



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 01:50 am BST

PDB ID : 5ZZ1  
Title : Probing the active center of catalase-phenol oxidase from *Scytalidium thermophilum*  
Authors : Yuzugullu Karakus, Y.; Trinh, C.H.; Pearson, A.R.; Ogel, Z.B.; McPherson, M.J.  
Deposited on : 2018-05-29  
Resolution : 1.91 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](mailto: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.

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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 : 2.11  
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) : 2.11

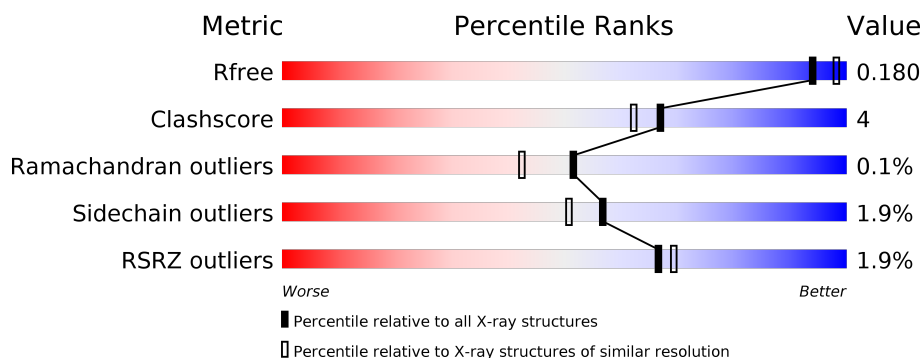
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.91 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	719	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>8%</div> <div>6%</div> </div> </div>
1	B	719	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>6%</div> </div> </div>
1	C	719	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>6%</div> </div> </div>
1	D	719	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>6%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23217 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	677	Total	C	N	O	S	0	14	0
			5372	3397	940	1023	12			
1	B	678	Total	C	N	O	S	0	4	0
			5314	3356	930	1017	11			
1	C	678	Total	C	N	O	S	0	6	0
			5327	3365	931	1019	12			
1	D	678	Total	C	N	O	S	0	7	0
			5329	3363	932	1022	12			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
B	-20	GLY	-	expression tag	UNP M4GGR7

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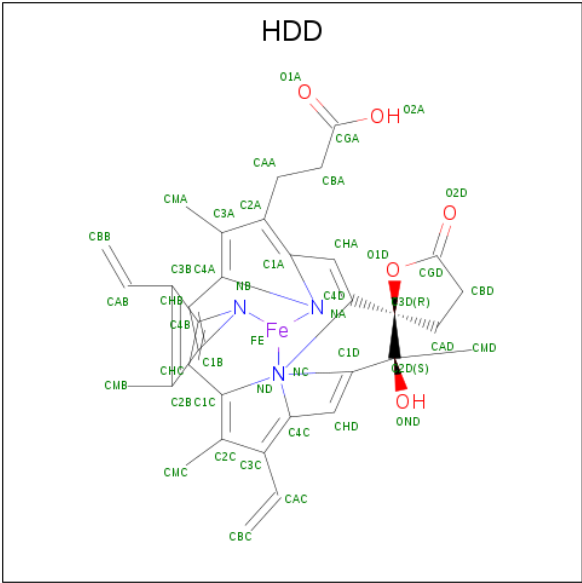
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	SER	-	expression tag	UNP M4GGR7
B	-18	SER	-	expression tag	UNP M4GGR7
B	-17	HIS	-	expression tag	UNP M4GGR7
B	-16	HIS	-	expression tag	UNP M4GGR7
B	-15	HIS	-	expression tag	UNP M4GGR7
B	-14	HIS	-	expression tag	UNP M4GGR7
B	-13	HIS	-	expression tag	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
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
C	-2	GLY	-	expression tag	UNP M4GGR7
C	-1	HIS	-	expression tag	UNP M4GGR7
D	-20	GLY	-	expression tag	UNP M4GGR7
D	-19	SER	-	expression tag	UNP M4GGR7
D	-18	SER	-	expression tag	UNP M4GGR7

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- Molecule 2 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (three-letter code: HDD) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>5</sub>).



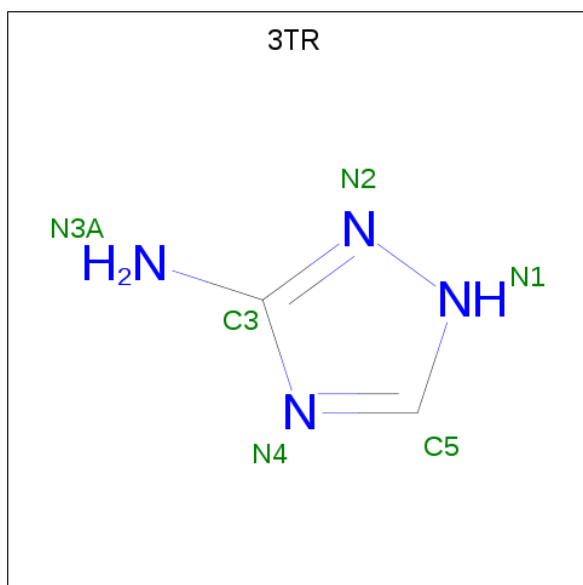
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		
2	B	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		

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

- Molecule 3 is 3-AMINO-1,2,4-TRIAZOLE (three-letter code: 3TR) (formula: C<sub>2</sub>H<sub>4</sub>N<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			6	2	4		
3	A	1	Total	C	N	0	0
			6	2	4		
3	B	1	Total	C	N	0	0
			6	2	4		
3	B	1	Total	C	N	0	0
			6	2	4		
3	B	1	Total	C	N	0	0
			6	2	4		
3	C	1	Total	C	N	0	0
			6	2	4		
3	C	1	Total	C	N	0	0
			6	2	4		
3	D	1	Total	C	N	0	0
			6	2	4		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

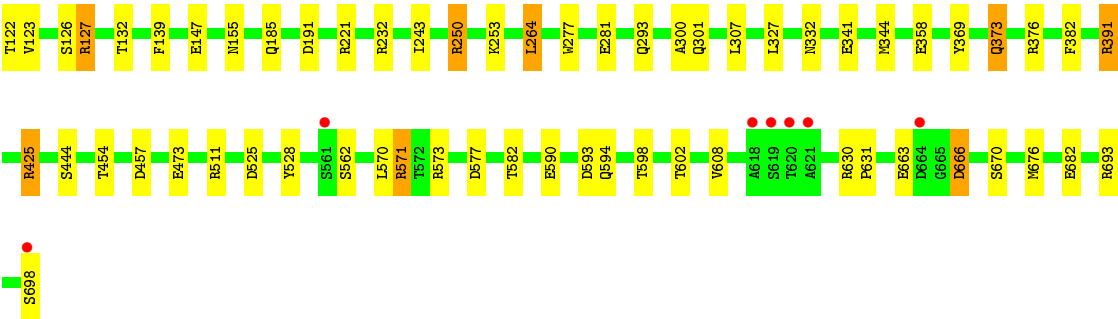
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Ca 2 2	0	0
4	A	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0

- Molecule 5 is water.

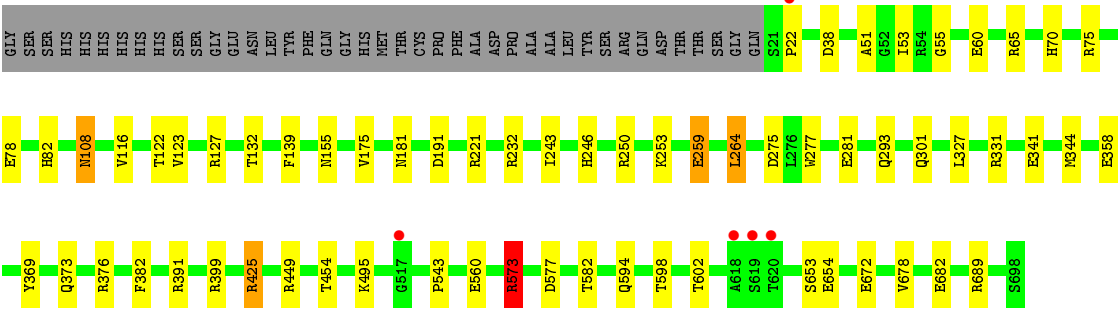
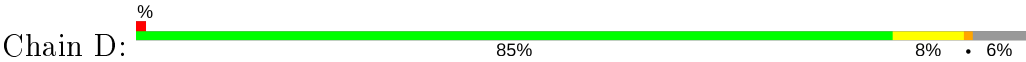
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	409	Total O 409 409	0	0
5	B	411	Total O 411 411	0	0
5	C	432	Total O 432 432	0	0
5	D	394	Total O 394 394	0	0







● Molecule 1: Catalase



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.53Å 121.68Å 185.45Å 90.00° 102.16° 90.00°	Depositor
Resolution (Å)	29.40 – 1.91 29.38 – 1.91	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.40-1.91) 98.8 (29.38-1.91)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.16 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, $R_{free}$	0.142 , 0.174 0.152 , 0.180	Depositor DCC
$R_{free}$ test set	10381 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.6	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	23217	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.66 % 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 3.5656e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CA, HDD, 3TR

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	0.80	8/5539 (0.1%)	0.92	13/7530 (0.2%)
1	B	0.78	4/5457 (0.1%)	0.91	11/7420 (0.1%)
1	C	0.82	5/5473 (0.1%)	0.94	17/7443 (0.2%)
1	D	0.81	8/5476 (0.1%)	0.94	15/7445 (0.2%)
All	All	0.80	25/21945 (0.1%)	0.93	56/29838 (0.2%)

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	A	0	4
1	B	0	6
1	C	0	4
1	D	0	3
All	All	0	17

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	341	GLU	CD-OE2	8.57	1.35	1.25
1	B	358	GLU	CD-OE1	7.54	1.33	1.25
1	A	78	GLU	CD-OE1	6.61	1.32	1.25
1	D	672	GLU	CD-OE2	-6.56	1.18	1.25
1	C	281	GLU	CD-OE2	6.50	1.32	1.25
1	C	358	GLU	CD-OE1	6.49	1.32	1.25
1	C	473	GLU	CD-OE1	6.42	1.32	1.25
1	C	341	GLU	CD-OE2	6.23	1.32	1.25
1	D	281	GLU	CD-OE2	5.93	1.32	1.25
1	A	78	GLU	CD-OE2	5.92	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	GLU	CD-OE1	5.89	1.32	1.25
1	A	281	GLU	CD-OE2	5.76	1.31	1.25
1	D	358	GLU	CD-OE1	5.69	1.31	1.25
1	B	621	ALA	C-O	-5.60	1.12	1.23
1	D	78	GLU	CD-OE1	5.47	1.31	1.25
1	A	680	GLU	CD-OE2	-5.43	1.19	1.25
1	C	147	GLU	CD-OE1	5.38	1.31	1.25
1	D	573[A]	ARG	CD-NE	-5.32	1.37	1.46
1	D	573[B]	ARG	CD-NE	-5.32	1.37	1.46
1	A	542	GLY	N-CA	5.26	1.53	1.46
1	B	127[A]	ARG	C-O	-5.23	1.13	1.23
1	B	127[B]	ARG	C-O	-5.23	1.13	1.23
1	D	341	GLU	CD-OE2	5.17	1.31	1.25
1	D	60	GLU	CD-OE1	5.06	1.31	1.25
1	A	484	GLU	CD-OE1	5.06	1.31	1.25

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	573[A]	ARG	NE-CZ-NH2	-13.96	113.32	120.30
1	D	573[B]	ARG	NE-CZ-NH2	-13.96	113.32	120.30
1	A	425[A]	ARG	NE-CZ-NH1	-9.30	115.65	120.30
1	A	425[B]	ARG	NE-CZ-NH1	-9.30	115.65	120.30
1	D	573[A]	ARG	CG-CD-NE	-9.28	92.32	111.80
1	D	573[B]	ARG	CG-CD-NE	-9.28	92.32	111.80
1	B	65	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	B	573	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	B	425	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	B	573	ARG	NE-CZ-NH1	8.59	124.60	120.30
1	A	391	ARG	NE-CZ-NH1	-8.24	116.18	120.30
1	A	425[A]	ARG	NE-CZ-NH2	8.22	124.41	120.30
1	A	425[B]	ARG	NE-CZ-NH2	8.22	124.41	120.30
1	D	399	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	A	573	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	B	391	ARG	NE-CZ-NH1	-8.10	116.25	120.30
1	A	573	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	D	65	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	C	573	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	C	573	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	B	425	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	C	391	ARG	NE-CZ-NH2	6.86	123.73	120.30
1	D	425	ARG	NE-CZ-NH1	6.77	123.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	D	376	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	C	232	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	C	127[A]	ARG	NE-CZ-NH1	-6.57	117.02	120.30
1	C	127[B]	ARG	NE-CZ-NH1	-6.57	117.02	120.30
1	C	65	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	C	425	ARG	CG-CD-NE	-6.38	98.41	111.80
1	B	21	SER	O-C-N	-6.05	109.61	121.10
1	A	331[A]	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	A	331[B]	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	C	693	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	D	425	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	D	449	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	C	391	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	A	65	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	D	221	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	C	250	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	C	511	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	C	221	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	B	399	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	D	232	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	D	259	GLU	CB-CA-C	-5.23	99.93	110.40
1	C	571	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	D	259	GLU	CB-CG-CD	5.18	128.17	114.20
1	B	571	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	C	425	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	C	666	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	C	376	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	232	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	21	SER	O-C-N	-5.11	111.40	121.10
1	A	220	TYR	CB-CG-CD1	5.03	124.02	121.00
1	B	232	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	D	689	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	250	ARG	Sidechain
1	A	425[A]	ARG	Sidechain
1	A	573	ARG	Sidechain
1	A	75	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	21	SER	Peptide
1	B	250	ARG	Sidechain
1	B	331	ARG	Sidechain
1	B	409	ARG	Sidechain
1	B	640	ARG	Sidechain
1	B	75	ARG	Sidechain
1	C	127[A]	ARG	Sidechain
1	C	250	ARG	Sidechain
1	C	425	ARG	Sidechain
1	C	75	ARG	Sidechain
1	D	250	ARG	Sidechain
1	D	425	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	5372	0	5178	50	0
1	B	5314	0	5094	36	1
1	C	5327	0	5108	40	0
1	D	5329	0	5113	33	0
2	A	44	0	31	5	0
2	B	44	0	31	1	0
2	C	44	0	31	2	0
2	D	44	0	31	3	0
3	A	12	0	8	0	0
3	B	18	0	12	0	0
3	C	12	0	8	1	0
3	D	6	0	4	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	409	0	0	17	0
5	B	411	0	0	10	0
5	C	432	0	0	9	0
5	D	394	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	23217	0	20649	163	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 4.

All (163) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589[B]:ARG:CG	1:A:589[B]:ARG:HH11	1.42	1.26
1:B:127[B]:ARG:NH2	5:B:1802:HOH:O	1.65	1.26
1:B:21:SER:HA	5:B:2086:HOH:O	1.41	1.20
1:A:589[B]:ARG:NH1	1:A:589[B]:ARG:HG2	1.27	1.19
1:D:127[A]:ARG:O	5:D:801:HOH:O	1.77	1.03
1:B:389:MET:SD	5:B:2144:HOH:O	2.19	1.00
1:B:313:ILE:H	1:B:461:GLN:HE22	1.20	0.88
1:C:663:GLU:OE1	5:C:801:HOH:O	1.91	0.88
2:A:701:HDD:HBD2	5:A:803:HOH:O	1.73	0.88
1:A:676:MET:SD	5:A:983:HOH:O	2.36	0.84
2:A:701:HDD:CGD	5:A:803:HOH:O	2.26	0.83
1:A:648:CYS:SG	5:A:873:HOH:O	2.35	0.83
2:A:701:HDD:CBD	5:A:803:HOH:O	2.27	0.82
3:C:703:3TR:H5	5:C:1071:HOH:O	1.79	0.81
1:C:253:LYS:HD2	5:C:1203:HOH:O	1.82	0.80
1:A:253:LYS:HG2	5:A:1109:HOH:O	1.83	0.79
1:A:475:GLN:NE2	1:A:697:ASP:H	1.81	0.78
1:A:127[B]:ARG:O	5:A:802:HOH:O	2.02	0.77
1:A:160:PHE:CD1	5:A:1167:HOH:O	2.38	0.75
1:B:70:HIS:CD2	5:B:1863:HOH:O	2.38	0.75
1:B:253:LYS:HE3	5:B:1955:HOH:O	1.88	0.74
1:D:253:LYS:HG3	5:D:1138:HOH:O	1.87	0.74
1:B:655:VAL:HG23	5:B:2065:HOH:O	1.89	0.73
1:B:264:LEU:HG	1:B:602:THR:HB	1.72	0.72
1:D:22:PRO:HB3	1:D:391:ARG:NH2	2.05	0.72
1:A:264:LEU:HG	1:A:602:THR:HB	1.73	0.70
1:C:373:GLN:HE21	1:C:373:GLN:HA	1.57	0.69
1:A:582:THR:HG21	1:A:594:GLN:HE21	1.57	0.69
1:A:589[B]:ARG:CG	1:A:589[B]:ARG:NH1	2.14	0.69
1:B:373:GLN:HA	1:B:373:GLN:HE21	1.56	0.69
1:D:654:GLU:OE1	5:D:802:HOH:O	2.11	0.68
1:B:389:MET:HE3	5:B:2211:HOH:O	1.94	0.67
1:C:22:PRO:HB3	1:C:391:ARG:NH2	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:LYS:HG2	5:C:1202:HOH:O	1.96	0.66
1:B:38:ASP:OD2	1:B:70:HIS:HE1	1.76	0.66
1:A:100:ASN:HB2	5:A:1183:HOH:O	1.96	0.65
1:D:264:LEU:HG	1:D:602:THR:HB	1.78	0.65
1:A:373:GLN:HE21	1:A:373:GLN:HA	1.61	0.64
1:A:160:PHE:CE1	5:A:1167:HOH:O	2.51	0.64
1:B:22:PRO:O	1:B:26:TYR:HD2	1.82	0.62
2:D:701:HDD:HBC1	2:D:701:HDD:HMC1	1.80	0.61
1:C:126:SER:H	1:C:185:GLN:HE22	1.49	0.61
1:C:264:LEU:HG	1:C:602:THR:HB	1.81	0.60
1:C:570:LEU:HD11	1:C:608:VAL:HG11	1.84	0.60
1:B:160:PHE:CE1	5:B:2186:HOH:O	2.54	0.60
1:C:70:HIS:CE1	5:C:805:HOH:O	2.55	0.59
1:C:253:LYS:CG	5:C:1202:HOH:O	2.50	0.59
1:B:277[A]:TRP:CZ3	1:D:181:ASN:HB3	2.39	0.58
1:D:582:THR:HG21	1:D:594:GLN:HE21	1.69	0.58
1:B:160:PHE:CD1	5:B:2186:HOH:O	2.53	0.57
1:B:181:ASN:HB3	1:D:277:TRP:CZ3	2.40	0.56
1:A:181:ASN:HB3	1:C:277[A]:TRP:CZ3	2.40	0.56
1:B:38:ASP:OD2	1:B:70:HIS:CE1	2.58	0.56
1:B:573:ARG:HG3	1:B:678:VAL:HG11	1.86	0.55
1:B:132:THR:HG21	1:B:264:LEU:HD13	1.89	0.54
1:B:277[A]:TRP:CE3	1:D:181:ASN:HB3	2.42	0.54
1:C:132:THR:HG21	1:C:264:LEU:HD13	1.89	0.54
1:D:132:THR:HG21	1:D:264:LEU:HD13	1.89	0.54
1:A:259:GLU:HG3	5:A:1097:HOH:O	2.06	0.54
1:C:126:SER:H	1:C:185:GLN:NE2	2.05	0.54
1:A:680:GLU:HG3	5:A:894:HOH:O	2.07	0.54
1:B:253:LYS:HD2	5:B:2182:HOH:O	2.07	0.53
1:A:132:THR:HG21	1:A:264:LEU:HD13	1.91	0.53
1:A:108:ASN:HD22	1:A:108:ASN:C	2.13	0.52
1:D:301:GLN:HE22	1:D:454:THR:HG21	1.73	0.52
1:A:611:ASP:CG	1:A:649:GLY:HA3	2.30	0.52
2:B:1702:HDD:HMB1	2:B:1702:HDD:HBB1	1.92	0.52
1:C:22:PRO:CB	1:C:391:ARG:NH2	2.73	0.51
1:A:22:PRO:O	1:A:26:TYR:HD2	1.94	0.51
1:C:82:HIS:HA	1:C:122:THR:O	2.11	0.51
1:C:301:GLN:HE22	1:C:454:THR:HG21	1.76	0.50
1:A:475:GLN:HE22	1:A:697:ASP:H	1.54	0.50
2:C:701:HDD:HMB1	2:C:701:HDD:HBB1	1.94	0.50
1:A:525:ASP:HA	1:A:528:TYR:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ASN:C	1:B:108:ASN:HD22	2.16	0.49
1:D:560:GLU:CD	5:D:957:HOH:O	2.51	0.49
1:A:376:ARG:CD	5:A:803:HOH:O	2.61	0.49
1:A:582:THR:HG21	1:A:594:GLN:NE2	2.28	0.48
1:A:82:HIS:HA	1:A:122:THR:O	2.13	0.48
1:C:27:GLU:OE2	5:C:802:HOH:O	2.20	0.48
1:C:594:GLN:HG3	1:C:598:THR:OG1	2.14	0.48
1:C:670:SER:HB2	5:C:1122:HOH:O	2.14	0.48
1:D:82:HIS:HA	1:D:122:THR:O	2.14	0.48
1:B:301:GLN:HE22	1:B:454:THR:HG21	1.79	0.48
1:C:155:ASN:CG	2:C:701:HDD:HMB2	2.33	0.48
1:D:82:HIS:CE1	1:D:123:VAL:HG22	2.48	0.48
1:C:373:GLN:HE21	1:C:373:GLN:CA	2.22	0.47
1:A:181:ASN:HB3	1:C:277[A]:TRP:CE3	2.50	0.47
1:B:373:GLN:HA	1:B:373:GLN:NE2	2.27	0.47
1:A:570:LEU:HD11	1:A:608:VAL:HG11	1.95	0.47
1:B:313:ILE:N	1:B:461:GLN:HE22	1.99	0.47
2:D:701:HDD:HBB1	2:D:701:HDD:HMB1	1.95	0.47
1:D:51:ALA:O	1:D:55:GLY:HA3	2.14	0.47
1:B:82:HIS:HA	1:B:122:THR:O	2.14	0.47
1:C:82:HIS:CE1	1:C:123:VAL:HG22	2.49	0.47
1:A:450[B]:GLU:HB2	1:C:53:ILE:CD1	2.45	0.47
1:C:300:ALA:HA	1:C:307:LEU:HD12	1.97	0.47
1:D:331:ARG:HD3	5:D:1122:HOH:O	2.14	0.47
1:C:108:ASN:HD22	1:C:108:ASN:C	2.18	0.46
1:D:243:ILE:HA	1:D:293:GLN:O	2.15	0.46
1:A:659:ALA:O	1:A:660:ASP:HB2	2.15	0.46
1:C:577:ASP:OD2	1:C:682:GLU:OE2	2.33	0.46
1:A:100:ASN:CB	5:A:1183:HOH:O	2.60	0.46
1:A:676:MET:O	1:A:680:GLU:HG2	2.14	0.46
1:C:676:MET:HE3	5:C:1053:HOH:O	2.15	0.46
1:B:472:VAL:HG11	1:B:691:THR:HB	1.98	0.46
1:A:277[A]:TRP:CH2	1:A:332:ASN:HB3	2.51	0.46
1:A:680:GLU:HA	1:A:680:GLU:OE1	2.16	0.46
1:A:594:GLN:HG3	1:A:598:THR:OG1	2.16	0.45
1:A:116:VAL:HG21	1:A:327[A]:LEU:HD11	1.99	0.45
1:B:525:ASP:HA	1:B:528:TYR:CD2	2.51	0.45
1:A:277[A]:TRP:CZ3	1:A:332:ASN:HB3	2.52	0.45
1:B:23:LEU:N	1:B:23:LEU:HD23	2.31	0.45
1:D:246:HIS:HD2	5:D:1091:HOH:O	1.99	0.45
1:D:573[B]:ARG:NH1	1:D:577:ASP:OD2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:TYR:O	1:A:373:GLN:HG2	2.17	0.45
1:D:344:MET:SD	1:D:382:PHE:HB2	2.57	0.45
1:D:155:ASN:CG	2:D:701:HDD:HMB2	2.37	0.45
1:D:108:ASN:HD22	1:D:108:ASN:C	2.21	0.44
1:A:373:GLN:NE2	1:A:373:GLN:HA	2.31	0.44
1:D:495:LYS:HE2	5:D:1180:HOH:O	2.17	0.44
1:A:585:ALA:O	1:A:595:THR:HA	2.18	0.44
1:B:51:ALA:O	1:B:55:GLY:HA3	2.18	0.44
1:C:369:TYR:O	1:C:373:GLN:HG2	2.18	0.44
1:A:376:ARG:HD2	5:A:803:HOH:O	2.17	0.44
1:C:571:ARG:NH2	1:C:593:ASP:OD2	2.38	0.44
1:D:38:ASP:OD2	1:D:70:HIS:NE2	2.49	0.44
1:B:573:ARG:HG2	1:B:678:VAL:HG21	2.00	0.44
1:C:373:GLN:NE2	1:C:373:GLN:HA	2.29	0.44
1:D:253:LYS:CG	5:D:1138:HOH:O	2.55	0.43
2:A:701:HDD:O2D	5:A:803:HOH:O	2.21	0.43
1:A:243:ILE:HA	1:A:293:GLN:O	2.18	0.43
1:D:175:VAL:HB	5:D:829:HOH:O	2.17	0.43
1:D:301:GLN:NE2	1:D:454:THR:HG21	2.33	0.43
1:B:344:MET:SD	1:B:382:PHE:HB2	2.58	0.43
1:B:659:ALA:HB1	1:B:661:VAL:HG23	2.00	0.43
1:D:577:ASP:OD2	1:D:682:GLU:OE2	2.37	0.42
1:B:582:THR:HG21	1:B:594:GLN:HE21	1.84	0.42
1:C:630:ARG:HB3	1:C:631:PRO:HD3	2.01	0.42
1:D:22:PRO:CB	1:D:391:ARG:NH2	2.78	0.42
1:C:116:VAL:HG21	1:C:327:LEU:HD11	2.00	0.42
1:D:594:GLN:HG3	1:D:598:THR:OG1	2.18	0.42
1:A:301:GLN:NE2	1:A:454:THR:HG21	2.34	0.42
1:C:277[A]:TRP:CZ3	1:C:332:ASN:HB3	2.54	0.42
2:A:701:HDD:HBB1	2:A:701:HDD:HMB1	2.01	0.42
1:C:582:THR:HG21	1:C:594:GLN:HE21	1.83	0.42
1:A:331[B]:ARG:HD3	1:A:331[B]:ARG:HH21	1.66	0.42
1:D:369:TYR:O	1:D:373:GLN:HG2	2.20	0.41
1:A:492[A]:GLU:CG	5:A:838:HOH:O	2.67	0.41
1:C:373:GLN:NE2	1:C:373:GLN:CA	2.84	0.41
1:C:457:ASP:OD1	1:C:457:ASP:C	2.59	0.41
1:D:116:VAL:HG21	1:D:327:LEU:HD11	2.02	0.41
1:C:525:ASP:HA	1:C:528:TYR:CD2	2.56	0.41
1:A:472:VAL:HG11	1:A:691:THR:HB	2.02	0.41
1:C:243:ILE:HA	1:C:293:GLN:O	2.21	0.41
1:D:573[B]:ARG:HG3	1:D:678:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:573:ARG:CG	1:B:678:VAL:HG21	2.52	0.40
1:B:64:PHE:CZ	1:B:68:ILE:HG13	2.56	0.40
1:A:589[B]:ARG:HH11	1:A:589[B]:ARG:HG2	0.48	0.40
1:C:344:MET:SD	1:C:382:PHE:HB2	2.61	0.40
1:A:331[A]:ARG:HG2	1:A:331[A]:ARG:NH2	2.36	0.40
1:A:108:ASN:ND2	1:A:108:ASN:C	2.74	0.40
1:A:301:GLN:HE22	1:A:454:THR:HG21	1.86	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)
1:B:21:SER:OG	1:B:675:ASP:OD2[2_555]	1.72	0.48

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	689/719 (96%)	671 (97%)	17 (2%)	1 (0%)	51	42
1	B	680/719 (95%)	656 (96%)	22 (3%)	2 (0%)	41	31
1	C	682/719 (95%)	661 (97%)	21 (3%)	0	100	100
1	D	683/719 (95%)	665 (97%)	18 (3%)	0	100	100
All	All	2734/2876 (95%)	2653 (97%)	78 (3%)	3 (0%)	51	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	622	SER
1	B	621	ALA
1	A	649	GLY

### 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	574/596 (96%)	560 (98%)	14 (2%)	49	41
1	B	565/596 (95%)	557 (99%)	8 (1%)	67	63
1	C	567/596 (95%)	557 (98%)	10 (2%)	59	53
1	D	568/596 (95%)	557 (98%)	11 (2%)	57	51
All	All	2274/2384 (95%)	2231 (98%)	43 (2%)	57	51

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	SER
1	A	23	LEU
1	A	70	HIS
1	A	108	ASN
1	A	139	PHE
1	A	191	ASP
1	A	264	LEU
1	A	373	GLN
1	A	559	SER
1	A	562	SER
1	A	573	ARG
1	A	651	LYS
1	A	660	ASP
1	A	676	MET
1	B	23	LEU
1	B	70	HIS
1	B	108	ASN
1	B	139	PHE
1	B	191	ASP
1	B	253	LYS
1	B	264	LEU
1	B	373	GLN
1	C	108	ASN
1	C	139	PHE

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Mol	Chain	Res	Type
1	C	191	ASP
1	C	264	LEU
1	C	373	GLN
1	C	444	SER
1	C	562	SER
1	C	590	GLU
1	C	666	ASP
1	C	698	SER
1	D	53	ILE
1	D	108	ASN
1	D	139	PHE
1	D	191	ASP
1	D	259	GLU
1	D	264	LEU
1	D	275	ASP
1	D	543	PRO
1	D	573[A]	ARG
1	D	573[B]	ARG
1	D	653	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	199	GLN
1	A	301	GLN
1	A	373	GLN
1	A	375	ASN
1	A	475	GLN
1	A	594	GLN
1	B	70	HIS
1	B	108	ASN
1	B	301	GLN
1	B	342	GLN
1	B	373	GLN
1	B	375	ASN
1	B	461	GLN
1	B	594	GLN
1	C	108	ASN
1	C	185	GLN
1	C	301	GLN
1	C	342	GLN

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Mol	Chain	Res	Type
1	C	373	GLN
1	C	375	ASN
1	C	594	GLN
1	D	108	ASN
1	D	246	HIS
1	D	301	GLN
1	D	375	ASN
1	D	594	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 5 are monoatomic - leaving 12 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	$\# Z  > 2$
3	3TR	D	702	-	4,6,6	1.68	1 (25%)	0,7,7	0.00	-
3	3TR	C	703	-	4,6,6	3.84	3 (75%)	0,7,7	0.00	-
3	3TR	B	1704	-	4,6,6	4.12	4 (100%)	0,7,7	0.00	-
3	3TR	B	1706	-	4,6,6	2.92	3 (75%)	0,7,7	0.00	-
3	3TR	C	702	-	4,6,6	1.24	0	0,7,7	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HDD	B	1702	1	38,52,52	1.80	9 (23%)	28,89,89	2.55	10 (35%)
3	3TR	B	1703	-	4,6,6	1.29	0	0,7,7	0.00	-
2	HDD	A	701	1,5	38,52,52	1.66	7 (18%)	28,89,89	2.31	15 (53%)
2	HDD	C	701	1,5	38,52,52	1.70	10 (26%)	28,89,89	2.57	11 (39%)
2	HDD	D	701	1,5	38,52,52	1.77	9 (23%)	28,89,89	3.04	13 (46%)
3	3TR	A	703	-	4,6,6	3.20	3 (75%)	0,7,7	0.00	-
3	3TR	A	702	-	4,6,6	0.95	0	0,7,7	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	3TR	D	702	-	-	-	0/1/1/1
3	3TR	C	703	-	-	-	0/1/1/1
3	3TR	B	1704	-	-	-	0/1/1/1
3	3TR	B	1706	-	-	-	0/1/1/1
3	3TR	C	702	-	-	-	0/1/1/1
2	HDD	B	1702	1	-	0/3/89/89	0/1/9/9
3	3TR	B	1703	-	-	-	0/1/1/1
2	HDD	A	701	1,5	-	0/3/89/89	0/1/9/9
2	HDD	C	701	1,5	-	0/3/89/89	0/1/9/9
2	HDD	D	701	1,5	-	0/3/89/89	0/1/9/9
3	3TR	A	703	-	-	-	0/1/1/1
3	3TR	A	702	-	-	-	0/1/1/1

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	703	3TR	C3-N3A	5.12	1.44	1.33
2	D	701	HDD	OND-C2D	4.94	1.52	1.42
2	B	1702	HDD	C3B-C2B	4.81	1.47	1.40
3	B	1704	3TR	C5-N1	4.81	1.41	1.32
3	B	1704	3TR	C3-N4	4.76	1.41	1.34
3	C	703	3TR	C3-N4	4.58	1.41	1.34
3	B	1704	3TR	C3-N3A	4.08	1.42	1.33
2	A	701	HDD	C3C-C2C	4.05	1.46	1.40
3	A	703	3TR	C3-N3A	3.98	1.41	1.33
3	B	1706	3TR	C5-N1	3.70	1.39	1.32
3	A	703	3TR	C5-N1	3.66	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	HDD	C3B-C2B	3.61	1.45	1.40
2	A	701	HDD	OND-C2D	3.50	1.49	1.42
2	C	701	HDD	C4A-NA	-3.40	1.29	1.36
2	B	1702	HDD	O1D-CGD	3.37	1.41	1.35
2	C	701	HDD	OND-C2D	3.35	1.49	1.42
2	C	701	HDD	CMD-C2D	-3.21	1.48	1.53
3	B	1706	3TR	C3-N3A	3.17	1.40	1.33
2	B	1702	HDD	OND-C2D	3.16	1.48	1.42
2	C	701	HDD	C1A-CHA	3.10	1.49	1.41
2	D	701	HDD	CBD-CGD	-3.10	1.43	1.50
3	B	1706	3TR	C3-N4	2.95	1.38	1.34
3	A	703	3TR	C3-N4	2.90	1.38	1.34
3	C	703	3TR	C5-N1	2.87	1.38	1.32
2	B	1702	HDD	C1B-C2B	2.83	1.49	1.42
2	D	701	HDD	CHD-C1D	-2.82	1.31	1.36
2	D	701	HDD	C3B-C2B	2.81	1.44	1.40
2	B	1702	HDD	C1A-CHA	2.81	1.48	1.41
2	A	701	HDD	C1A-CHA	2.80	1.48	1.41
2	D	701	HDD	CMB-C2B	-2.73	1.45	1.51
2	D	701	HDD	C3C-C2C	2.69	1.44	1.40
3	D	702	3TR	C5-N1	2.69	1.37	1.32
2	C	701	HDD	C3B-C2B	2.66	1.44	1.40
2	A	701	HDD	C4C-CHD	2.62	1.48	1.41
2	B	1702	HDD	CMD-C2D	-2.55	1.49	1.53
2	C	701	HDD	CBD-CGD	-2.51	1.45	1.50
2	B	1702	HDD	CAA-C2A	-2.49	1.48	1.52
2	C	701	HDD	C4A-CHB	2.44	1.47	1.41
2	D	701	HDD	C1A-CHA	2.38	1.47	1.41
3	B	1704	3TR	N1-N2	2.32	1.42	1.37
2	C	701	HDD	C1C-NC	-2.31	1.31	1.36
2	A	701	HDD	CHD-C1D	-2.28	1.32	1.36
2	C	701	HDD	C1C-CHC	2.23	1.47	1.41
2	B	1702	HDD	O1D-C3D	2.18	1.50	1.46
2	D	701	HDD	C4A-CHB	2.15	1.47	1.41
2	C	701	HDD	O1D-CGD	2.13	1.39	1.35
2	D	701	HDD	C1A-NA	-2.07	1.31	1.36
2	B	1702	HDD	CMB-C2B	-2.02	1.46	1.51
2	A	701	HDD	C4C-NC	-2.01	1.32	1.36

All (49) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	HDD	C4A-C3A-C2A	-7.96	101.46	107.00
2	D	701	HDD	O1D-CGD-CBD	-6.74	103.39	110.19
2	B	1702	HDD	O1D-CGD-CBD	-6.08	104.05	110.19
2	C	701	HDD	OND-C2D-CMD	-5.79	98.92	109.59
2	B	1702	HDD	O1D-CGD-O2D	5.34	125.57	120.80
2	C	701	HDD	O1D-CGD-O2D	5.19	125.43	120.80
2	A	701	HDD	C4A-C3A-C2A	-4.85	103.62	107.00
2	D	701	HDD	O1D-CGD-O2D	4.79	125.08	120.80
2	B	1702	HDD	CMC-C2C-C3C	4.53	133.15	124.68
2	B	1702	HDD	CAA-CBA-CGA	-4.40	105.28	112.67
2	D	701	HDD	OND-C2D-CMD	-4.26	101.75	109.59
2	C	701	HDD	CMC-C2C-C3C	4.09	132.33	124.68
2	D	701	HDD	C2D-C1D-CHD	-4.03	117.62	124.28
2	C	701	HDD	C4B-C3B-C2B	-4.00	104.10	106.90
2	A	701	HDD	OND-C2D-CMD	-3.86	102.48	109.59
2	D	701	HDD	CAA-CBA-CGA	-3.84	106.22	112.67
2	B	1702	HDD	CMB-C2B-C3B	3.84	131.86	124.68
2	D	701	HDD	CMC-C2C-C3C	3.73	131.65	124.68
2	C	701	HDD	O1D-CGD-CBD	-3.73	106.43	110.19
2	C	701	HDD	CAD-CBD-CGD	3.66	110.22	104.56
2	C	701	HDD	C2D-C1D-CHD	-3.64	118.27	124.28
2	D	701	HDD	CAD-CBD-CGD	3.38	109.79	104.56
2	B	1702	HDD	C4A-C3A-C2A	-3.36	104.66	107.00
2	A	701	HDD	CMC-C2C-C3C	3.34	130.94	124.68
2	B	1702	HDD	OND-C2D-CMD	-3.28	103.56	109.59
2	A	701	HDD	C2D-C1D-CHD	-3.25	118.92	124.28
2	A	701	HDD	O1D-CGD-CBD	-3.04	107.12	110.19
2	A	701	HDD	CMB-C2B-C3B	3.03	130.35	124.68
2	B	1702	HDD	C2D-C1D-CHD	-3.01	119.30	124.28
2	D	701	HDD	CMD-C2D-C1D	3.01	117.98	112.63
2	C	701	HDD	C4A-C3A-C2A	-3.01	104.90	107.00
2	C	701	HDD	CAA-CBA-CGA	-2.75	108.05	112.67
2	A	701	HDD	C4C-CHD-C1D	-2.71	124.74	130.12
2	A	701	HDD	CAA-CBA-CGA	-2.64	108.24	112.67
2	A	701	HDD	C3C-C4C-NC	2.50	112.44	109.21
2	A	701	HDD	OND-C2D-C1D	-2.47	106.91	111.92
2	A	701	HDD	C4B-C3B-C2B	-2.39	105.23	106.90
2	D	701	HDD	C4B-C3B-C2B	-2.37	105.24	106.90
2	C	701	HDD	C3D-C4D-CHA	-2.30	117.52	124.34
2	D	701	HDD	CMA-C3A-C2A	2.29	129.25	124.94
2	A	701	HDD	O1D-C3D-CAD	-2.26	98.77	103.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	HDD	C4C-CHD-C1D	-2.24	125.68	130.12
2	C	701	HDD	CMB-C2B-C3B	2.18	128.76	124.68
2	A	701	HDD	C3D-C4D-CHA	-2.13	118.02	124.34
2	A	701	HDD	CMA-C3A-C2A	2.11	128.93	124.94
2	B	1702	HDD	O1D-C3D-CAD	-2.08	99.10	103.01
2	B	1702	HDD	C4B-C3B-C2B	2.06	108.34	106.90
2	D	701	HDD	C1A-CHA-C4D	-2.05	126.07	130.12
2	A	701	HDD	CBA-CAA-C2A	-2.02	108.77	112.49

There are no chirality outliers.

There are no torsion outliers.

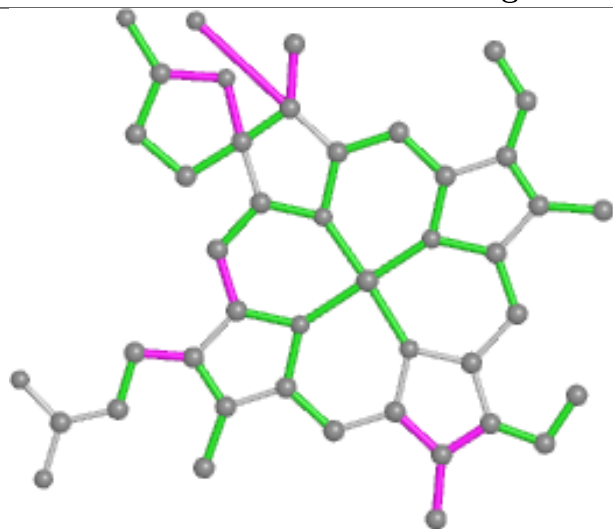
There are no ring outliers.

5 monomers are involved in 12 short contacts:

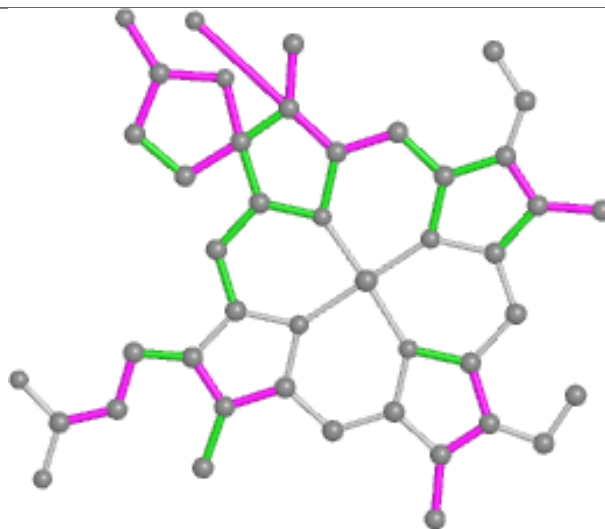
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	703	3TR	1	0
2	B	1702	HDD	1	0
2	A	701	HDD	5	0
2	C	701	HDD	2	0
2	D	701	HDD	3	0

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

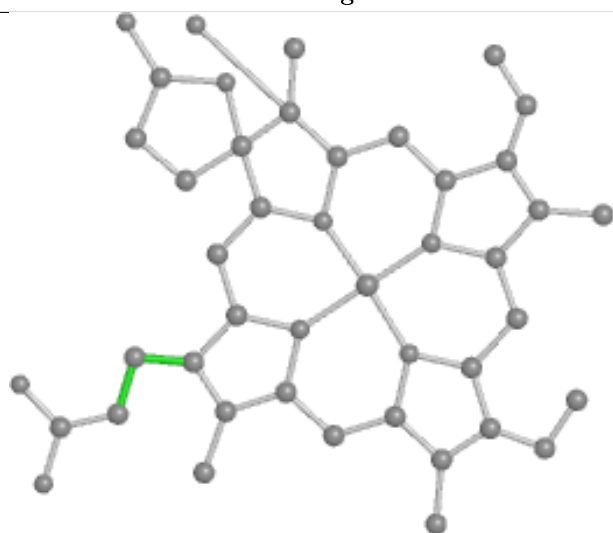
## Ligand HDD B 1702



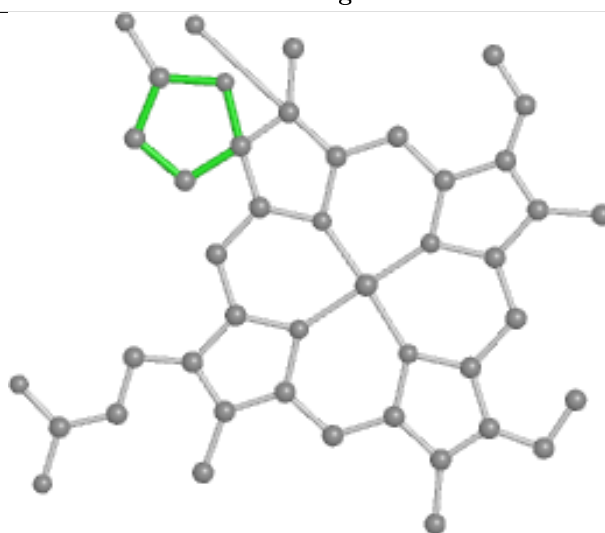
Bond lengths



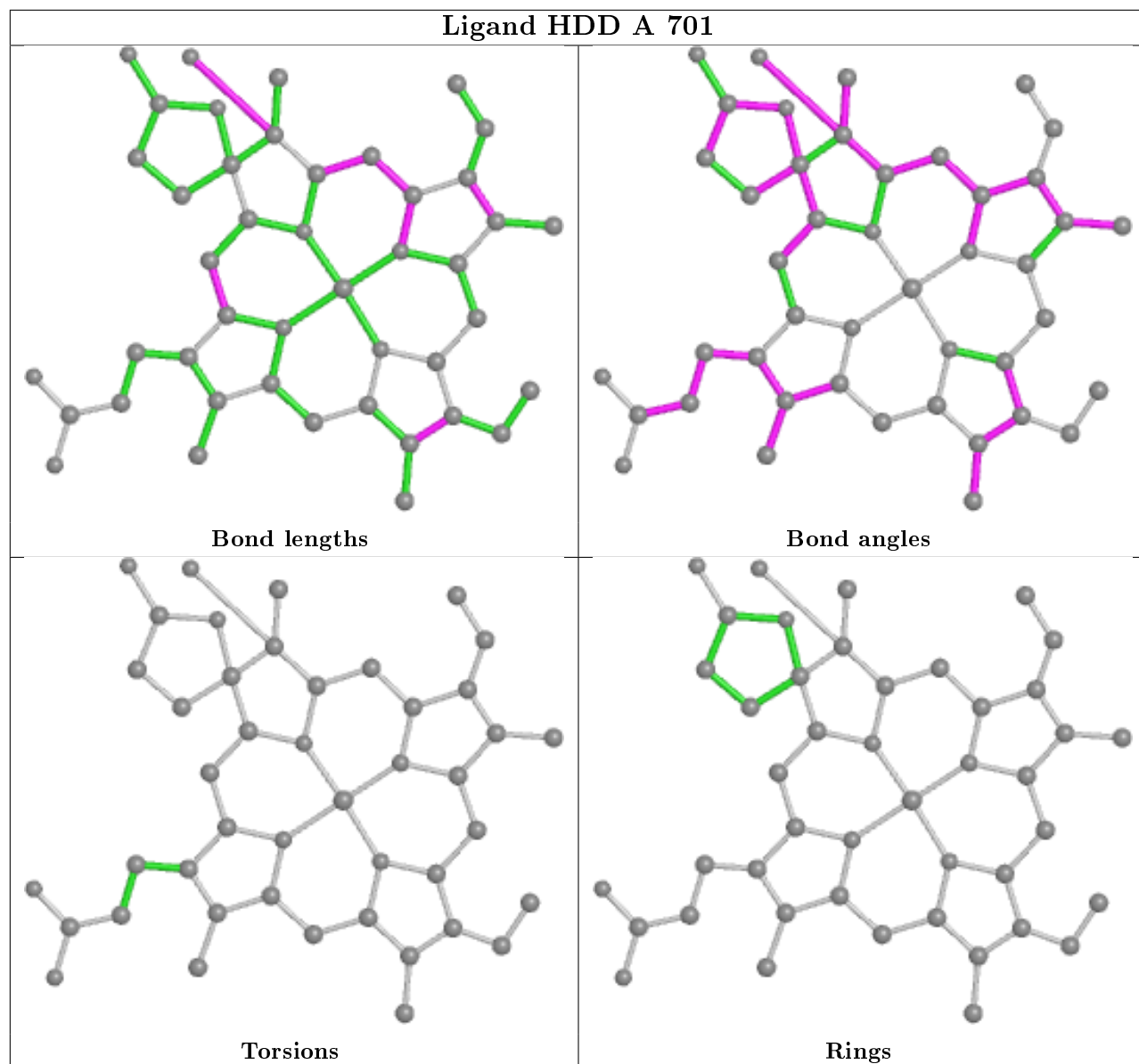
Bond angles

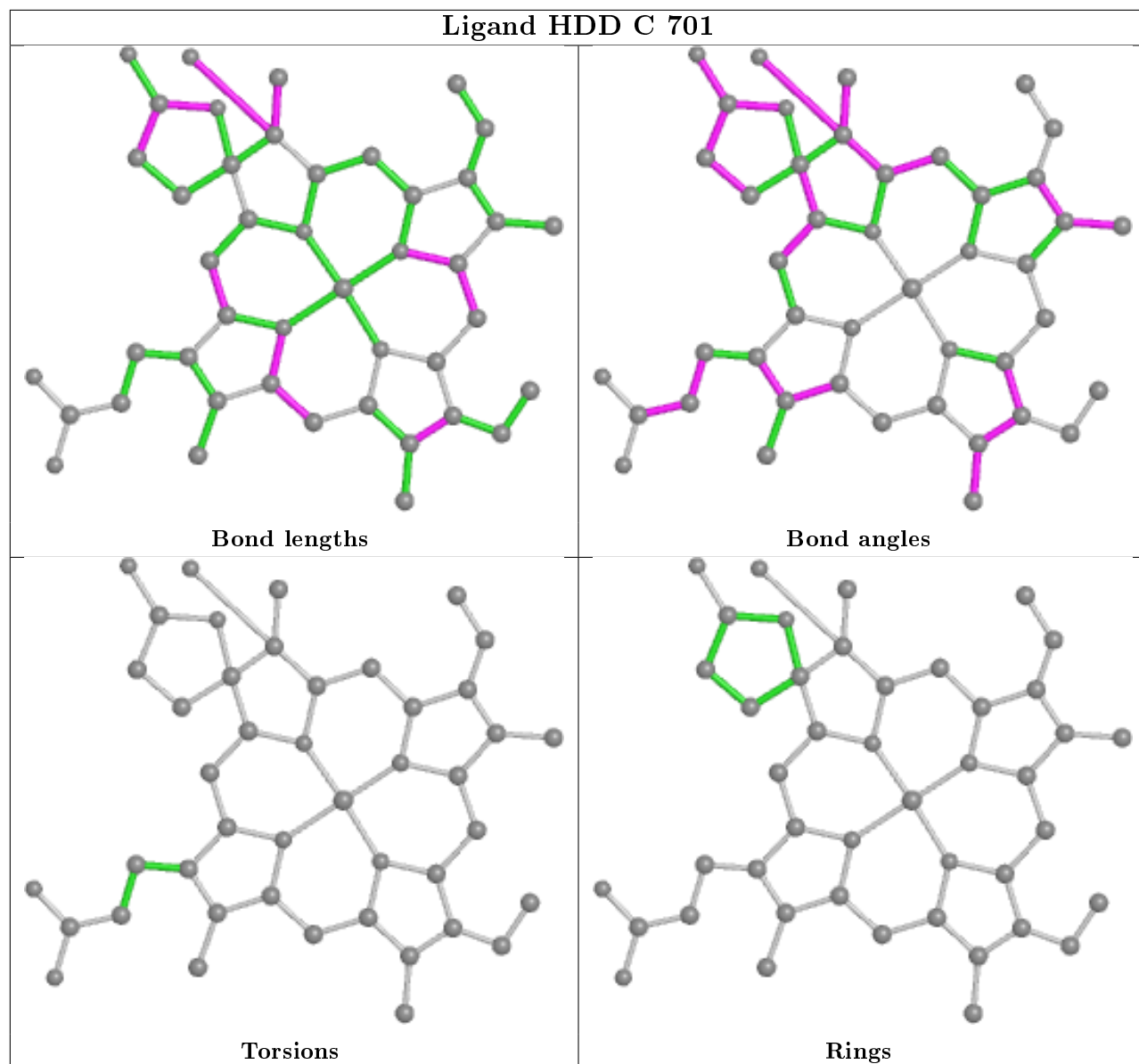


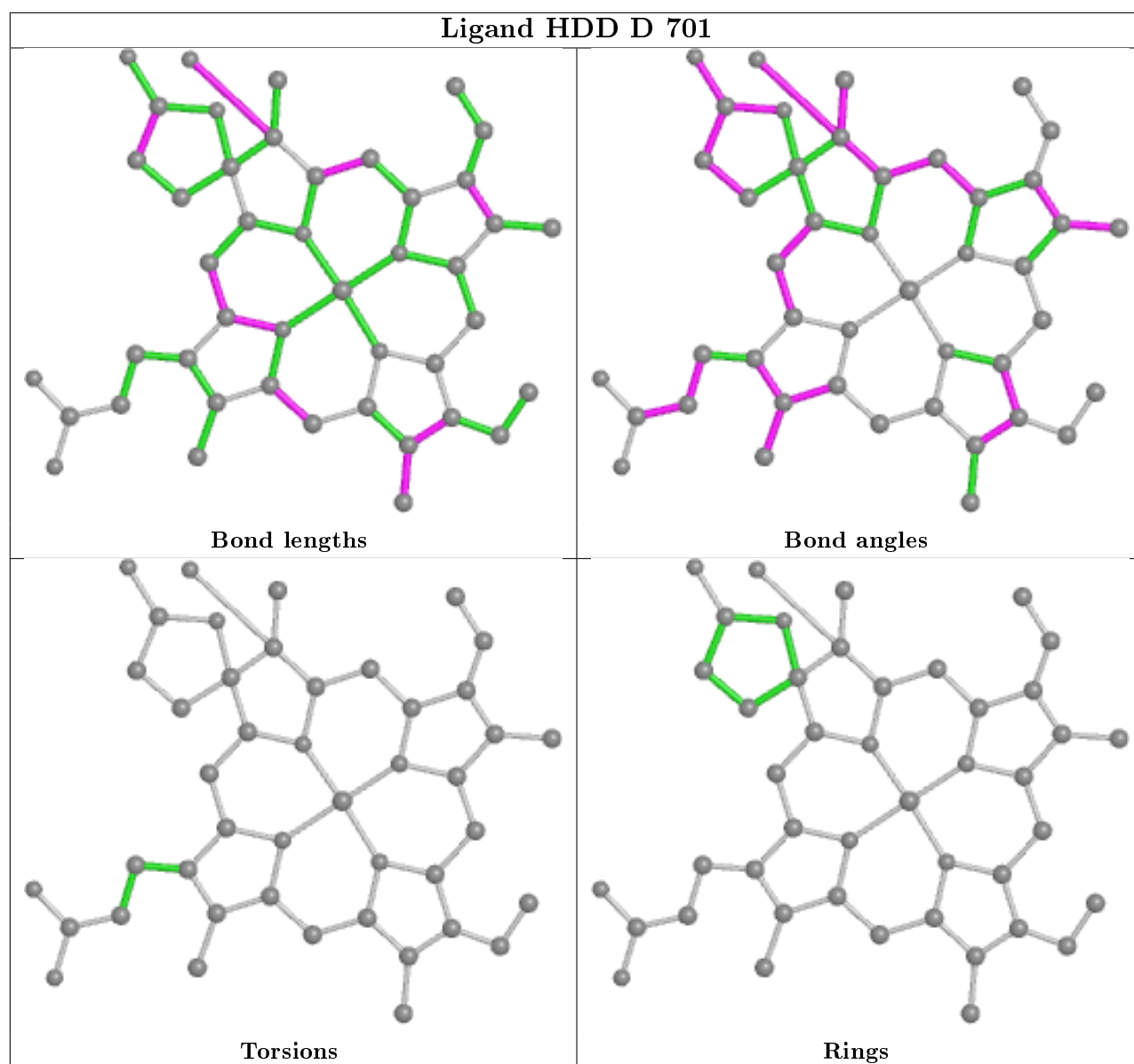
Torsions



Rings







## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	677/719 (94%)	-0.45	18 (2%) 54 57	9, 19, 46, 90	0
1	B	678/719 (94%)	-0.41	21 (3%) 49 52	10, 20, 49, 89	0
1	C	678/719 (94%)	-0.53	8 (1%) 79 81	9, 17, 34, 84	0
1	D	678/719 (94%)	-0.50	5 (0%) 87 89	10, 20, 39, 66	0
All	All	2711/2876 (94%)	-0.47	52 (1%) 66 69	9, 19, 41, 90	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	21	SER	15.7
1	A	21	SER	9.8
1	B	649	GLY	6.6
1	C	620	THR	5.1
1	A	672	GLU	5.0
1	B	620	THR	5.0
1	D	619	SER	4.9
1	C	618	ALA	4.8
1	B	672	GLU	4.7
1	B	653	SER	4.6
1	C	619	SER	4.5
1	B	650	GLY	4.2
1	A	651	LYS	4.1
1	B	651	LYS	4.1
1	D	620	THR	4.0
1	A	649	GLY	4.0
1	A	620	THR	3.9
1	C	621	ALA	3.7
1	B	22	PRO	3.7
1	A	650	GLY	3.6
1	C	698	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	621	ALA	3.5
1	D	618	ALA	3.4
1	A	619	SER	3.4
1	B	652	SER	3.3
1	B	698	SER	3.3
1	B	619	SER	3.2
1	A	618	ALA	3.1
1	A	653	SER	3.1
1	A	652	SER	3.0
1	D	22	PRO	3.0
1	D	517	GLY	2.9
1	C	22	PRO	2.8
1	B	621	ALA	2.8
1	B	590	GLU	2.8
1	B	560	GLU	2.6
1	B	23	LEU	2.6
1	A	22	PRO	2.5
1	B	561	SER	2.4
1	B	657	ASP	2.4
1	A	676	MET	2.3
1	B	618	ALA	2.2
1	B	654	GLU	2.2
1	A	560	GLU	2.1
1	B	675	ASP	2.1
1	C	664	ASP	2.1
1	A	657	ASP	2.1
1	A	318	TYR	2.1
1	A	654	GLU	2.1
1	B	611	ASP	2.1
1	C	561	SER	2.0
1	A	589[A]	ARG	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 carbohydrates in this entry.



## 6.4 Ligands

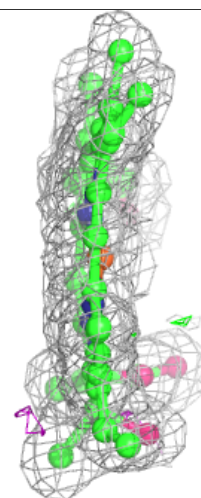
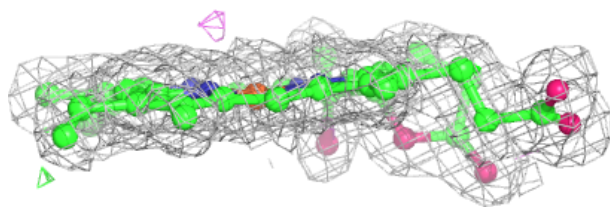
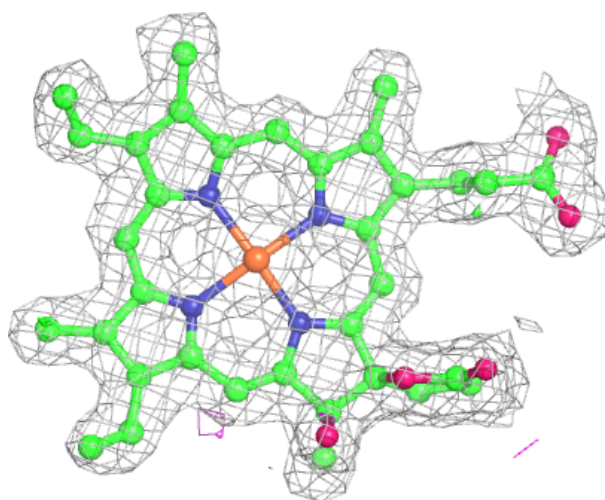
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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
3	3TR	C	703	6/6	0.87	0.13	29,29,30,32	0
3	3TR	B	1704	6/6	0.87	0.15	33,35,35,35	0
3	3TR	A	703	6/6	0.89	0.15	32,35,36,37	0
3	3TR	B	1706	6/6	0.91	0.13	29,31,32,32	0
3	3TR	B	1703	6/6	0.95	0.10	24,25,25,26	0
3	3TR	D	702	6/6	0.96	0.13	22,23,24,24	0
3	3TR	C	702	6/6	0.98	0.07	22,22,22,22	0
2	HDD	A	701	44/44	0.98	0.09	10,12,16,20	0
2	HDD	C	701	44/44	0.98	0.08	9,12,15,19	0
2	HDD	D	701	44/44	0.98	0.08	11,13,16,20	0
4	CA	B	1701	1/1	0.98	0.12	44,44,44,44	0
2	HDD	B	1702	44/44	0.98	0.09	10,12,16,20	0
3	3TR	A	702	6/6	0.98	0.06	21,22,23,23	0
4	CA	D	703	1/1	0.99	0.06	24,24,24,24	0
4	CA	A	704	1/1	1.00	0.05	19,19,19,19	0
4	CA	B	1705	1/1	1.00	0.06	23,23,23,23	0
4	CA	C	704	1/1	1.00	0.09	24,24,24,24	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.

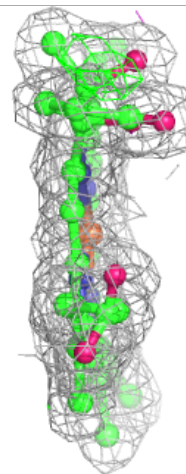
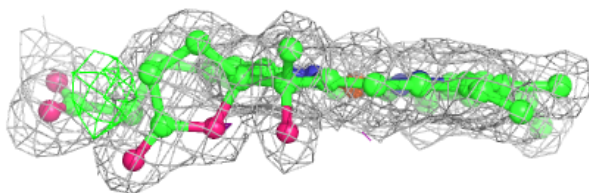
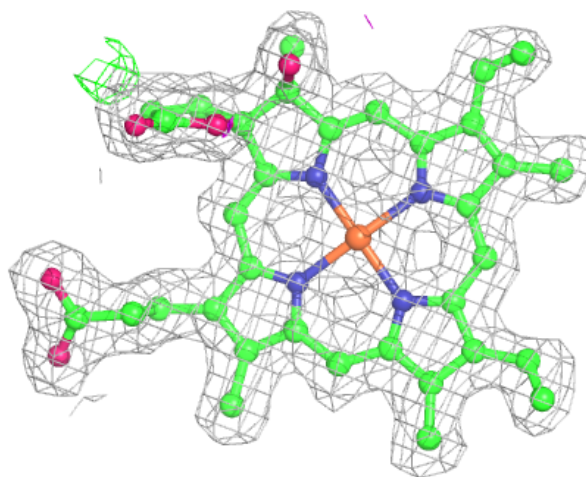
**Electron density around HDD A 701:**

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



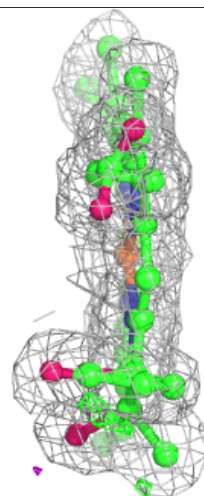
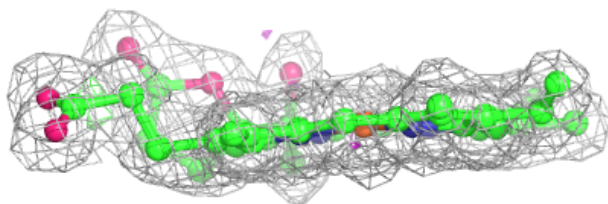
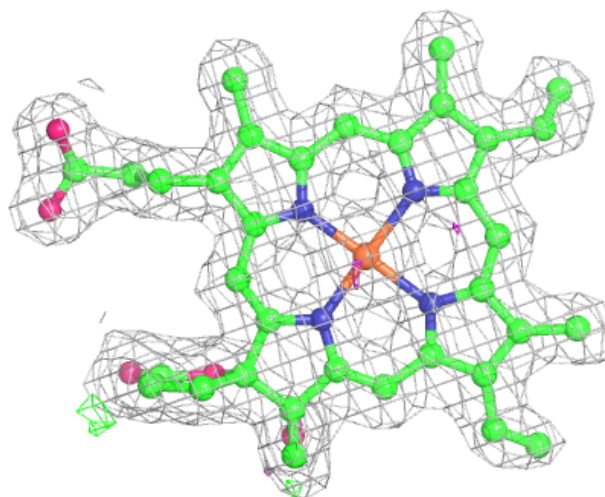
**Electron density around HDD C 701:**

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



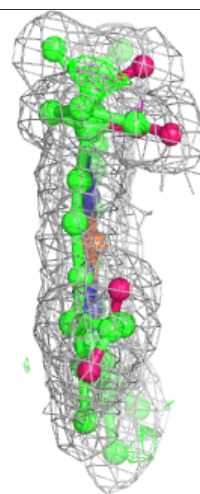
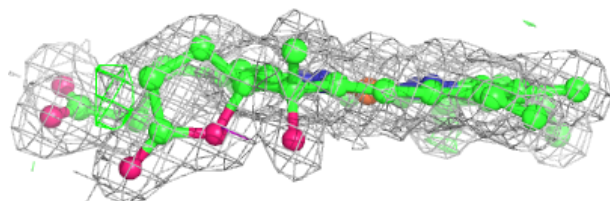
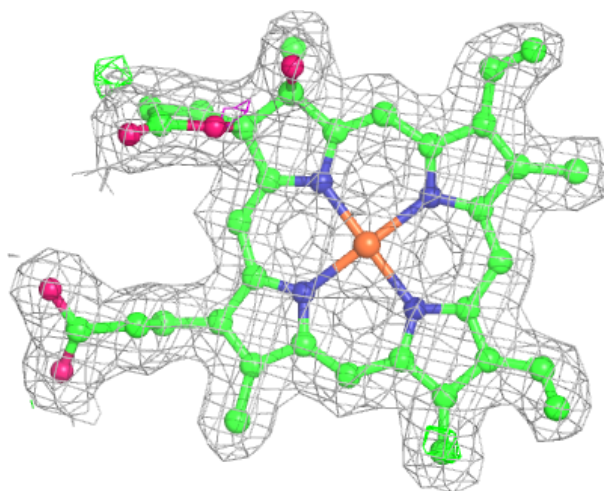
**Electron density around HDD D 701:**

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



**Electron density around HDD B 1702:**

$2mF_o-DF_c$  (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.