



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2022 – 12:23 PM JST

PDB ID : 7VN0
Title : CATPO mutant - T188A
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Deposited on : 2021-10-10
Resolution : 1.40 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.30
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

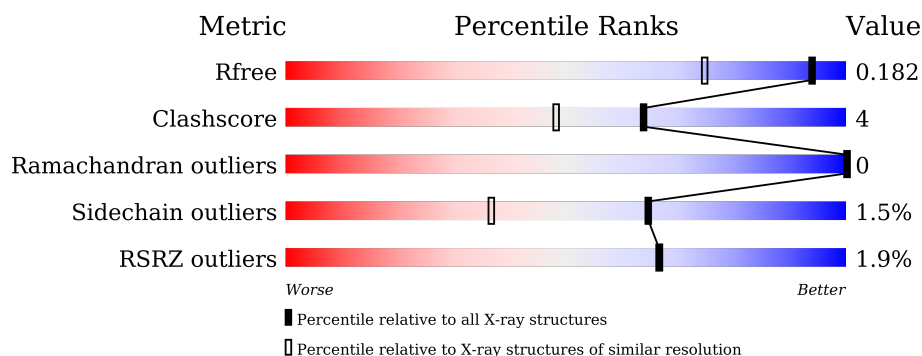
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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}	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	720	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>6%</div> </div> </div>
1	B	720	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>6%</div> </div> </div>
1	C	720	<div> <div></div> <div> <div></div> <div>87%</div> <div>7%</div> <div>6%</div> </div> </div>
1	D	720	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>6%</div> <div>6%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24123 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Catalase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	674	Total	C	N	O	S	0	35	0
			5562	3496	987	1067	12			
1	B	678	Total	C	N	O	S	0	31	0
			5548	3489	982	1065	12			
1	C	676	Total	C	N	O	S	0	26	0
			5486	3458	964	1052	12			
1	D	678	Total	C	N	O	S	0	18	0
			5434	3425	953	1045	11			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP M4GGR7
A	-20	GLY	-	expression tag	UNP M4GGR7
A	-19	SER	-	expression tag	UNP M4GGR7
A	-18	SER	-	expression tag	UNP M4GGR7
A	-17	HIS	-	expression tag	UNP M4GGR7
A	-16	HIS	-	expression tag	UNP M4GGR7
A	-15	HIS	-	expression tag	UNP M4GGR7
A	-14	HIS	-	expression tag	UNP M4GGR7
A	-13	HIS	-	expression tag	UNP M4GGR7
A	-12	HIS	-	expression tag	UNP M4GGR7
A	-11	SER	-	expression tag	UNP M4GGR7
A	-10	SER	-	expression tag	UNP M4GGR7
A	-9	GLY	-	expression tag	UNP M4GGR7
A	-8	GLU	-	expression tag	UNP M4GGR7
A	-7	ASN	-	expression tag	UNP M4GGR7
A	-6	LEU	-	expression tag	UNP M4GGR7
A	-5	TYR	-	expression tag	UNP M4GGR7
A	-4	PHE	-	expression tag	UNP M4GGR7
A	-3	GLN	-	expression tag	UNP M4GGR7
A	-2	GLY	-	expression tag	UNP M4GGR7
A	-1	HIS	-	expression tag	UNP M4GGR7

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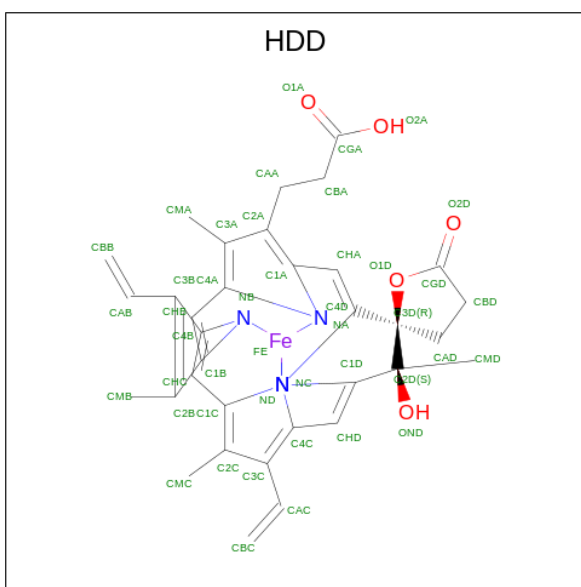
Chain	Residue	Modelled	Actual	Comment	Reference
A	188	ALA	THR	engineered mutation	UNP M4GGR7
B	-21	MET	-	initiating methionine	UNP M4GGR7
B	-20	GLY	-	expression tag	UNP M4GGR7
B	-19	SER	-	expression tag	UNP M4GGR7
B	-18	SER	-	expression tag	UNP M4GGR7
B	-17	HIS	-	expression tag	UNP M4GGR7
B	-16	HIS	-	expression tag	UNP M4GGR7
B	-15	HIS	-	expression tag	UNP M4GGR7
B	-14	HIS	-	expression tag	UNP M4GGR7
B	-13	HIS	-	expression tag	UNP M4GGR7
B	-12	HIS	-	expression tag	UNP M4GGR7
B	-11	SER	-	expression tag	UNP M4GGR7
B	-10	SER	-	expression tag	UNP M4GGR7
B	-9	GLY	-	expression tag	UNP M4GGR7
B	-8	GLU	-	expression tag	UNP M4GGR7
B	-7	ASN	-	expression tag	UNP M4GGR7
B	-6	LEU	-	expression tag	UNP M4GGR7
B	-5	TYR	-	expression tag	UNP M4GGR7
B	-4	PHE	-	expression tag	UNP M4GGR7
B	-3	GLN	-	expression tag	UNP M4GGR7
B	-2	GLY	-	expression tag	UNP M4GGR7
B	-1	HIS	-	expression tag	UNP M4GGR7
B	188	ALA	THR	engineered mutation	UNP M4GGR7
C	-21	MET	-	initiating methionine	UNP M4GGR7
C	-20	GLY	-	expression tag	UNP M4GGR7
C	-19	SER	-	expression tag	UNP M4GGR7
C	-18	SER	-	expression tag	UNP M4GGR7
C	-17	HIS	-	expression tag	UNP M4GGR7
C	-16	HIS	-	expression tag	UNP M4GGR7
C	-15	HIS	-	expression tag	UNP M4GGR7
C	-14	HIS	-	expression tag	UNP M4GGR7
C	-13	HIS	-	expression tag	UNP M4GGR7
C	-12	HIS	-	expression tag	UNP M4GGR7
C	-11	SER	-	expression tag	UNP M4GGR7
C	-10	SER	-	expression tag	UNP M4GGR7
C	-9	GLY	-	expression tag	UNP M4GGR7
C	-8	GLU	-	expression tag	UNP M4GGR7
C	-7	ASN	-	expression tag	UNP M4GGR7
C	-6	LEU	-	expression tag	UNP M4GGR7
C	-5	TYR	-	expression tag	UNP M4GGR7
C	-4	PHE	-	expression tag	UNP M4GGR7
C	-3	GLN	-	expression tag	UNP M4GGR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP M4GGR7
C	-1	HIS	-	expression tag	UNP M4GGR7
C	188	ALA	THR	engineered mutation	UNP M4GGR7
D	-21	MET	-	initiating methionine	UNP M4GGR7
D	-20	GLY	-	expression tag	UNP M4GGR7
D	-19	SER	-	expression tag	UNP M4GGR7
D	-18	SER	-	expression tag	UNP M4GGR7
D	-17	HIS	-	expression tag	UNP M4GGR7
D	-16	HIS	-	expression tag	UNP M4GGR7
D	-15	HIS	-	expression tag	UNP M4GGR7
D	-14	HIS	-	expression tag	UNP M4GGR7
D	-13	HIS	-	expression tag	UNP M4GGR7
D	-12	HIS	-	expression tag	UNP M4GGR7
D	-11	SER	-	expression tag	UNP M4GGR7
D	-10	SER	-	expression tag	UNP M4GGR7
D	-9	GLY	-	expression tag	UNP M4GGR7
D	-8	GLU	-	expression tag	UNP M4GGR7
D	-7	ASN	-	expression tag	UNP M4GGR7
D	-6	LEU	-	expression tag	UNP M4GGR7
D	-5	TYR	-	expression tag	UNP M4GGR7
D	-4	PHE	-	expression tag	UNP M4GGR7
D	-3	GLN	-	expression tag	UNP M4GGR7
D	-2	GLY	-	expression tag	UNP M4GGR7
D	-1	HIS	-	expression tag	UNP M4GGR7
D	188	ALA	THR	engineered mutation	UNP M4GGR7

- Molecule 2 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (three-letter code: HDD) (formula: $C_{34}H_{32}FeN_4O_5$) (labeled as "Ligand of Interest" by depositor).

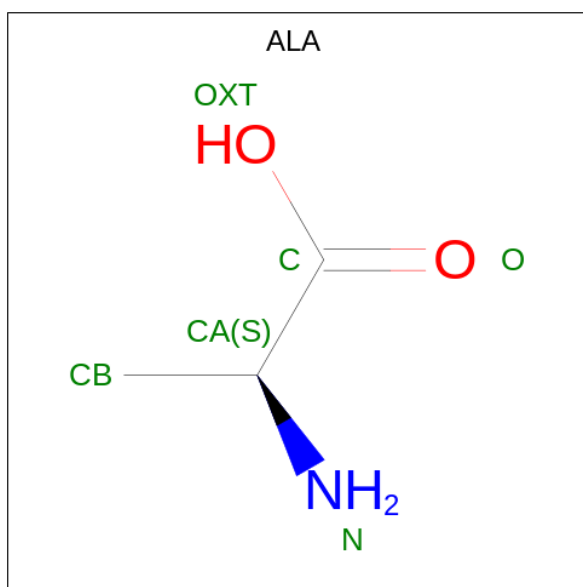


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 44	C 34	Fe 1	N 4	O 5	0	0
2	B	1	Total 44	C 34	Fe 1	N 4	O 5	0	0
2	C	1	Total 44	C 34	Fe 1	N 4	O 5	0	0
2	D	1	Total 44	C 34	Fe 1	N 4	O 5	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Ca 3 3	0	0
3	B	2	Total Ca 2 2	0	0
3	C	2	Total Ca 2 2	0	0
3	D	2	Total Ca 2 2	0	0

- Molecule 4 is ALANINE (three-letter code: ALA) (formula: $\text{C}_3\text{H}_7\text{NO}_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			5	3	1	1		

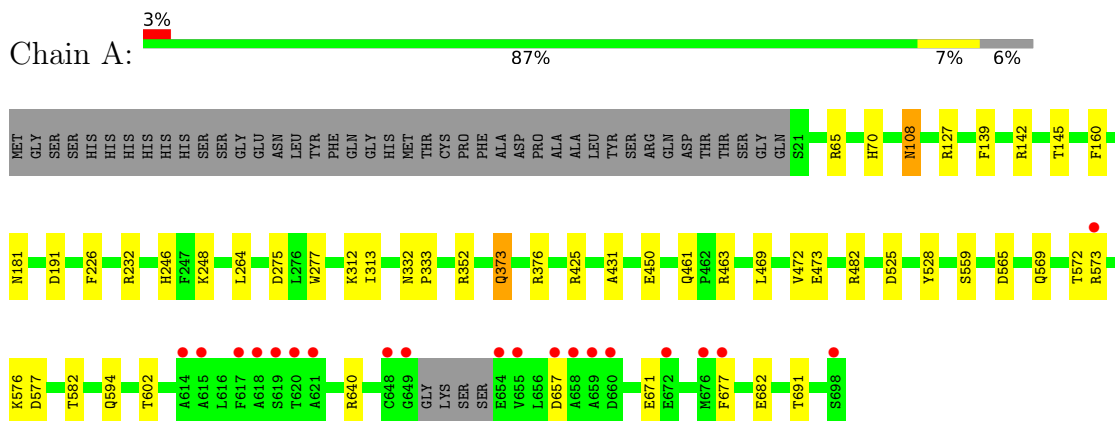
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	470	Total	O	0	0
			470	470		
5	B	464	Total	O	0	0
			464	464		
5	C	493	Total	O	0	0
			493	493		
5	D	475	Total	O	0	1
			476	476		

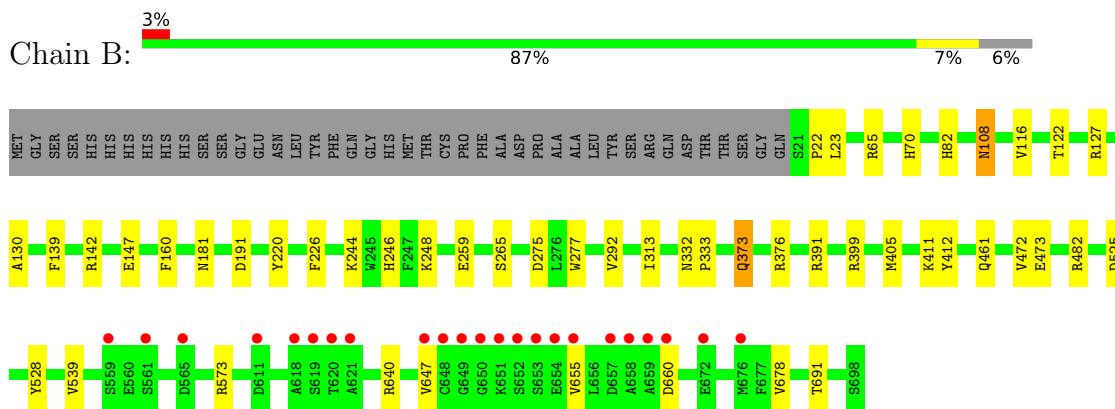
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

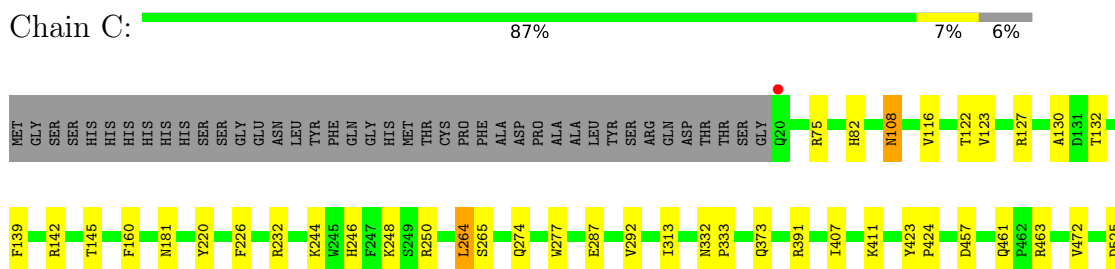
• Molecule 1: Catalase

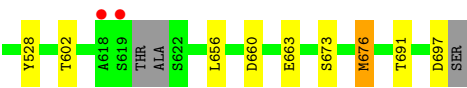


• Molecule 1: Catalase

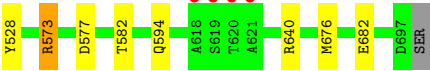
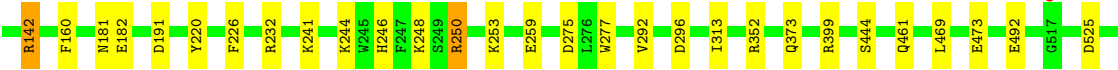
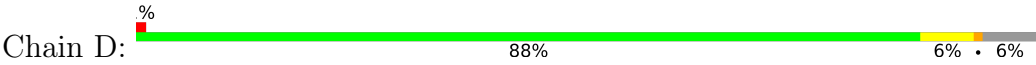


• Molecule 1: Catalase





● Molecule 1: Catalase



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	124.94Å 120.79Å 184.75Å 90.00° 101.90° 90.00°	Depositor
Resolution (Å)	56.37 – 1.40 56.31 – 1.40	Depositor EDS
% Data completeness (in resolution range)	98.9 (56.37-1.40) 98.9 (56.31-1.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 1.40Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.161 , 0.182 0.162 , 0.182	Depositor DCC
R_{free} test set	25989 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	10.3	Xtrriage
Anisotropy	0.121	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	24123	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.9150e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, CA

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	0.74	0/5699	0.91	11/7738 (0.1%)
1	B	0.73	0/5686	0.90	6/7721 (0.1%)
1	C	0.74	0/5626	0.90	6/7643 (0.1%)
1	D	0.77	2/5572 (0.0%)	0.93	7/7575 (0.1%)
All	All	0.74	2/22583 (0.0%)	0.91	30/30677 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	492[A]	GLU	CD-OE2	7.94	1.34	1.25
1	D	492[B]	GLU	CD-OE2	7.94	1.34	1.25

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	399	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	A	232	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	B	399	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	B	482	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	D	232	ARG	NE-CZ-NH1	6.60	123.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	232	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	B	220	TYR	CB-CG-CD1	6.44	124.87	121.00
1	A	142	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	D	220	TYR	CB-CG-CD2	-6.20	117.28	121.00
1	D	399	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	232	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	C	220	TYR	CB-CG-CD1	6.00	124.60	121.00
1	B	220	TYR	CB-CG-CD2	-5.86	117.48	121.00
1	A	352	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	A	65	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	463	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	D	142	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	376	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	D	352	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	C	391	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	C	697	ASP	CA-C-O	-5.47	108.62	120.10
1	A	463	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	376	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	65	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	D	573	ARG	NE-CZ-NH1	-5.33	117.63	120.30
1	A	142	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	B	65	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	C	391	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	C	463	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	482	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	75	ARG	Sidechain
1	D	75	ARG	Sidechain

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	5562	0	5296	46	0
1	B	5548	0	5292	52	0
1	C	5486	0	5238	49	0
1	D	5434	0	5177	41	0
2	A	44	0	31	2	0
2	B	44	0	31	1	0
2	C	44	0	31	1	0
2	D	44	0	31	2	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	D	5	0	4	0	0
5	A	470	0	0	9	0
5	B	464	0	0	14	0
5	C	493	0	0	8	0
5	D	476	0	0	10	0
All	All	24123	0	21131	183	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 4.

All (183) 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:405[B]:MET:CE	5:B:1029:HOH:O	1.71	1.29
1:A:246[B]:HIS:CE1	1:A:248[B]:LYS:NZ	2.00	1.29
1:B:246[B]:HIS:ND1	1:B:248[B]:LYS:HD3	1.52	1.22
1:B:246[B]:HIS:CE1	1:B:248[B]:LYS:NZ	2.06	1.22
1:C:127[A]:ARG:O	5:C:802:HOH:O	1.58	1.22
1:B:246[B]:HIS:CE1	1:B:248[B]:LYS:HD3	1.76	1.21
1:B:246[B]:HIS:CE1	1:B:248[B]:LYS:CD	2.26	1.18
1:B:246[B]:HIS:HE1	1:B:248[B]:LYS:NZ	1.40	1.16
1:B:246[B]:HIS:CE1	1:B:248[B]:LYS:HZ3	1.63	1.13
1:B:246[B]:HIS:ND1	1:B:248[B]:LYS:CD	2.19	1.05
1:A:246[B]:HIS:ND1	1:A:248[B]:LYS:HD3	1.72	1.05
1:A:246[B]:HIS:CE1	1:A:248[B]:LYS:CD	2.40	1.04
1:D:127[B]:ARG:NH1	5:D:803:HOH:O	1.93	1.01
1:A:246[B]:HIS:CE1	1:A:248[B]:LYS:HD3	1.98	0.98
1:A:127[A]:ARG:NH2	5:A:802:HOH:O	1.97	0.97
1:B:313:ILE:H	1:B:461:GLN:HE22	1.12	0.97
1:B:259[A]:GLU:HG3	5:B:807:HOH:O	1.64	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246[B]:HIS:ND1	1:A:248[B]:LYS:CD	2.28	0.96
1:A:246[B]:HIS:CE1	1:A:248[B]:LYS:HZ3	1.72	0.95
1:A:576:LYS:HE3	5:A:812:HOH:O	1.66	0.94
1:A:127[A]:ARG:NH1	5:A:802:HOH:O	1.99	0.92
1:C:127[B]:ARG:NH1	5:C:803:HOH:O	1.96	0.92
1:B:246[B]:HIS:HE1	1:B:248[B]:LYS:HZ2	1.12	0.92
1:B:246[B]:HIS:CE1	1:B:248[B]:LYS:CE	2.52	0.92
1:A:246[B]:HIS:CE1	1:A:248[B]:LYS:HZ2	1.74	0.92
1:A:313:ILE:H	1:A:461:GLN:HE22	1.15	0.91
1:A:246[B]:HIS:HE1	1:A:248[B]:LYS:NZ	1.46	0.90
1:C:313:ILE:H	1:C:461:GLN:HE22	1.11	0.90
1:D:313:ILE:H	1:D:461:GLN:HE22	1.18	0.86
1:C:246[B]:HIS:CD2	1:C:248:LYS:HD3	2.10	0.86
1:C:127[B]:ARG:NH2	5:C:803:HOH:O	2.09	0.86
1:D:127[B]:ARG:NH2	5:D:803:HOH:O	2.10	0.84
1:C:246[B]:HIS:CD2	1:C:248:LYS:CD	2.61	0.84
1:C:246[B]:HIS:NE2	1:C:248:LYS:NZ	2.25	0.84
1:A:246[B]:HIS:HE1	1:A:248[B]:LYS:HZ2	0.88	0.83
1:A:246[B]:HIS:CE1	1:A:248[B]:LYS:CE	2.62	0.82
1:D:246[B]:HIS:CE1	1:D:248:LYS:NZ	2.48	0.82
1:D:127[B]:ARG:CZ	5:D:803:HOH:O	2.26	0.81
1:D:246[B]:HIS:CE1	1:D:248:LYS:HZ3	1.97	0.81
1:B:127[A]:ARG:NH1	5:B:802:HOH:O	1.97	0.81
1:C:656:LEU:HD12	1:C:663[B]:GLU:HG3	1.64	0.80
1:C:127[B]:ARG:CZ	5:C:803:HOH:O	2.30	0.79
1:D:226:PHE:CE1	1:D:246[B]:HIS:CE1	2.71	0.78
1:D:246[B]:HIS:CE1	1:D:248:LYS:CD	2.66	0.78
1:B:405[B]:MET:HE2	5:B:1029:HOH:O	1.56	0.77
1:D:246[B]:HIS:CE1	1:D:248:LYS:HD3	2.19	0.77
1:D:160:PHE:CD1	5:D:1192:HOH:O	2.36	0.76
1:A:127[A]:ARG:CZ	5:A:802:HOH:O	2.23	0.76
1:C:127[A]:ARG:NH1	5:C:804:HOH:O	2.17	0.76
1:C:656:LEU:CD1	1:C:663[B]:GLU:HG3	2.16	0.76
1:C:226:PHE:CE1	1:C:246[B]:HIS:CD2	2.74	0.75
1:A:264:LEU:HG	1:A:602:THR:HB	1.71	0.73
1:A:640[B]:ARG:NH1	5:A:803:HOH:O	2.19	0.72
1:C:246[B]:HIS:CE1	1:C:248:LYS:HZ2	2.07	0.71
1:B:246[B]:HIS:CG	1:B:248[B]:LYS:HD3	2.24	0.71
1:B:405[B]:MET:HE1	5:B:1029:HOH:O	1.53	0.71
1:A:246[B]:HIS:ND1	1:A:248[B]:LYS:HD2	2.04	0.70
1:C:246[B]:HIS:CD2	1:C:248:LYS:HD2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:PHE:CD1	5:C:1203:HOH:O	2.43	0.70
1:D:127[A]:ARG:NH2	5:D:806:HOH:O	2.23	0.70
1:A:576:LYS:CE	5:A:812:HOH:O	2.30	0.70
1:A:127[B]:ARG:NH1	5:A:805:HOH:O	2.24	0.69
1:B:127[A]:ARG:NH2	5:B:802:HOH:O	2.25	0.69
1:B:573[A]:ARG:HG3	1:B:678:VAL:HG11	1.75	0.68
1:B:259[A]:GLU:OE2	5:B:803:HOH:O	2.12	0.68
1:B:246[B]:HIS:ND1	1:B:248[B]:LYS:HD2	2.08	0.67
1:A:246[B]:HIS:CG	1:A:248[B]:LYS:HD3	2.29	0.67
1:C:160:PHE:CE1	5:C:1203:HOH:O	2.47	0.66
1:D:241:LYS:NZ	1:D:296[A]:ASP:OD1	2.25	0.66
1:B:127[A]:ARG:CZ	5:B:802:HOH:O	2.40	0.65
1:B:147[B]:GLU:OE1	5:B:804:HOH:O	2.14	0.65
1:C:264:LEU:HG	1:C:602:THR:HB	1.77	0.65
1:D:226:PHE:HE1	1:D:246[B]:HIS:CE1	2.12	0.65
1:D:259[B]:GLU:OE2	5:D:804:HOH:O	2.13	0.65
1:D:160:PHE:CE1	5:D:1192:HOH:O	2.47	0.65
1:C:246[B]:HIS:CG	1:C:248:LYS:HD3	2.33	0.64
1:A:373:GLN:HE21	1:A:373:GLN:HA	1.63	0.63
1:C:274[B]:GLN:NE2	5:C:806:HOH:O	2.27	0.62
1:A:313:ILE:N	1:A:461:GLN:HE22	1.95	0.62
1:D:373:GLN:HE21	1:D:373:GLN:HA	1.64	0.62
1:A:565[B]:ASP:OD2	1:A:569:GLN:NE2	2.33	0.62
1:D:582:THR:HG21	1:D:594[A]:GLN:HE21	1.65	0.62
1:B:160:PHE:CE1	5:B:1188:HOH:O	2.53	0.61
1:B:472:VAL:HG11	1:B:691:THR:HB	1.82	0.61
1:B:373:GLN:HE21	1:B:373:GLN:HA	1.65	0.60
1:D:246[B]:HIS:ND1	1:D:248:LYS:HD3	2.16	0.60
1:B:246[B]:HIS:CE1	1:B:248[B]:LYS:HD2	2.31	0.59
1:B:160:PHE:CD1	5:B:1188:HOH:O	2.52	0.58
1:C:226:PHE:HE1	1:C:246[B]:HIS:CD2	2.22	0.58
1:C:246[B]:HIS:NE2	1:C:248:LYS:CD	2.66	0.58
1:B:127[B]:ARG:NH1	5:B:806:HOH:O	2.35	0.58
1:C:373:GLN:HE21	1:C:373:GLN:HA	1.69	0.57
1:B:277[A]:TRP:CE3	1:D:181:ASN:HB3	2.40	0.56
1:B:130:ALA:CB	1:B:265[B]:SER:HB2	2.35	0.56
1:C:226:PHE:CE1	1:C:246[B]:HIS:NE2	2.73	0.56
1:C:313:ILE:N	1:C:461:GLN:HE22	1.92	0.56
2:A:701:HDD:HBC1	2:A:701:HDD:HMC1	1.88	0.56
1:C:250[B]:ARG:HD3	1:C:287:GLU:HB3	1.88	0.55
1:C:246[B]:HIS:CE1	1:C:248:LYS:NZ	2.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ASN:C	1:B:108:ASN:HD22	2.11	0.54
1:B:313:ILE:N	1:B:461:GLN:HE22	1.95	0.54
1:D:226:PHE:CE1	1:D:246[B]:HIS:ND1	2.76	0.54
2:C:701:HDD:HMC1	2:C:701:HDD:HBC1	1.92	0.52
1:B:277[A]:TRP:CZ3	1:B:333:PRO:HD2	2.44	0.52
1:D:246[B]:HIS:HE1	1:D:248:LYS:NZ	2.04	0.52
1:D:246[B]:HIS:ND1	1:D:248:LYS:CD	2.73	0.52
1:B:277[A]:TRP:CZ3	1:D:181:ASN:HB3	2.44	0.51
1:D:108:ASN:HD22	1:D:108:ASN:C	2.14	0.51
1:A:246[B]:HIS:CE1	1:A:248[B]:LYS:HD2	2.35	0.51
1:C:108:ASN:C	1:C:108:ASN:HD22	2.14	0.51
1:C:246[B]:HIS:NE2	1:C:248:LYS:HD3	2.25	0.51
1:A:277[A]:TRP:CZ3	1:C:181:ASN:HB3	2.46	0.50
1:B:22:PRO:HD2	1:B:391[B]:ARG:NE	2.26	0.50
1:D:525:ASP:HA	1:D:528:TYR:CD2	2.45	0.50
2:A:701:HDD:HMB1	2:A:701:HDD:HBB1	1.92	0.50
1:A:469:LEU:HB3	1:A:473:GLU:HB3	1.92	0.50
1:B:640[B]:ARG:CG	5:B:812:HOH:O	2.60	0.50
1:A:431:ALA:HB1	5:D:807:HOH:O	2.11	0.49
2:D:702:HDD:HMB1	2:D:702:HDD:HBB1	1.95	0.49
1:D:469:LEU:HB3	1:D:473:GLU:HB3	1.94	0.49
1:C:226:PHE:HE1	1:C:246[B]:HIS:NE2	2.11	0.49
1:A:181:ASN:HB3	1:C:277[A]:TRP:CE3	2.48	0.48
1:A:525:ASP:HA	1:A:528:TYR:CD2	2.48	0.48
1:C:226:PHE:HE1	1:C:246[B]:HIS:CE1	2.32	0.48
1:D:259[B]:GLU:OE2	5:D:805:HOH:O	2.19	0.48
1:A:472:VAL:HG11	1:A:691:THR:HB	1.94	0.48
1:C:673:SER:HB3	1:C:676[A]:MET:HB2	1.94	0.47
1:D:82:HIS:CE1	1:D:123:VAL:HG22	2.49	0.47
1:A:277[A]:TRP:CE3	1:C:181:ASN:HB3	2.50	0.47
1:B:525:ASP:HA	1:B:528:TYR:CD2	2.49	0.47
1:A:450[B]:GLU:OE1	5:A:804:HOH:O	2.20	0.47
1:B:411[B]:LYS:HG2	1:B:412:TYR:CE2	2.49	0.47
1:C:116:VAL:HA	1:C:142:ARG:O	2.15	0.47
2:B:701:HDD:HMC1	2:B:701:HDD:HBC1	1.97	0.47
1:D:250:ARG:HH11	1:D:250:ARG:HB3	1.80	0.47
5:B:1019:HOH:O	1:C:411[B]:LYS:HD2	2.16	0.46
1:A:108:ASN:C	1:A:108:ASN:HD22	2.19	0.46
1:C:132:THR:HG21	1:C:264:LEU:HD13	1.97	0.46
1:B:181:ASN:HB3	1:D:277[A]:TRP:CE3	2.52	0.45
1:D:253:LYS:HE3	5:D:1103:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:PHE:CE1	1:A:246[B]:HIS:CE1	3.03	0.45
1:D:246[B]:HIS:CG	1:D:248:LYS:HD3	2.51	0.45
1:D:244:LYS:O	1:D:292:VAL:HA	2.17	0.45
1:A:425[A]:ARG:HB3	1:D:34:TYR:CD1	2.52	0.45
1:A:277[A]:TRP:CZ3	1:A:332:ASN:HB3	2.52	0.45
1:A:160:PHE:CE1	5:A:1183:HOH:O	2.68	0.44
1:B:127[B]:ARG:NH1	1:D:182:GLU:OE2	2.50	0.44
1:A:577:ASP:OD2	1:A:682:GLU:OE2	2.36	0.44
1:C:82:HIS:HA	1:C:122:THR:O	2.18	0.43
1:A:181:ASN:HB3	1:C:277[A]:TRP:CZ3	2.53	0.43
1:D:246[B]:HIS:HE1	1:D:248:LYS:HZ2	1.66	0.43
1:B:181:ASN:HB3	1:D:277[A]:TRP:CZ3	2.53	0.43
1:B:244:LYS:O	1:B:292:VAL:HA	2.18	0.42
1:C:277[A]:TRP:CZ3	1:C:332:ASN:HB3	2.54	0.42
1:C:130:ALA:CB	1:C:265[B]:SER:HB2	2.50	0.42
1:D:246[B]:HIS:CE1	1:D:248:LYS:HD2	2.50	0.42
1:B:116:VAL:HA	1:B:142:ARG:O	2.20	0.42
1:C:525:ASP:HA	1:C:528:TYR:CD2	2.54	0.42
1:B:647:VAL:HG21	1:B:655:VAL:HB	2.02	0.42
1:C:472:VAL:HG11	1:C:691:THR:HB	2.01	0.42
1:D:577:ASP:OD2	1:D:682:GLU:OE2	2.37	0.42
2:D:702:HDD:HBC1	2:D:702:HDD:HMC1	2.02	0.42
1:B:373:GLN:HA	1:B:373:GLN:NE2	2.34	0.42
1:D:116:VAL:HA	1:D:142:ARG:O	2.20	0.42
1:B:277[A]:TRP:CH2	1:B:332:ASN:HB3	2.54	0.41
1:C:82:HIS:CE1	1:C:123:VAL:HG22	2.55	0.41
1:A:277[A]:TRP:CZ3	1:A:333:PRO:HD2	2.56	0.41
1:A:425[B]:ARG:HA	1:A:425[B]:ARG:HD2	1.86	0.41
1:C:244:LYS:O	1:C:292:VAL:HA	2.21	0.41
1:C:277[A]:TRP:CZ3	1:C:333:PRO:HD2	2.55	0.41
1:B:108:ASN:C	1:B:108:ASN:ND2	2.74	0.41
1:B:23:LEU:HG	1:C:407:ILE:HD11	2.02	0.41
1:B:82:HIS:HA	1:B:122:THR:O	2.21	0.41
1:D:373:GLN:HA	1:D:373:GLN:NE2	2.32	0.41
1:A:373:GLN:HA	1:A:373:GLN:NE2	2.33	0.41
1:A:671:GLU:HB2	1:A:677:PHE:HB2	2.03	0.40
1:C:457:ASP:OD1	1:C:457:ASP:C	2.60	0.40
1:B:226:PHE:CE1	1:B:246[B]:HIS:CE1	3.10	0.40
1:B:473:GLU:HG3	1:B:539:VAL:CG2	2.51	0.40
1:A:312:LYS:HA	1:A:461:GLN:NE2	2.36	0.40
1:B:277[A]:TRP:CZ3	1:B:332:ASN:HB3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:THR:HG21	1:A:594[A]:GLN:HE21	1.86	0.40
1:C:423:TYR:HA	1:C:424:PRO:C	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	705/720 (98%)	685 (97%)	20 (3%)	0	100	100
1	B	707/720 (98%)	685 (97%)	22 (3%)	0	100	100
1	C	698/720 (97%)	682 (98%)	16 (2%)	0	100	100
1	D	694/720 (96%)	678 (98%)	16 (2%)	0	100	100
All	All	2804/2880 (97%)	2730 (97%)	74 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	592/596 (99%)	580 (98%)	12 (2%)	55	23
1	B	591/596 (99%)	584 (99%)	7 (1%)	71	47
1	C	585/596 (98%)	578 (99%)	7 (1%)	71	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	577/596 (97%)	567 (98%)	10 (2%)	60	31
All	All	2345/2384 (98%)	2309 (98%)	36 (2%)	65	37

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	108	ASN
1	A	139	PHE
1	A	145	THR
1	A	191	ASP
1	A	275	ASP
1	A	373	GLN
1	A	559[A]	SER
1	A	559[B]	SER
1	A	572	THR
1	A	573	ARG
1	A	657	ASP
1	B	70	HIS
1	B	108	ASN
1	B	139	PHE
1	B	191	ASP
1	B	275	ASP
1	B	373	GLN
1	B	660	ASP
1	C	108	ASN
1	C	139	PHE
1	C	145	THR
1	C	264	LEU
1	C	660	ASP
1	C	676[A]	MET
1	C	676[B]	MET
1	D	70	HIS
1	D	108	ASN
1	D	139	PHE
1	D	191	ASP
1	D	250	ARG
1	D	275	ASP
1	D	444	SER
1	D	573	ARG
1	D	640	ARG
1	D	676	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	167	GLN
1	A	373	GLN
1	A	375	ASN
1	A	430	ASN
1	A	461	GLN
1	B	108	ASN
1	B	167	GLN
1	B	373	GLN
1	B	375	ASN
1	B	461	GLN
1	C	108	ASN
1	C	373	GLN
1	C	375	ASN
1	C	461	GLN
1	D	108	ASN
1	D	373	GLN
1	D	375	ASN
1	D	461	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 9 are monoatomic - leaving 5 for Mogul analysis.

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	C	701	5,1	41,52,52	1.21	4 (9%)	31,89,89	1.81	9 (29%)
2	HDD	B	701	1	41,52,52	1.43	9 (21%)	31,89,89	1.86	11 (35%)
2	HDD	A	701	5,1	41,52,52	1.22	6 (14%)	31,89,89	1.72	11 (35%)
4	ALA	D	701	-	3,4,5	1.31	0	2,4,6	2.39	1 (50%)
2	HDD	D	702	5,1	41,52,52	1.42	6 (14%)	31,89,89	1.73	5 (16%)

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	C	701	5,1	-	2/5/89/89	0/1/9/9
2	HDD	B	701	1	-	2/5/89/89	0/1/9/9
2	HDD	A	701	5,1	-	2/5/89/89	0/1/9/9
4	ALA	D	701	-	-	0/0/2/4	-
2	HDD	D	702	5,1	-	2/5/89/89	0/1/9/9

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	702	HDD	CBD-CGD	-3.40	1.43	1.50
2	B	701	HDD	C3B-C2B	3.23	1.44	1.40
2	D	702	HDD	C3B-C2B	3.13	1.44	1.40
2	A	701	HDD	C1A-CHA	2.75	1.48	1.41
2	C	701	HDD	CMD-C2D	-2.64	1.49	1.53
2	A	701	HDD	C3B-C2B	2.63	1.44	1.40
2	B	701	HDD	CAA-C2A	-2.63	1.48	1.52
2	B	701	HDD	C3C-CAC	-2.61	1.42	1.47
2	B	701	HDD	C1A-CHA	2.58	1.48	1.41
2	A	701	HDD	FE-ND	2.58	2.05	1.95
2	C	701	HDD	OND-C2D	2.54	1.47	1.42
2	A	701	HDD	C3C-C2C	2.53	1.43	1.40
2	D	702	HDD	CMA-C3A	-2.39	1.46	1.51
2	D	702	HDD	CAA-C2A	-2.26	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	HDD	FE-ND	2.24	2.04	1.95
2	B	701	HDD	C1D-ND	-2.22	1.34	1.37
2	C	701	HDD	C1A-CHA	2.21	1.47	1.41
2	B	701	HDD	O1A-CGA	2.20	1.29	1.22
2	B	701	HDD	C2B-C1B	2.16	1.47	1.42
2	A	701	HDD	C1D-ND	-2.10	1.34	1.37
2	C	701	HDD	C3B-C2B	2.07	1.43	1.40
2	A	701	HDD	C4A-CHB	2.06	1.46	1.41
2	B	701	HDD	C4C-NC	-2.02	1.32	1.36
2	D	702	HDD	OND-C2D	2.02	1.46	1.42
2	D	702	HDD	CMD-C2D	-2.00	1.50	1.53

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	702	HDD	C4A-C3A-C2A	-5.06	103.48	107.00
2	D	702	HDD	C2B-C3B-C4B	-4.84	103.52	106.90
2	C	701	HDD	C2B-C3B-C4B	-4.19	103.97	106.90
2	B	701	HDD	C3C-C4C-NC	4.08	114.48	109.21
2	B	701	HDD	CMB-C2B-C3B	3.60	131.41	124.68
2	A	701	HDD	C3C-C4C-NC	3.58	113.84	109.21
2	C	701	HDD	CMA-C3A-C4A	-3.23	123.50	128.46
4	D	701	ALA	O-C-CA	-3.17	114.24	124.28
2	C	701	HDD	CAA-CBA-CGA	-3.17	104.87	113.76
2	B	701	HDD	CAA-CBA-CGA	-3.13	104.99	113.76
2	C	701	HDD	CMA-C3A-C2A	3.12	130.82	124.94
2	C	701	HDD	C4C-CHD-C1D	-3.09	124.00	130.12
2	A	701	HDD	CMB-C2B-C3B	3.02	130.34	124.68
2	B	701	HDD	OND-C2D-CMD	-2.87	104.30	109.59
2	C	701	HDD	OND-C2D-CMD	-2.87	104.31	109.59
2	B	701	HDD	C2B-C3B-C4B	2.69	108.78	106.90
2	A	701	HDD	CAA-CBA-CGA	-2.69	106.22	113.76
2	A	701	HDD	CMA-C3A-C4A	-2.66	124.37	128.46
2	A	701	HDD	OND-C2D-CMD	-2.63	104.75	109.59
2	B	701	HDD	O1D-CGD-O2D	2.58	123.10	120.80
2	C	701	HDD	CMC-C2C-C3C	2.57	129.48	124.68
2	B	701	HDD	CMC-C2C-C3C	2.50	129.36	124.68
2	D	702	HDD	C2D-C1D-CHD	-2.50	120.15	124.28
2	A	701	HDD	O1D-CGD-O2D	-2.47	118.59	120.80
2	C	701	HDD	C2D-C1D-CHD	-2.41	120.29	124.28
2	B	701	HDD	CMA-C3A-C4A	-2.39	124.80	128.46
2	A	701	HDD	C2D-C1D-CHD	-2.37	120.36	124.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	702	HDD	OND-C2D-CMD	-2.31	105.33	109.59
2	B	701	HDD	CMA-C3A-C2A	2.30	129.27	124.94
2	A	701	HDD	CMC-C2C-C3C	2.29	128.96	124.68
2	A	701	HDD	CMA-C3A-C2A	2.23	129.14	124.94
2	B	701	HDD	O1A-CGA-CBA	-2.16	116.15	123.08
2	A	701	HDD	O1A-CGA-CBA	-2.14	116.21	123.08
2	B	701	HDD	O2A-CGA-CBA	2.11	120.81	114.03
2	C	701	HDD	O1D-CGD-O2D	-2.09	118.94	120.80
2	D	702	HDD	CAA-CBA-CGA	-2.04	108.04	113.76
2	A	701	HDD	C1A-CHA-C4D	-2.02	126.11	130.12

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	HDD	CAA-CBA-CGA-O1A
2	C	701	HDD	CAA-CBA-CGA-O1A
2	C	701	HDD	CAA-CBA-CGA-O2A
2	D	702	HDD	CAA-CBA-CGA-O1A
2	A	701	HDD	CAA-CBA-CGA-O1A
2	D	702	HDD	CAA-CBA-CGA-O2A
2	B	701	HDD	CAA-CBA-CGA-O2A
2	A	701	HDD	CAA-CBA-CGA-O2A

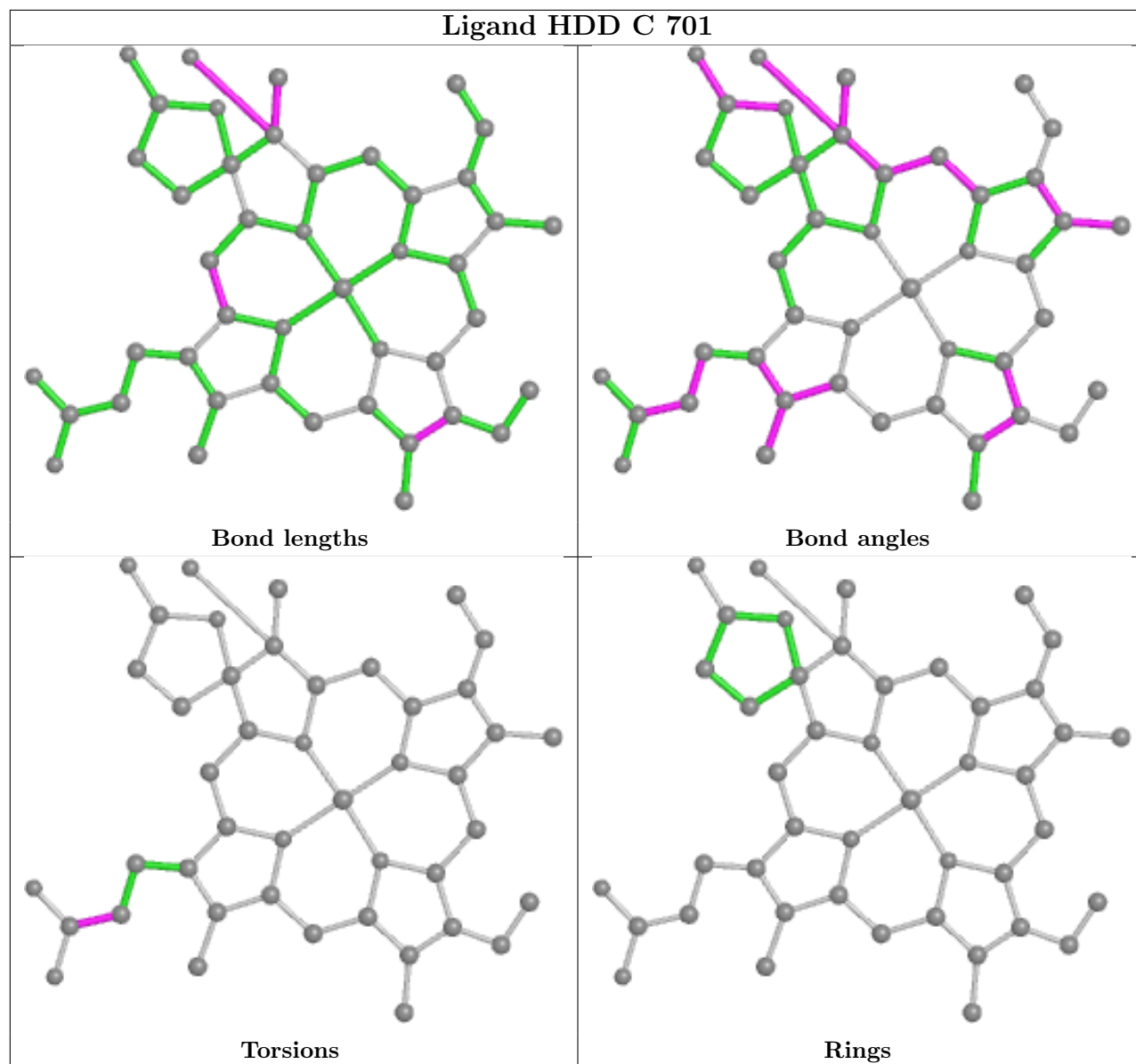
There are no ring outliers.

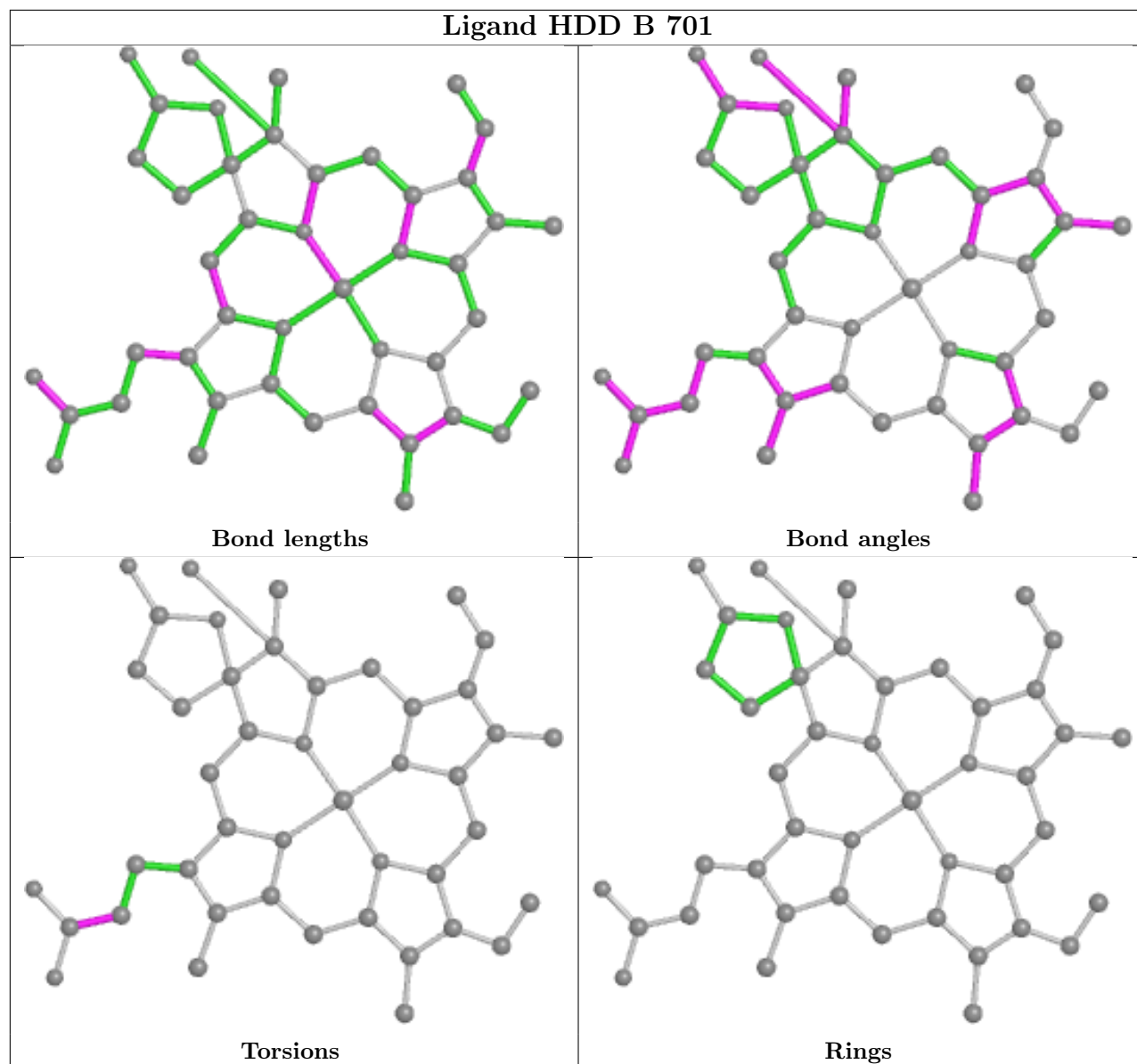
4 monomers are involved in 6 short contacts:

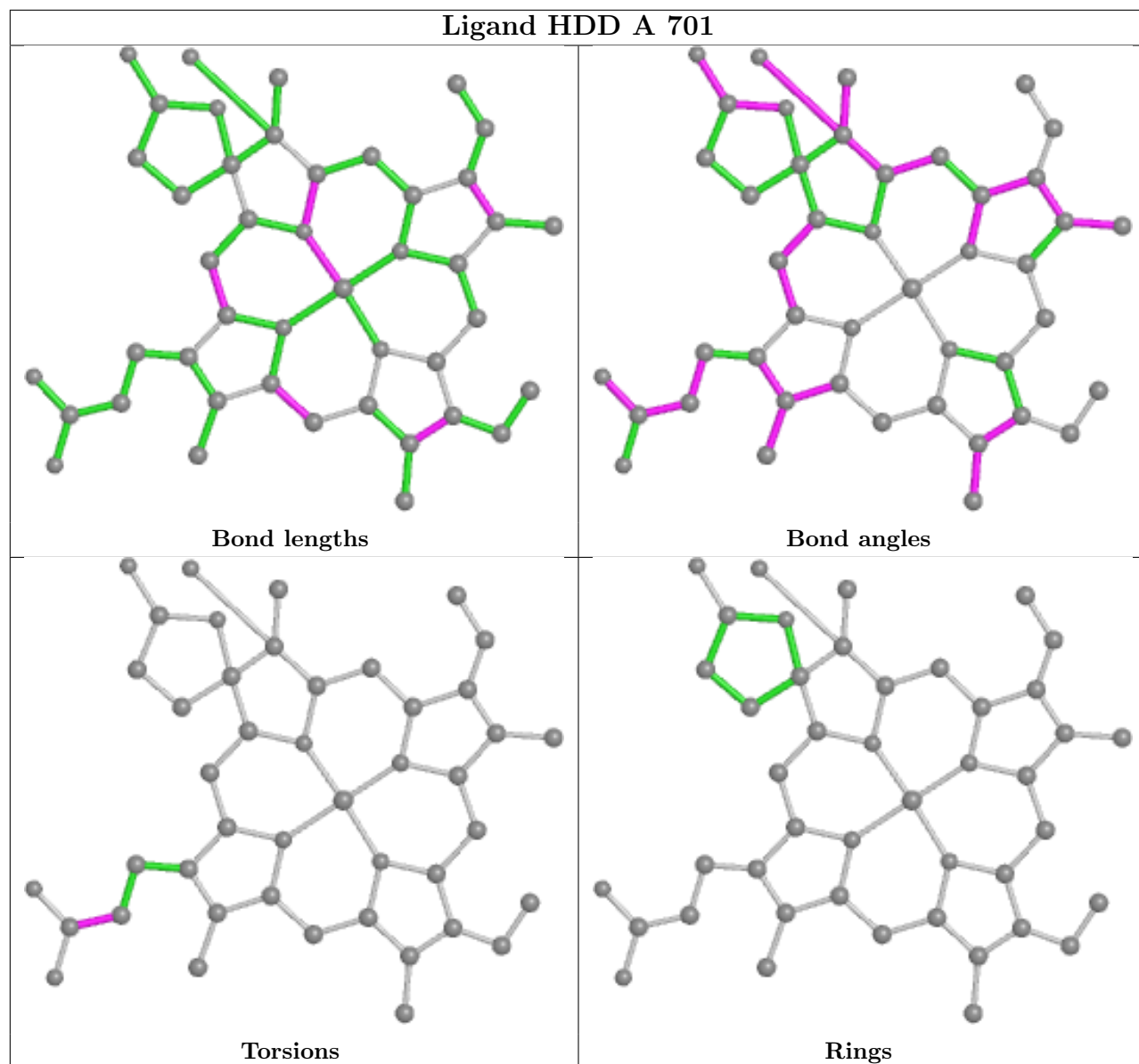
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	701	HDD	1	0
2	B	701	HDD	1	0
2	A	701	HDD	2	0
2	D	702	HDD	2	0

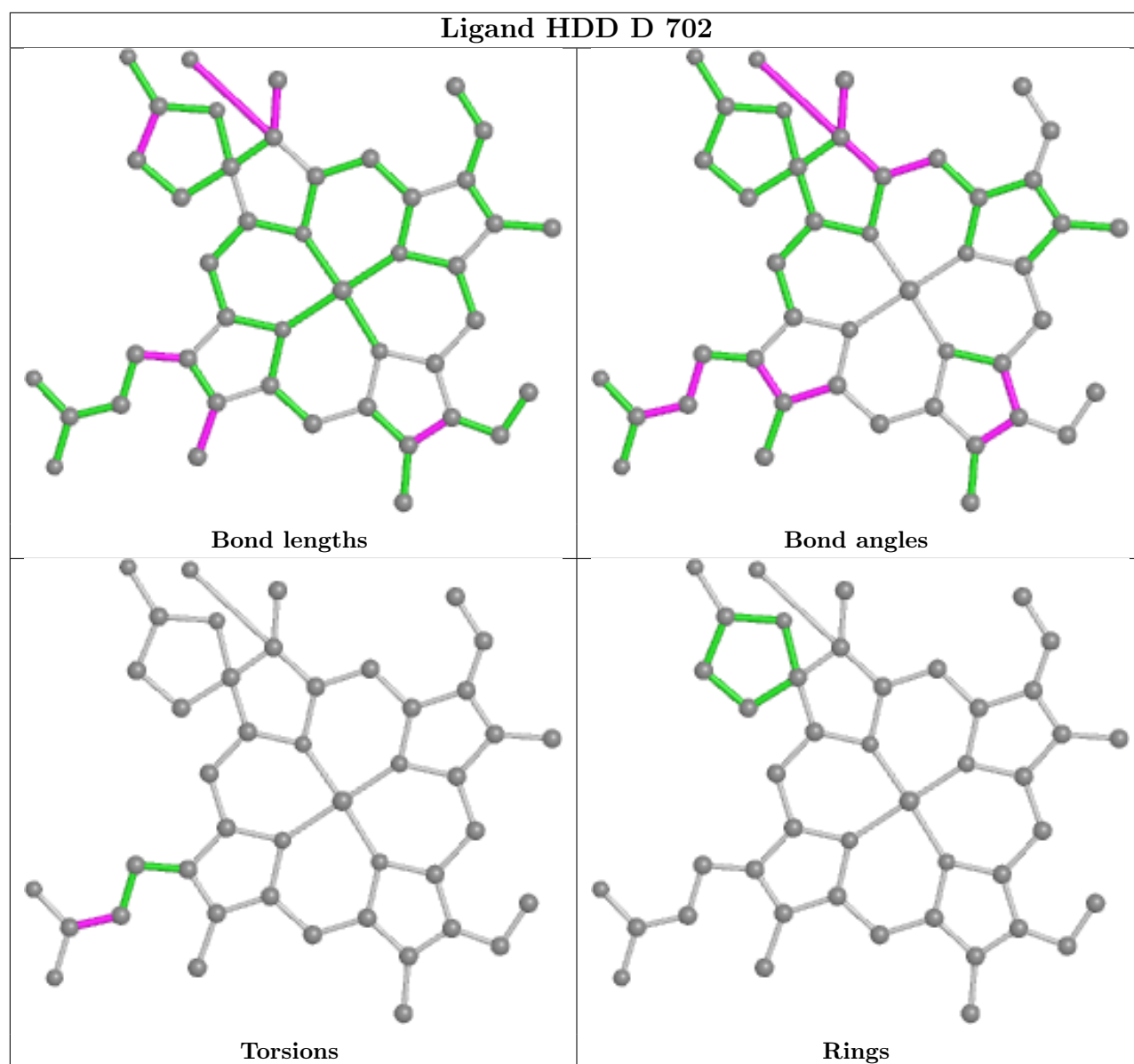
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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	674/720 (93%)	-0.24	20 (2%) 50 49	6, 12, 32, 59	0
1	B	678/720 (94%)	-0.22	23 (3%) 45 44	6, 13, 34, 72	0
1	C	676/720 (93%)	-0.42	3 (0%) 92 91	6, 12, 22, 62	0
1	D	678/720 (94%)	-0.31	5 (0%) 87 86	7, 13, 26, 46	0
All	All	2706/2880 (93%)	-0.30	51 (1%) 66 67	6, 12, 28, 72	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	619	SER	6.8
1	A	618	ALA	6.6
1	A	621	ALA	6.2
1	B	652	SER	6.2
1	D	619	SER	5.9
1	C	618	ALA	5.6
1	B	653	SER	5.5
1	A	620	THR	5.4
1	A	619	SER	5.3
1	A	655	VAL	4.8
1	B	655	VAL	4.7
1	B	619	SER	4.5
1	D	620	THR	4.5
1	B	659	ALA	4.5
1	D	621	ALA	4.3
1	B	651	LYS	3.8
1	A	573	ARG	3.8
1	B	657	ASP	3.7
1	B	620	THR	3.7
1	B	654	GLU	3.4
1	A	654	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	649	GLY	3.4
1	B	658	ALA	3.4
1	D	618	ALA	3.2
1	A	657	ASP	3.0
1	A	698	SER	3.0
1	A	672	GLU	3.0
1	B	621	ALA	2.9
1	B	647	VAL	2.8
1	A	648	CYS	2.7
1	B	660	ASP	2.7
1	B	611	ASP	2.7
1	B	672	GLU	2.7
1	A	660	ASP	2.6
1	A	659	ALA	2.5
1	B	618	ALA	2.5
1	D	517	GLY	2.5
1	B	650	GLY	2.3
1	A	676[A]	MET	2.3
1	B	648	CYS	2.2
1	B	559[A]	SER	2.2
1	B	561	SER	2.2
1	A	614	ALA	2.2
1	C	20	GLN	2.2
1	A	677	PHE	2.1
1	A	617	PHE	2.1
1	A	649	GLY	2.1
1	B	676	MET	2.1
1	A	615	ALA	2.1
1	B	565	ASP	2.0
1	A	658	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands

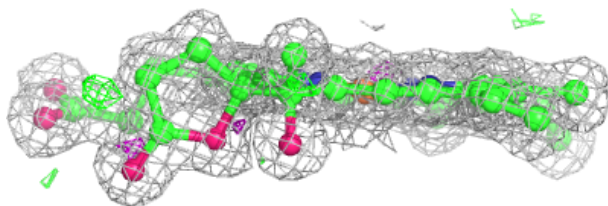
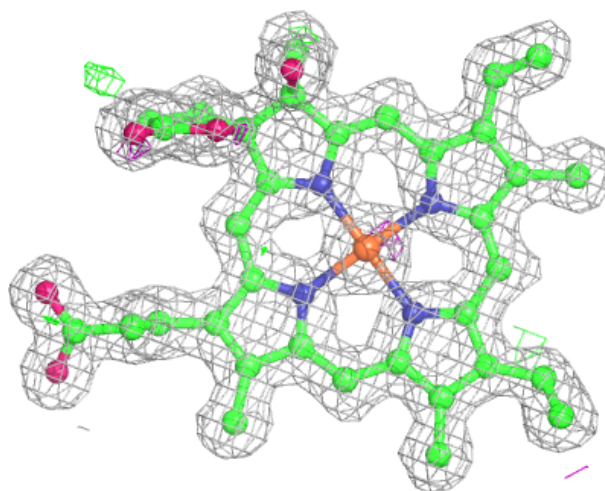
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ALA	D	701	5/6	0.83	0.11	22,24,25,26	0
3	CA	B	703	1/1	0.96	0.07	18,18,18,18	1
2	HDD	C	701	44/44	0.99	0.06	6,7,10,11	0
2	HDD	D	702	44/44	0.99	0.06	7,8,10,12	0
3	CA	A	703	1/1	0.99	0.04	14,14,14,14	1
3	CA	A	704	1/1	0.99	0.04	11,11,11,11	1
3	CA	B	702	1/1	0.99	0.04	14,14,14,14	0
2	HDD	A	701	44/44	0.99	0.07	7,8,10,13	0
3	CA	C	703	1/1	0.99	0.05	14,14,14,14	1
3	CA	D	704	1/1	0.99	0.08	15,15,15,15	1
2	HDD	B	701	44/44	0.99	0.07	7,8,10,12	0
3	CA	D	703	1/1	1.00	0.03	15,15,15,15	0
3	CA	C	702	1/1	1.00	0.05	9,9,9,9	1
3	CA	A	702	1/1	1.00	0.03	12,12,12,12	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.

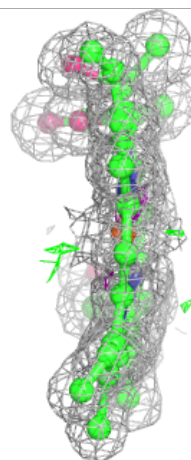
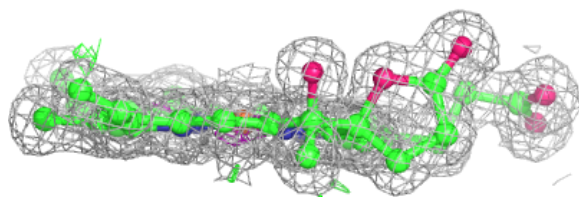
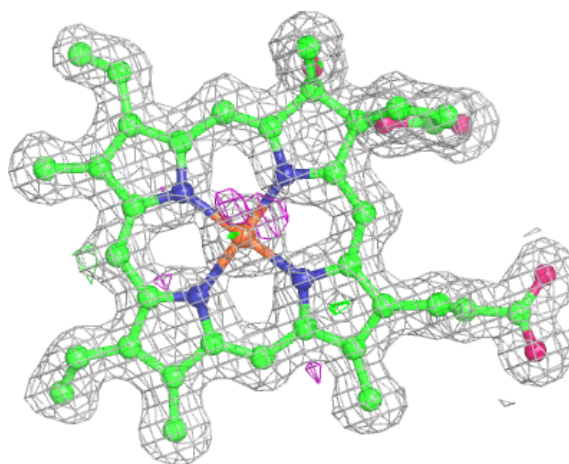
Electron density around HDD C 701:

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



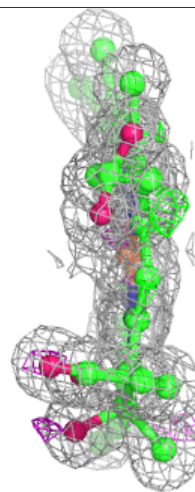
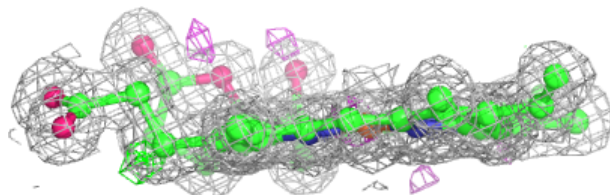
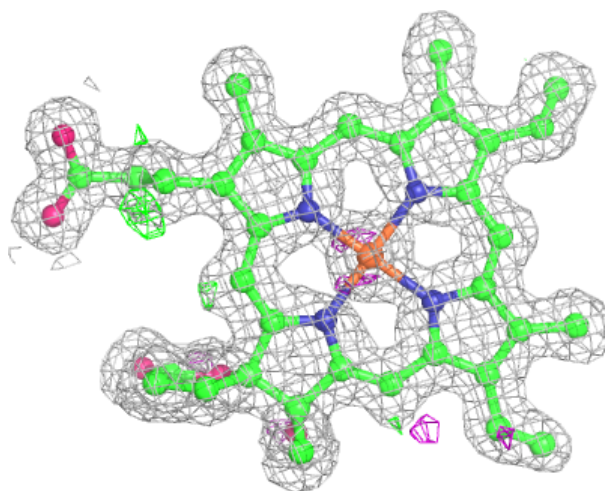
Electron density around HDD D 702:

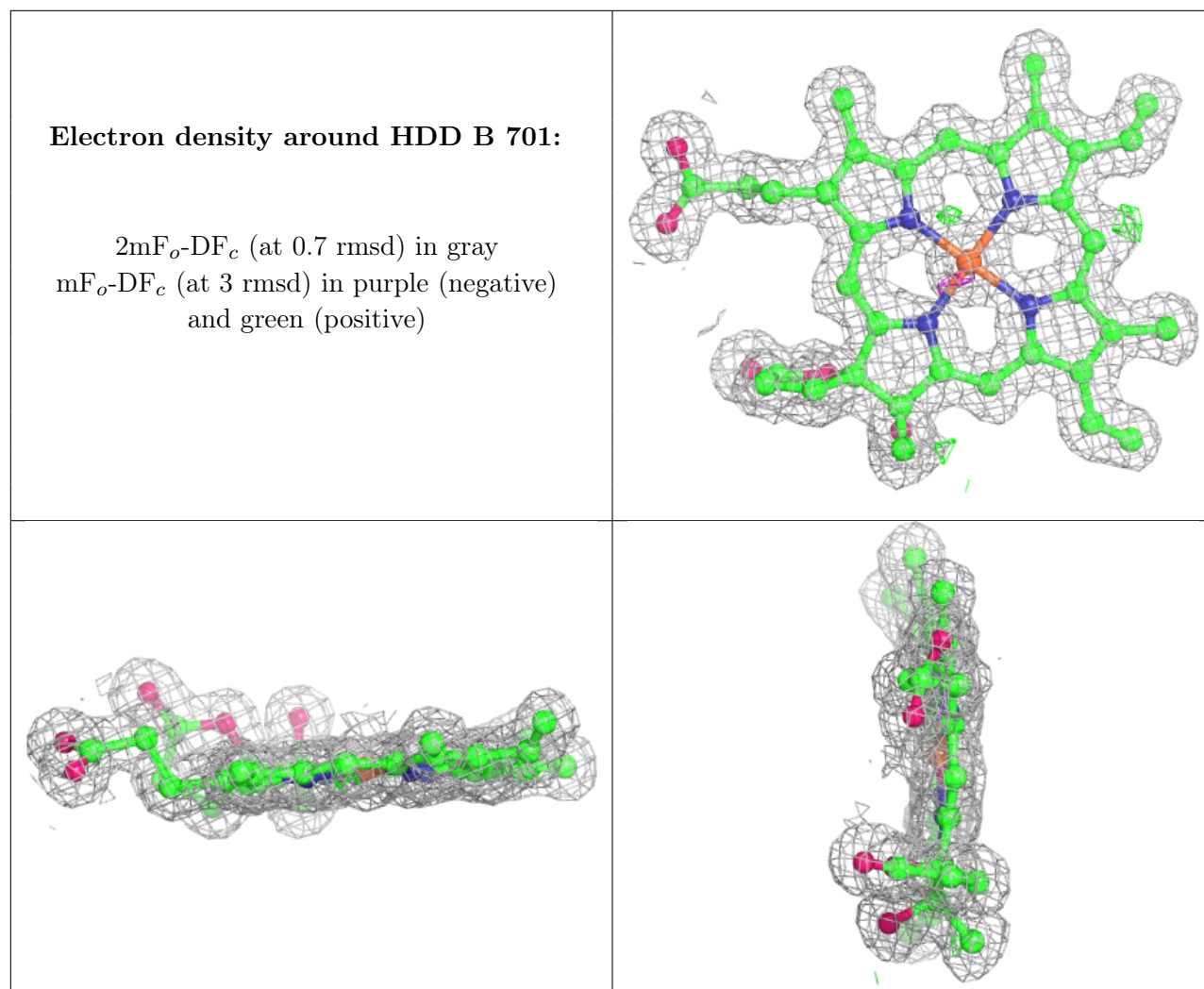
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HDD A 701:

$2mF_o-DF_c$ (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.