565	GLU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	610	GLU
1	B	633	LEU
1	B	709	LYS
1	B	749	ASP
1	B	750	LYS
1	B	751	ILE
1	C	37	ARG
1	C	159	ILE
1	C	181	GLU
1	C	205	ILE
1	C	252	ASN

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Mol	Chain	Res	Type
1	C	285	LYS
1	C	375	LEU
1	C	377	ARG
1	C	415	TYR
1	C	440	TYR
1	C	459	ASN
1	C	478	LYS
1	C	488	ARG
1	C	521	ARG
1	C	531	LEU
1	C	568	ASP
1	C	571	LEU
1	C	584	LYS
1	C	593	ILE
1	C	606	LEU
1	C	612	ARG
1	C	616	LEU
1	C	633	LEU
1	C	648	LEU
1	C	660	LEU
1	C	685	LEU
1	C	725	ASP
1	C	733	LEU
1	C	750	LYS
1	D	28	SER
1	D	41	GLU
1	D	48	GLN
1	D	73	LYS
1	D	181	GLU
1	D	191	THR
1	D	205	ILE
1	D	252	ASN
1	D	340	LEU
1	D	344	GLU
1	D	375	LEU
1	D	415	TYR
1	D	440	TYR
1	D	459	ASN
1	D	490	GLU
1	D	552	LEU
1	D	554	LEU
1	D	582	LEU

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Mol	Chain	Res	Type
1	D	583	LYS
1	D	598	VAL
1	D	616	LEU
1	D	633	LEU
1	D	648	LEU
1	D	708	ILE
1	D	713	GLN
1	D	747	LYS
1	D	749	ASP
1	D	750	LYS
1	D	751	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	252	ASN
1	A	449	HIS
1	A	459	ASN
1	A	515	GLN
1	A	556	GLN
1	A	713	GLN
1	B	84	GLN
1	B	157	ASN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	546	GLN
1	B	629	HIS
1	C	252	ASN
1	C	459	ASN
1	C	486	GLN
1	C	507	HIS
1	C	546	GLN
1	C	556	GLN
1	C	572	ASN
1	C	629	HIS
1	D	48	GLN
1	D	252	ASN
1	D	459	ASN
1	D	507	HIS
1	D	556	GLN

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Mol	Chain	Res	Type
1	D	629	HIS
1	D	671	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 ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HDD	B	760	3,1	46,52,52	2.98	20 (43%)	62,89,89	4.00	36 (58%)
2	HDD	A	760	3,1	46,52,52	3.10	16 (34%)	62,89,89	3.91	38 (61%)
2	HDD	D	760	3,1	46,52,52	3.16	17 (36%)	62,89,89	4.19	35 (56%)
2	HDD	C	760	3,1	46,52,52	3.10	17 (36%)	62,89,89	3.90	35 (56%)

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	HDD	B	760	3,1	-	2/9/89/89	0/1/9/9
2	HDD	A	760	3,1	-	2/9/89/89	0/1/9/9
2	HDD	D	760	3,1	-	2/9/89/89	0/1/9/9
2	HDD	C	760	3,1	-	2/9/89/89	0/1/9/9

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	760	HDD	CMD-C2D	11.71	1.69	1.53
2	B	760	HDD	C3D-C2D	-11.50	1.27	1.55
2	C	760	HDD	C3D-C2D	-11.38	1.28	1.55
2	A	760	HDD	C3D-C2D	-10.96	1.29	1.55
2	D	760	HDD	C3D-C2D	-10.94	1.29	1.55
2	C	760	HDD	CAD-C3D	-10.49	1.35	1.53
2	A	760	HDD	CAD-C3D	10.25	1.71	1.53
2	B	760	HDD	O1D-C3D	7.99	1.59	1.46
2	C	760	HDD	O1D-C3D	7.63	1.59	1.46
2	A	760	HDD	O1D-C3D	7.26	1.58	1.46
2	D	760	HDD	O1D-C3D	6.97	1.57	1.46
2	B	760	HDD	CMD-C2D	6.75	1.62	1.53
2	A	760	HDD	OND-C2D	5.88	1.53	1.42
2	D	760	HDD	OND-C2D	5.52	1.53	1.42
2	B	760	HDD	OND-C2D	4.96	1.52	1.42
2	C	760	HDD	OND-C2D	4.40	1.51	1.42
2	B	760	HDD	CAD-C3D	3.63	1.60	1.53
2	D	760	HDD	O1D-CGD	-3.62	1.30	1.35
2	B	760	HDD	O1D-CGD	-3.30	1.30	1.35
2	C	760	HDD	CMC-C2C	3.27	1.57	1.50
2	C	760	HDD	CAB-C3B	3.09	1.55	1.47
2	A	760	HDD	C4A-C3A	3.06	1.50	1.43
2	D	760	HDD	CMC-C2C	3.05	1.57	1.50
2	A	760	HDD	CMC-C2C	3.03	1.57	1.50
2	C	760	HDD	C4A-C3A	2.99	1.50	1.43
2	B	760	HDD	C4A-C3A	2.98	1.50	1.43
2	D	760	HDD	C1A-C2A	2.92	1.50	1.44
2	A	760	HDD	C1B-NB	-2.91	1.34	1.39
2	C	760	HDD	CMD-C2D	2.88	1.57	1.53
2	C	760	HDD	CBA-CGA	2.86	1.57	1.50
2	B	760	HDD	CMC-C2C	2.86	1.56	1.50
2	A	760	HDD	CBA-CGA	2.77	1.57	1.50
2	A	760	HDD	O1D-CGD	-2.76	1.31	1.35
2	B	760	HDD	CBA-CGA	2.71	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	760	HDD	CAC-C3C	2.71	1.54	1.47
2	C	760	HDD	C1B-NB	-2.70	1.34	1.39
2	B	760	HDD	C1A-C2A	2.59	1.49	1.44
2	A	760	HDD	CMB-C2B	2.59	1.56	1.50
2	D	760	HDD	CAB-C3B	2.52	1.54	1.47
2	B	760	HDD	CAB-C3B	2.48	1.54	1.47
2	A	760	HDD	O2A-CGA	-2.47	1.22	1.30
2	C	760	HDD	O1D-CGD	-2.47	1.31	1.35
2	A	760	HDD	C1A-C2A	2.46	1.49	1.44
2	A	760	HDD	C3C-C4C	2.46	1.49	1.42
2	D	760	HDD	CBA-CGA	2.45	1.56	1.50
2	B	760	HDD	C1B-NB	-2.44	1.35	1.39
2	B	760	HDD	CAC-C3C	2.44	1.53	1.47
2	C	760	HDD	CMB-C2B	2.44	1.55	1.50
2	D	760	HDD	C4A-C3A	2.43	1.48	1.43
2	C	760	HDD	C1A-C2A	2.40	1.49	1.44
2	C	760	HDD	CBA-CAA	2.39	1.60	1.51
2	D	760	HDD	C3C-C4C	2.37	1.49	1.42
2	D	760	HDD	CAC-C3C	2.35	1.53	1.47
2	D	760	HDD	C1B-NB	-2.35	1.35	1.39
2	B	760	HDD	C1C-C2C	2.34	1.48	1.43
2	B	760	HDD	CMB-C2B	2.27	1.55	1.50
2	B	760	HDD	C2A-C3A	-2.27	1.33	1.38
2	D	760	HDD	C2A-C3A	-2.22	1.33	1.38
2	B	760	HDD	C1D-ND	2.22	1.41	1.37
2	A	760	HDD	CAB-C3B	2.21	1.53	1.47
2	C	760	HDD	CAC-C3C	2.14	1.53	1.47
2	C	760	HDD	CHA-C4D	2.10	1.44	1.37
2	D	760	HDD	CMA-C3A	2.09	1.55	1.50
2	D	760	HDD	CHA-C4D	2.09	1.44	1.37
2	B	760	HDD	C4C-NC	-2.09	1.35	1.39
2	B	760	HDD	C3C-C4C	2.08	1.48	1.42
2	C	760	HDD	C3C-C4C	2.08	1.48	1.42
2	B	760	HDD	C3C-C2C	-2.05	1.34	1.41
2	A	760	HDD	CBA-CAA	2.03	1.59	1.51
2	D	760	HDD	CBA-CAA	2.02	1.58	1.51

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	760	HDD	OND-C2D-CMD	-12.56	85.17	109.45
2	D	760	HDD	C3D-O1D-CGD	12.52	122.82	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	760	HDD	OND-C2D-CMD	-11.06	88.06	109.45
2	B	760	HDD	C4B-C3B-C2B	10.45	115.88	106.81
2	C	760	HDD	CHD-C1D-ND	10.23	138.38	124.28
2	B	760	HDD	CHD-C1D-ND	10.17	138.31	124.28
2	D	760	HDD	C4B-C3B-C2B	9.90	115.40	106.81
2	A	760	HDD	C4B-C3B-C2B	9.67	115.20	106.81
2	A	760	HDD	CHD-C1D-ND	9.51	137.39	124.28
2	A	760	HDD	C3C-C4C-NC	-9.24	102.02	109.80
2	C	760	HDD	C4B-C3B-C2B	9.16	114.75	106.81
2	A	760	HDD	O1D-CGD-CBD	-9.14	101.83	110.17
2	C	760	HDD	CHC-C4B-NB	8.77	134.00	124.45
2	A	760	HDD	CBD-CAD-C3D	-8.34	92.09	103.98
2	D	760	HDD	O1D-CGD-O2D	7.91	127.47	120.81
2	D	760	HDD	CHD-C1D-ND	7.89	135.16	124.28
2	D	760	HDD	C3C-C4C-NC	-7.78	103.25	109.80
2	B	760	HDD	C3D-O1D-CGD	7.68	118.31	111.14
2	C	760	HDD	OND-C2D-CMD	-7.42	95.10	109.45
2	C	760	HDD	O1D-CGD-CBD	-7.33	103.48	110.17
2	B	760	HDD	CHC-C4B-NB	7.02	132.09	124.45
2	D	760	HDD	O1D-C3D-CAD	-6.98	90.15	103.06
2	B	760	HDD	C3B-C2B-C1B	-6.97	100.45	107.05
2	D	760	HDD	O1D-CGD-CBD	-6.92	103.86	110.17
2	A	760	HDD	CHC-C4B-NB	6.92	131.99	124.45
2	C	760	HDD	C3B-C2B-C1B	-6.83	100.58	107.05
2	B	760	HDD	C3C-C4C-NC	-6.56	104.28	109.80
2	D	760	HDD	C4B-NB-C1B	6.30	116.09	105.82
2	B	760	HDD	O1D-C3D-CAD	-6.08	91.81	103.06
2	C	760	HDD	C3C-C4C-NC	-6.04	104.71	109.80
2	D	760	HDD	CHC-C4B-NB	5.97	130.96	124.45
2	C	760	HDD	C2A-C1A-NA	-5.89	103.62	110.15
2	C	760	HDD	CHA-C4D-ND	-5.88	116.17	124.28
2	D	760	HDD	CBD-CAD-C3D	5.76	112.19	103.98
2	A	760	HDD	CHA-C4D-ND	-5.68	116.46	124.28
2	C	760	HDD	CBD-CAD-C3D	5.60	111.97	103.98
2	C	760	HDD	C3D-O1D-CGD	5.55	116.32	111.14
2	A	760	HDD	C4B-NB-C1B	5.41	114.63	105.82
2	C	760	HDD	C4B-NB-C1B	5.38	114.59	105.82
2	B	760	HDD	CHA-C4D-ND	-5.32	116.95	124.28
2	D	760	HDD	C3B-C2B-C1B	-5.20	102.12	107.05
2	D	760	HDD	C2A-C1A-NA	-5.17	104.42	110.15
2	B	760	HDD	C2D-C1D-CHD	-5.14	116.28	124.27
2	A	760	HDD	C3B-C2B-C1B	-5.11	102.21	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	760	HDD	C4C-CHD-C1D	-4.97	116.14	125.81
2	D	760	HDD	CHA-C4D-ND	-4.89	117.55	124.28
2	A	760	HDD	O1D-C3D-CAD	-4.87	94.05	103.06
2	C	760	HDD	CAB-C3B-C4B	-4.87	113.19	124.82
2	A	760	HDD	C2A-C1A-NA	-4.86	104.77	110.15
2	C	760	HDD	C4C-CHD-C1D	-4.83	116.42	125.81
2	A	760	HDD	C4C-CHD-C1D	-4.79	116.51	125.81
2	A	760	HDD	O2A-CGA-O1A	4.70	135.43	123.33
2	D	760	HDD	C4C-CHD-C1D	-4.63	116.80	125.81
2	A	760	HDD	C3D-O1D-CGD	4.57	115.41	111.14
2	B	760	HDD	C2A-C1A-NA	-4.57	105.08	110.15
2	B	760	HDD	O1D-CGD-CBD	-4.54	106.03	110.17
2	B	760	HDD	C4B-NB-C1B	4.46	113.10	105.82
2	B	760	HDD	O1D-CGD-O2D	4.45	124.56	120.81
2	D	760	HDD	CMD-C2D-C1D	4.43	120.19	112.68
2	C	760	HDD	CHB-C4A-NA	4.39	131.82	123.86
2	C	760	HDD	CHD-C4C-NC	4.32	131.70	123.86
2	A	760	HDD	CHC-C1C-NC	4.23	131.53	123.86
2	C	760	HDD	C1A-C2A-C3A	4.22	113.40	106.87
2	A	760	HDD	O1D-CGD-O2D	4.21	124.36	120.81
2	B	760	HDD	CAB-C3B-C4B	-4.17	114.87	124.82
2	C	760	HDD	O2A-CGA-O1A	4.07	133.79	123.33
2	B	760	HDD	CHC-C1C-NC	4.05	131.20	123.86
2	D	760	HDD	CHA-C1A-NA	4.02	131.15	123.86
2	A	760	HDD	C4C-NC-C1C	3.98	112.31	105.82
2	A	760	HDD	OND-C2D-CMD	-3.91	101.89	109.45
2	B	760	HDD	C4C-NC-C1C	3.90	112.18	105.82
2	C	760	HDD	C2D-C1D-CHD	-3.87	118.25	124.27
2	C	760	HDD	CMD-C2D-C3D	3.85	125.22	115.11
2	C	760	HDD	CAA-CBA-CGA	-3.83	103.50	113.67
2	A	760	HDD	C1A-C2A-C3A	3.79	112.74	106.87
2	D	760	HDD	O1A-CGA-CBA	-3.74	111.23	123.09
2	D	760	HDD	O2A-CGA-O1A	3.71	132.88	123.33
2	C	760	HDD	O1D-CGD-O2D	3.69	123.92	120.81
2	A	760	HDD	O1A-CGA-CBA	-3.68	111.42	123.09
2	A	760	HDD	C3D-C4D-CHA	3.67	134.80	124.14
2	A	760	HDD	CAA-CBA-CGA	-3.67	103.93	113.67
2	C	760	HDD	O1D-C3D-CAD	-3.64	96.32	103.06
2	C	760	HDD	C3D-C4D-CHA	3.63	134.68	124.14
2	B	760	HDD	CHD-C4C-NC	3.62	130.42	123.86
2	D	760	HDD	CAB-C3B-C4B	-3.52	116.41	124.82
2	D	760	HDD	C4C-NC-C1C	3.46	111.46	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	760	HDD	C1A-C2A-C3A	3.41	112.15	106.87
2	A	760	HDD	CHD-C4C-NC	3.37	129.97	123.86
2	A	760	HDD	CMA-C3A-C2A	3.36	132.75	125.62
2	D	760	HDD	CHD-C4C-NC	3.35	129.93	123.86
2	A	760	HDD	CHB-C4A-NA	3.34	129.91	123.86
2	C	760	HDD	C4A-C3A-C2A	-3.34	102.99	106.82
2	C	760	HDD	O1A-CGA-CBA	-3.33	112.52	123.09
2	A	760	HDD	C2C-C1C-NC	-3.33	104.81	110.14
2	A	760	HDD	C2D-C1D-CHD	-3.30	119.15	124.27
2	B	760	HDD	O1A-CGA-CBA	-3.25	112.77	123.09
2	D	760	HDD	CHB-C1B-NB	3.15	127.88	124.45
2	C	760	HDD	CMA-C3A-C2A	3.13	132.26	125.62
2	C	760	HDD	CHB-C4A-C3A	-3.12	118.36	127.43
2	B	760	HDD	O2A-CGA-O1A	3.08	131.25	123.33
2	C	760	HDD	C4C-C3C-C2C	3.05	111.10	107.30
2	A	760	HDD	OND-C2D-C3D	-3.04	103.33	110.46
2	D	760	HDD	CAA-CBA-CGA	-3.00	105.71	113.67
2	D	760	HDD	C1A-C2A-C3A	3.00	111.51	106.87
2	B	760	HDD	CAA-CBA-CGA	-2.99	105.73	113.67
2	C	760	HDD	OND-C2D-C3D	-2.98	103.48	110.46
2	A	760	HDD	CAB-C3B-C4B	-2.98	117.71	124.82
2	B	760	HDD	C4A-C3A-C2A	-2.95	103.44	106.82
2	D	760	HDD	C4C-C3C-C2C	2.94	110.96	107.30
2	D	760	HDD	OND-C2D-C3D	-2.91	103.63	110.46
2	A	760	HDD	C4C-C3C-C2C	2.90	110.91	107.30
2	D	760	HDD	C2D-C1D-CHD	-2.83	119.87	124.27
2	A	760	HDD	CMA-C3A-C4A	-2.81	121.13	125.42
2	D	760	HDD	CHC-C1C-NC	2.80	128.94	123.86
2	B	760	HDD	C3D-C4D-CHA	2.77	132.19	124.14
2	C	760	HDD	CHC-C1C-NC	2.75	128.84	123.86
2	B	760	HDD	CMD-C2D-C1D	2.74	117.33	112.68
2	B	760	HDD	CMA-C3A-C2A	2.72	131.40	125.62
2	D	760	HDD	C2C-C1C-NC	-2.72	105.78	110.14
2	A	760	HDD	CHB-C1B-NB	2.61	127.29	124.45
2	B	760	HDD	CHB-C4A-NA	2.60	128.58	123.86
2	A	760	HDD	C4A-C3A-C2A	-2.57	103.88	106.82
2	D	760	HDD	CAA-C2A-C1A	-2.55	119.95	124.94
2	B	760	HDD	C2C-C1C-NC	-2.54	106.08	110.14
2	C	760	HDD	C4C-NC-C1C	2.53	109.94	105.82
2	D	760	HDD	C4A-NA-C1A	2.52	109.93	105.82
2	D	760	HDD	C3D-C4D-CHA	2.51	131.42	124.14
2	A	760	HDD	CAA-C2A-C1A	-2.51	120.04	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	760	HDD	C4C-C3C-C2C	2.50	110.41	107.30
2	A	760	HDD	CBC-CAC-C3C	-2.43	115.38	127.53
2	A	760	HDD	CHB-C4A-C3A	-2.41	120.44	127.43
2	B	760	HDD	CHB-C4A-C3A	-2.40	120.45	127.43
2	C	760	HDD	C1C-CHC-C4B	-2.38	117.31	124.66
2	C	760	HDD	CMC-C2C-C1C	2.38	129.04	125.42
2	C	760	HDD	CBB-CAB-C3B	-2.29	116.07	127.53
2	B	760	HDD	CHA-C1A-NA	2.28	128.00	123.86
2	B	760	HDD	CHC-C1C-C2C	-2.19	121.08	127.43
2	B	760	HDD	CBD-CAD-C3D	2.16	107.07	103.98
2	B	760	HDD	CMD-C2D-C3D	2.16	120.80	115.11
2	D	760	HDD	CBC-CAC-C3C	-2.16	116.74	127.53
2	A	760	HDD	C4A-NA-C1A	2.16	109.34	105.82
2	A	760	HDD	C1A-CHA-C4D	2.16	129.99	125.81
2	D	760	HDD	CMB-C2B-C1B	2.10	128.43	124.73
2	B	760	HDD	CAA-C2A-C1A	-2.10	120.84	124.94

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	760	HDD	CAA-CBA-CGA-O1A
2	C	760	HDD	CAA-CBA-CGA-O2A
2	B	760	HDD	CAA-CBA-CGA-O2A
2	D	760	HDD	CAA-CBA-CGA-O2A
2	A	760	HDD	CAA-CBA-CGA-O1A
2	A	760	HDD	CAA-CBA-CGA-O2A
2	C	760	HDD	CAA-CBA-CGA-O1A
2	D	760	HDD	CAA-CBA-CGA-O1A

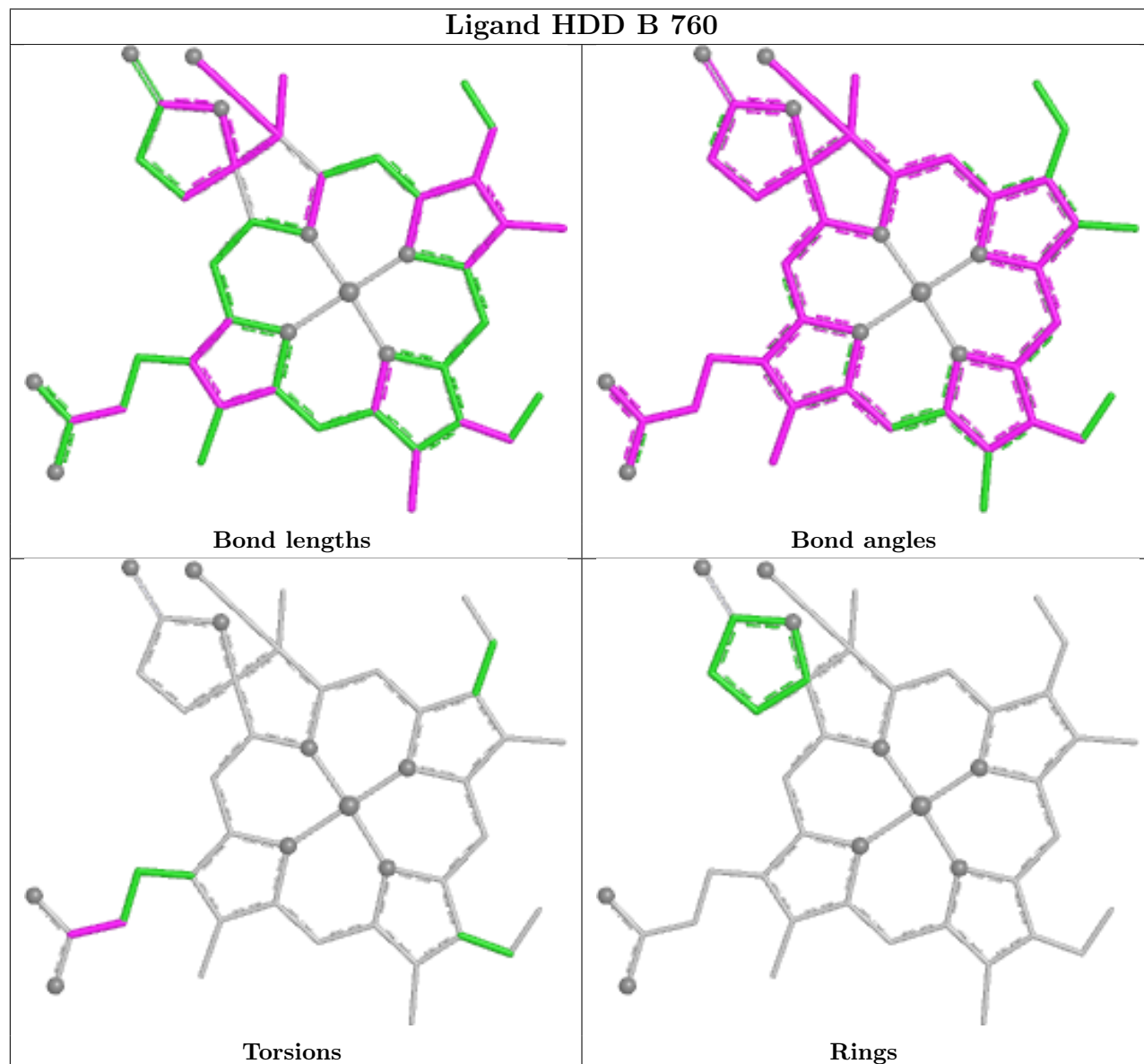
There are no ring outliers.

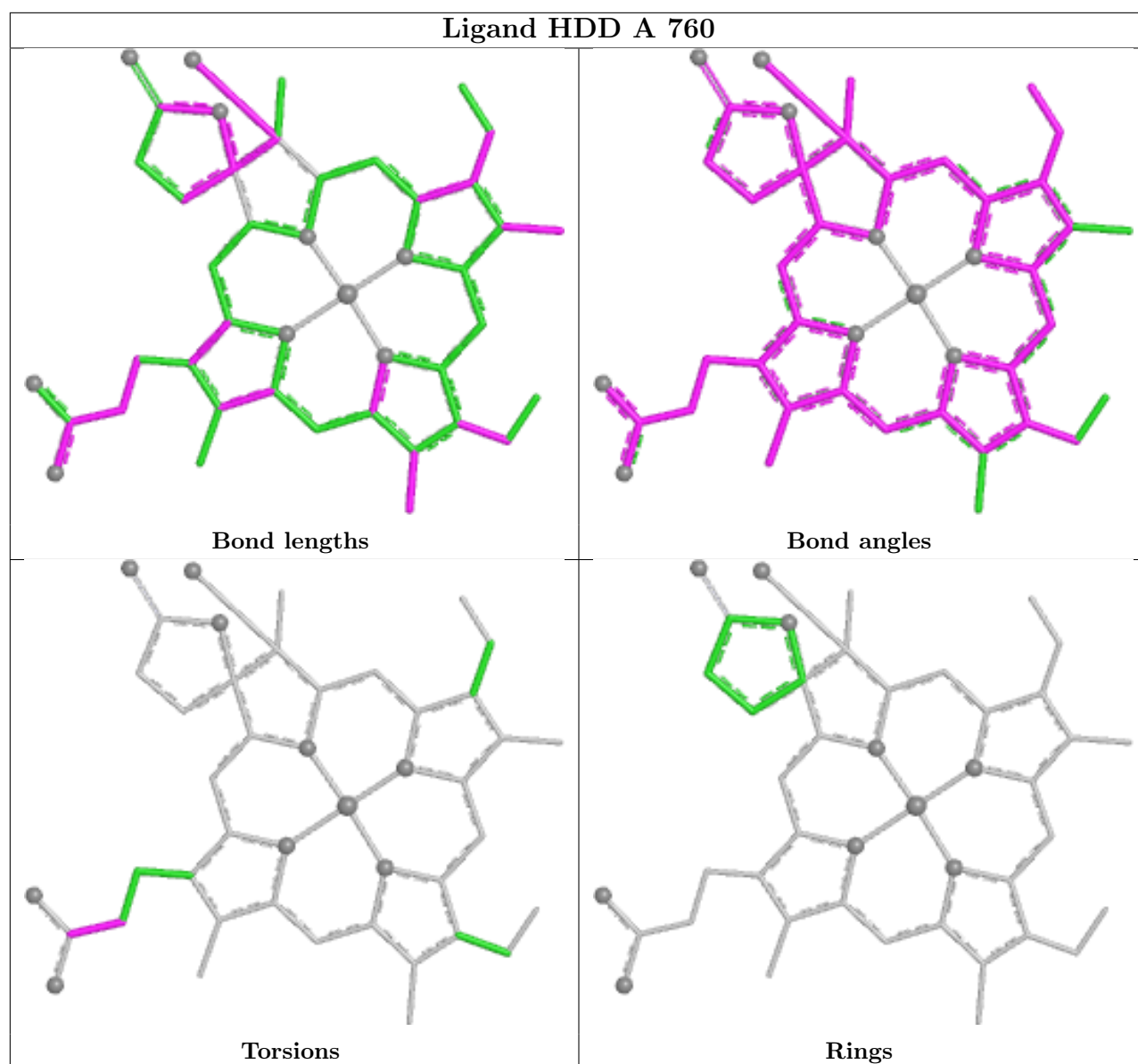
4 monomers are involved in 17 short contacts:

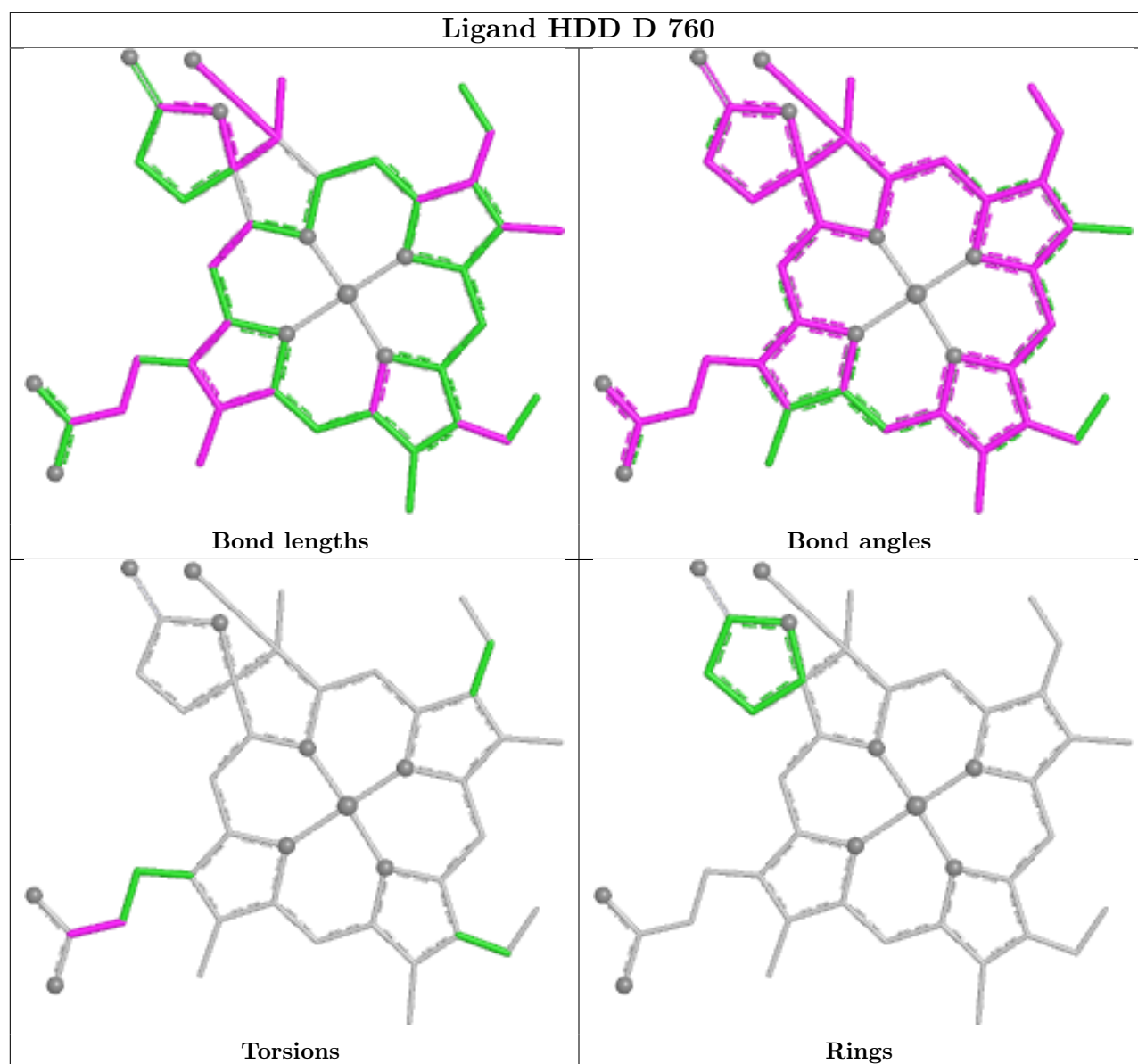
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	760	HDD	4	0
2	A	760	HDD	5	0
2	D	760	HDD	2	0
2	C	760	HDD	6	0

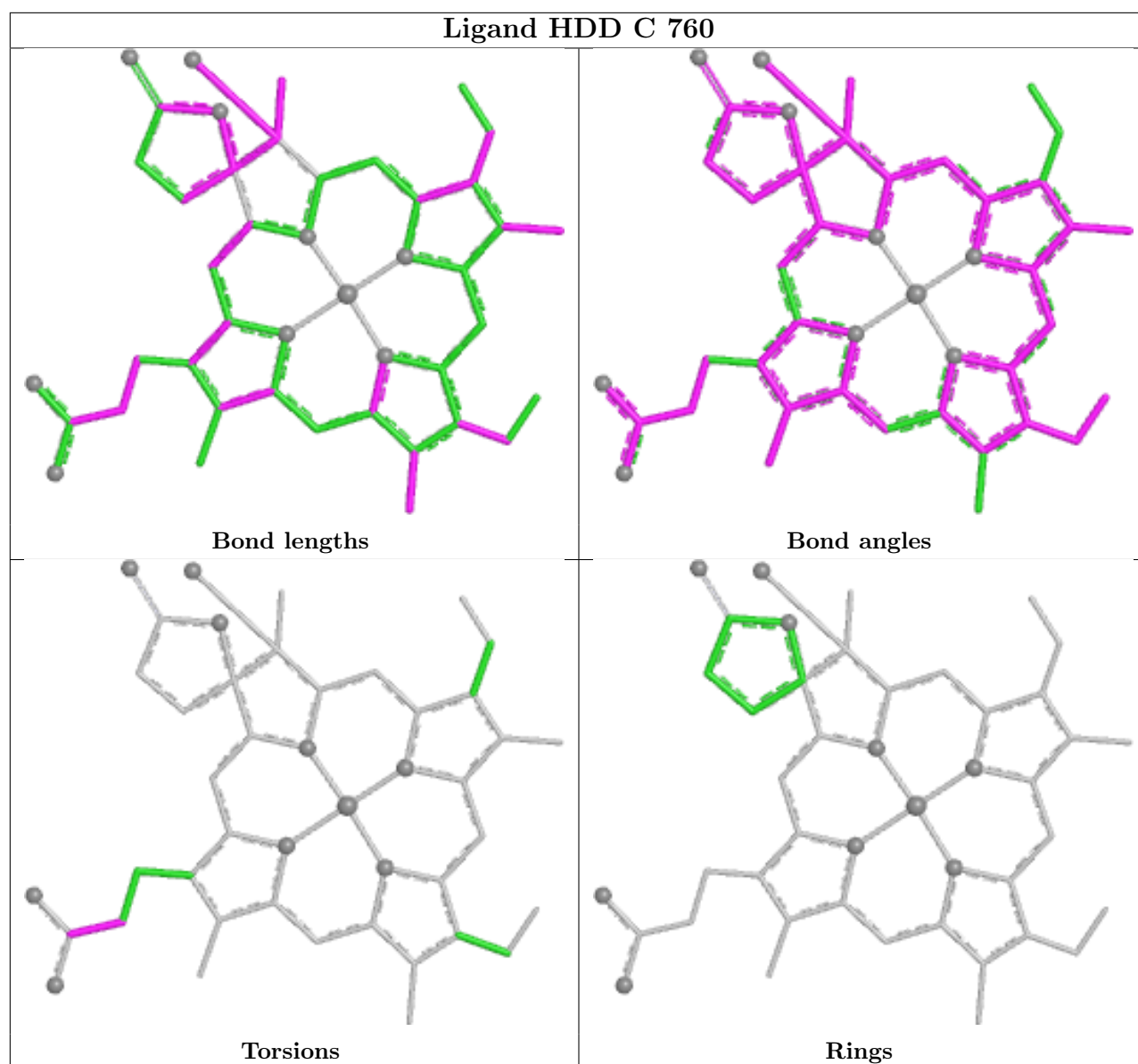
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.









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	727/753 (96%)	-0.32	18 (2%) 58 64	7, 13, 30, 55	1 (0%)
1	B	727/753 (96%)	-0.20	18 (2%) 58 64	7, 15, 36, 50	1 (0%)
1	C	727/753 (96%)	-0.24	11 (1%) 72 78	8, 15, 34, 47	1 (0%)
1	D	727/753 (96%)	-0.28	18 (2%) 58 64	7, 14, 32, 48	1 (0%)
All	All	2908/3012 (96%)	-0.26	65 (2%) 62 69	7, 14, 34, 55	4 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	27	ASP	7.5
1	A	28	SER	6.9
1	A	27	ASP	6.9
1	B	27	ASP	5.6
1	A	711	ALA	5.5
1	D	27	ASP	5.5
1	D	29	LEU	5.4
1	D	28	SER	5.3
1	B	29	LEU	4.3
1	C	28	SER	4.2
1	A	710	ILE	4.0
1	B	28	SER	4.0
1	D	39	ALA	3.8
1	A	29	LEU	3.7
1	B	30	ALA	3.7
1	D	31	PRO	3.6
1	C	29	LEU	3.5
1	D	751	ILE	3.3
1	A	712	ASP	3.3
1	D	30	ALA	3.3
1	A	749	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	726	GLY	3.3
1	A	37	ARG	3.2
1	D	750	LYS	3.1
1	B	34	GLY	3.1
1	C	724	ALA	3.0
1	A	31	PRO	3.0
1	B	710	ILE	2.9
1	A	34	GLY	2.9
1	B	37	ARG	2.9
1	B	568	ASP	2.8
1	D	36	HIS	2.8
1	C	751	ILE	2.8
1	D	35	SER	2.8
1	A	713	GLN	2.7
1	D	47	ALA	2.7
1	D	37	ARG	2.7
1	B	32	GLU	2.7
1	A	35	SER	2.7
1	A	38	PRO	2.7
1	B	670	GLY	2.6
1	C	595	ASP	2.5
1	C	725	ASP	2.5
1	D	38	PRO	2.5
1	D	749	ASP	2.5
1	B	38	PRO	2.4
1	A	30	ALA	2.4
1	B	611	VAL	2.4
1	B	36	HIS	2.4
1	C	34	GLY	2.4
1	A	750	LYS	2.4
1	B	612	ARG	2.3
1	D	60	THR	2.3
1	A	707	THR	2.3
1	B	583	LYS	2.3
1	D	32	GLU	2.2
1	B	40	ALA	2.2
1	B	709	LYS	2.1
1	A	32	GLU	2.1
1	C	749	ASP	2.1
1	D	61	ARG	2.1
1	D	41	GLU	2.1
1	A	716	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	751	ILE	2.0
1	C	596	GLY	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 [i](#)

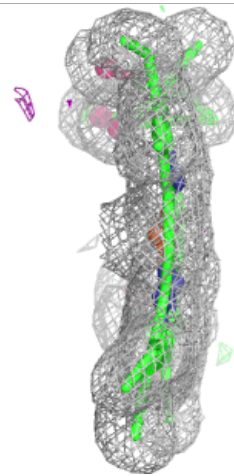
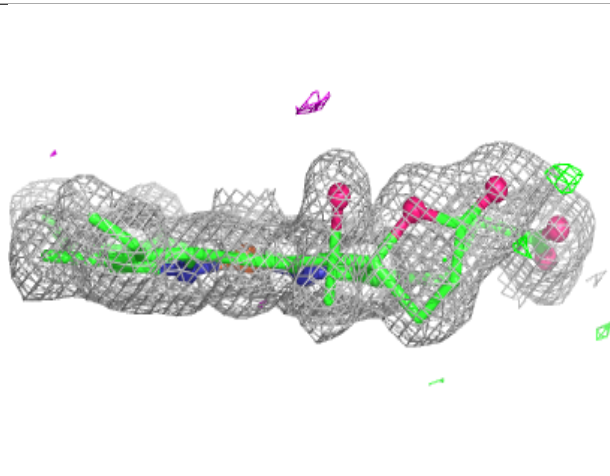
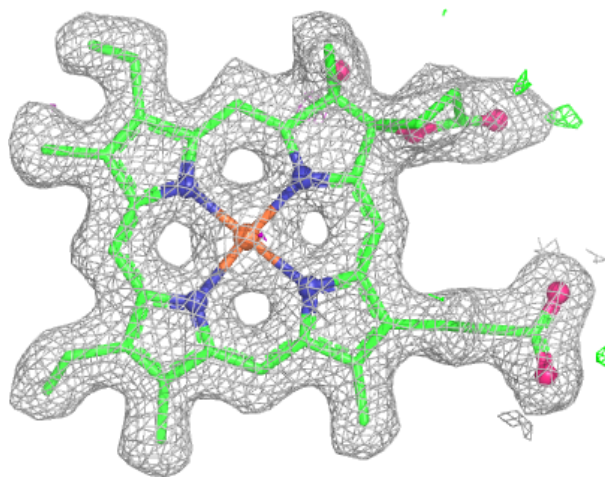
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HDD	A	760	44/44	0.98	0.05	7,9,14,17	0
2	HDD	B	760	44/44	0.98	0.05	7,10,15,18	0
2	HDD	C	760	44/44	0.98	0.05	8,11,15,16	0
2	HDD	D	760	44/44	0.98	0.05	7,9,15,16	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.

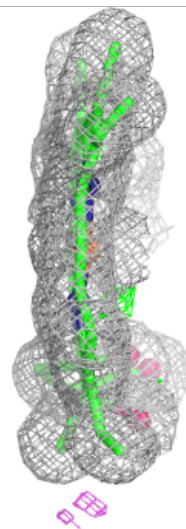
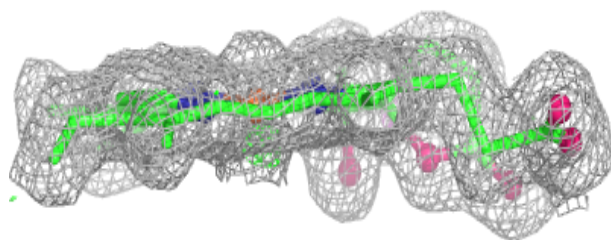
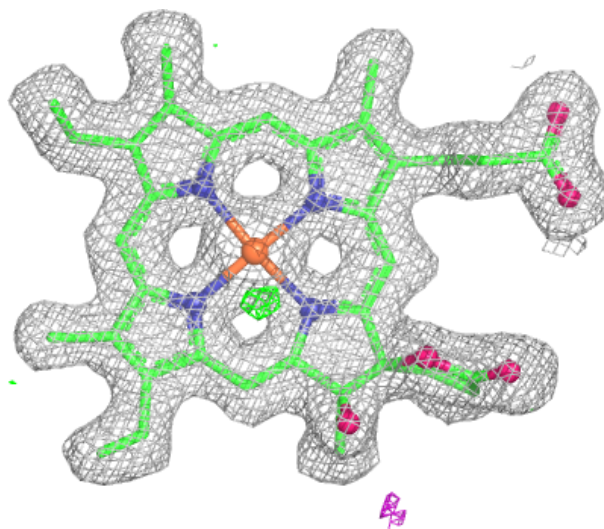
Electron density around HDD A 760:

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



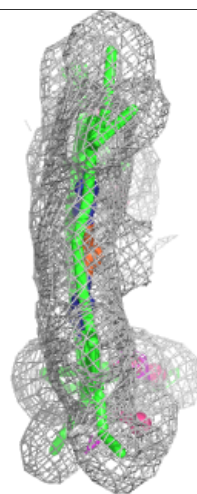
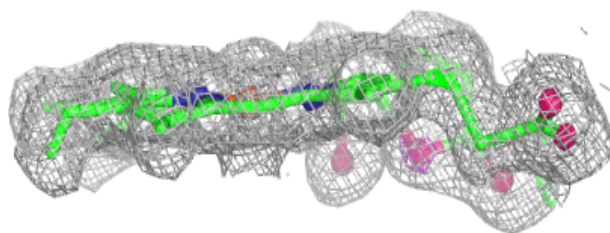
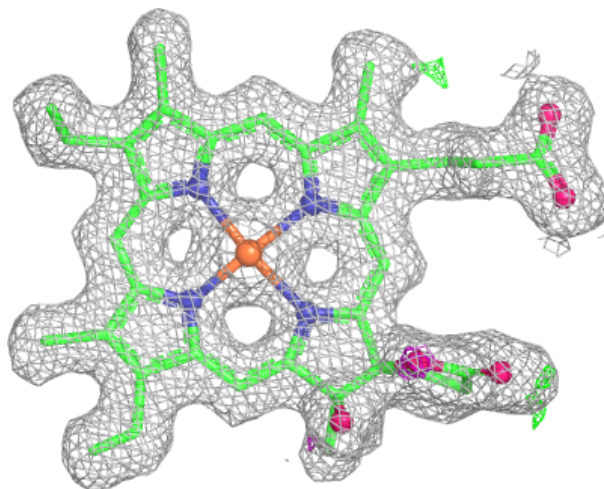
Electron density around HDD B 760:

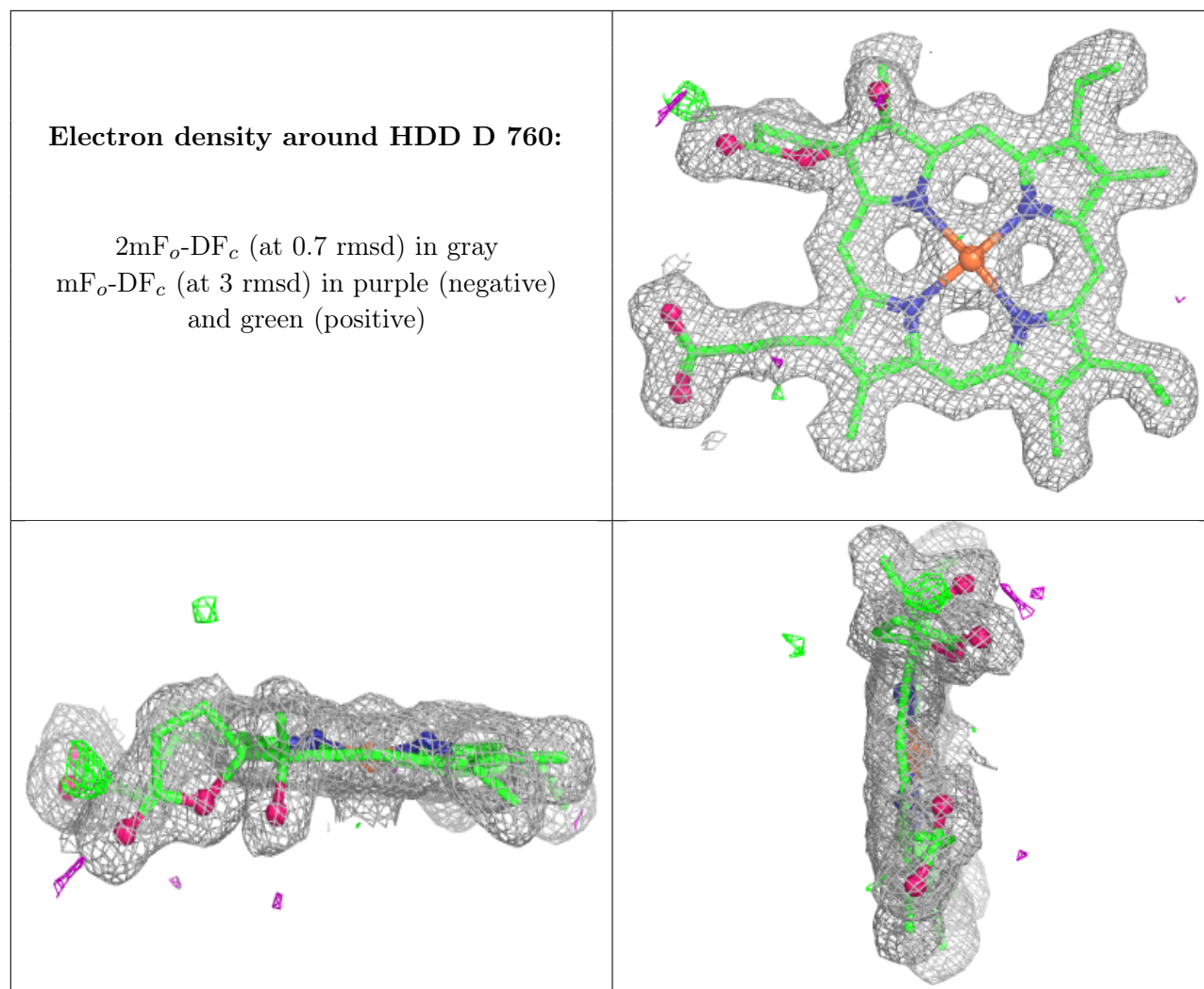
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HDD C 760:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.