



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 09:58 AM EDT

PDB ID : 3PQ5  
Title : Structure of I274C variant of E. coli KatE[] - Images 19-24  
Authors : Loewen, P.C.; Jha, V.; Louis, S.; Chelikani, P.; Carpena, X.; Fita, I.  
Deposited on : 2010-11-25  
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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.

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 : 2.35  
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) : 2.35

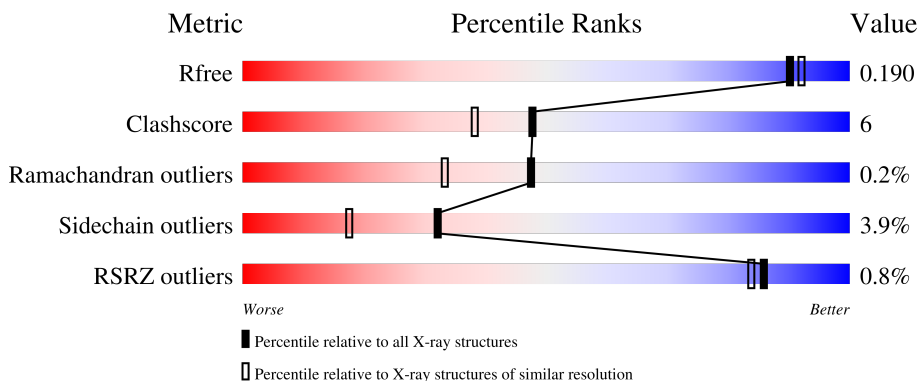
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	753	 85% 10% . .
1	B	753	 85% 10% . .
1	C	753	 83% 12% . .
1	D	753	 86% 9% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	H2S	A	754	-	-	X	-
4	H2S	B	754	-	-	X	-
4	H2S	C	754	-	-	X	-
4	H2S	D	754	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26829 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.

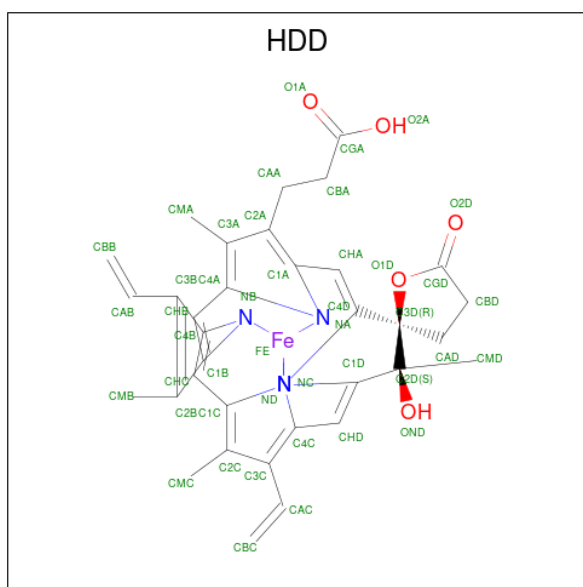
- Molecule 1 is a protein called Catalase HP11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	726	5755	3652	1009	1083	11	0	5	0
1	B	726	5757	3654	1009	1083	11	0	5	0
1	C	726	5747	3649	1007	1080	11	0	2	0
1	D	726	5771	3662	1013	1085	11	0	9	0

There are 12 discrepancies between the modelled and reference sequences:

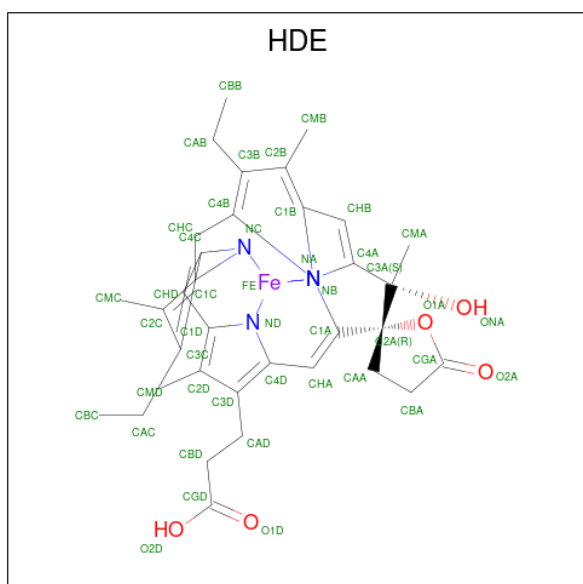
Chain	Residue	Modelled	Actual	Comment	Reference
A	274	CYS	ILE	engineered mutation	UNP P21179
A	438	ALA	CYS	engineered mutation	UNP P21179
A	669	ALA	CYS	engineered mutation	UNP P21179
B	274	CYS	ILE	engineered mutation	UNP P21179
B	438	ALA	CYS	engineered mutation	UNP P21179
B	669	ALA	CYS	engineered mutation	UNP P21179
C	274	CYS	ILE	engineered mutation	UNP P21179
C	438	ALA	CYS	engineered mutation	UNP P21179
C	669	ALA	CYS	engineered mutation	UNP P21179
D	274	CYS	ILE	engineered mutation	UNP P21179
D	438	ALA	CYS	engineered mutation	UNP P21179
D	669	ALA	CYS	engineered mutation	UNP P21179

- Molecule 2 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (three-letter code: HDD) (formula:  $C_{34}H_{32}FeN_4O_5$ ).



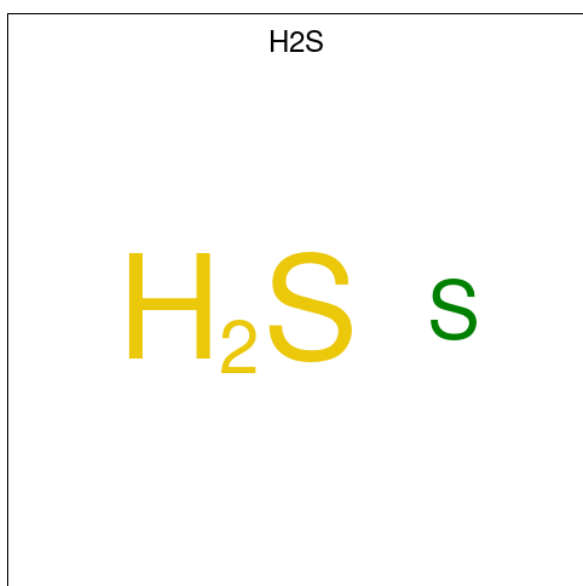
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
2	A	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
2	B	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
2	C	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
2	D	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		

- Molecule 3 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE 17R, 18S (three-letter code: HDE) (formula:  $C_{34}H_{38}FeN_4O_5$ ).



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

- Molecule 4 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H<sub>2</sub>S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	893	Total	O	0	0
			893	893		
5	B	790	Total	O	0	0
			790	790		

*Continued on next page...*

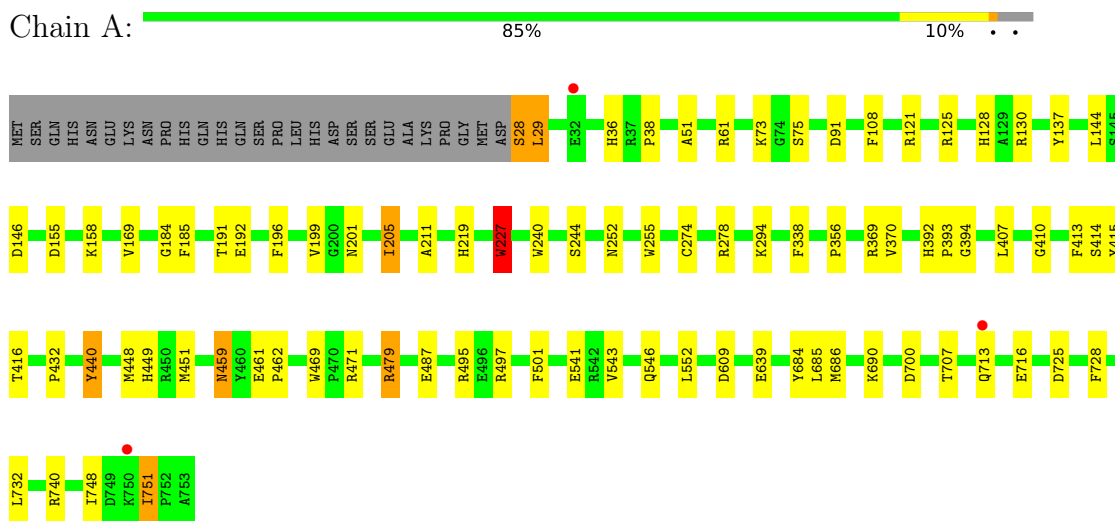
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	C	850	Total 850	O 850	0	0
5	D	910	Total 910	O 910	0	0

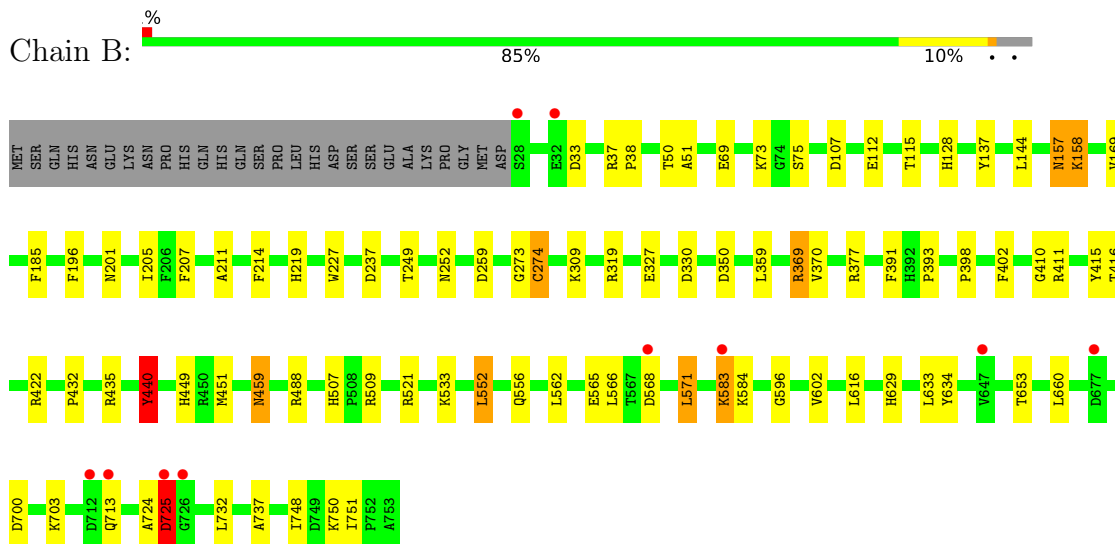
### 3 Residue-property plots i

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.

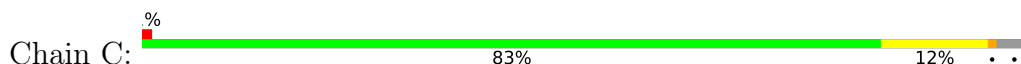
- Molecule 1: Catalase HPII



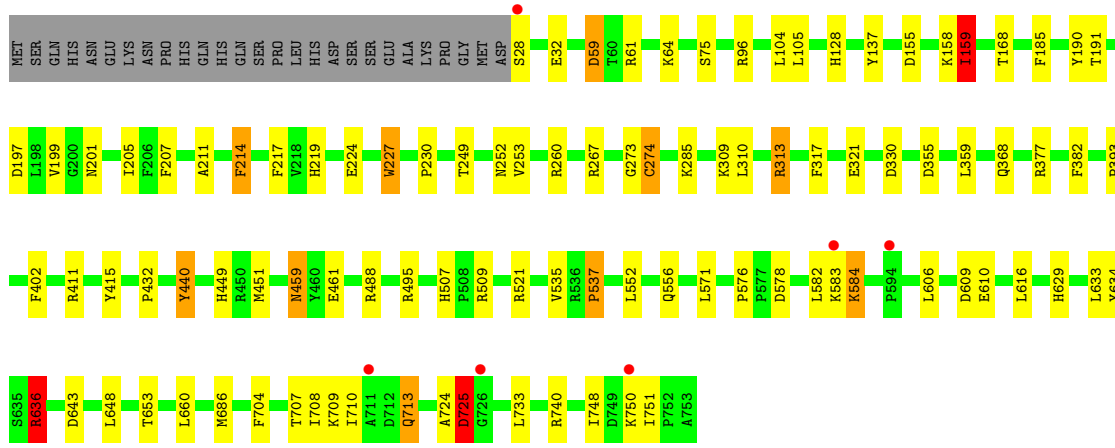
- Molecule 1: Catalase HPII



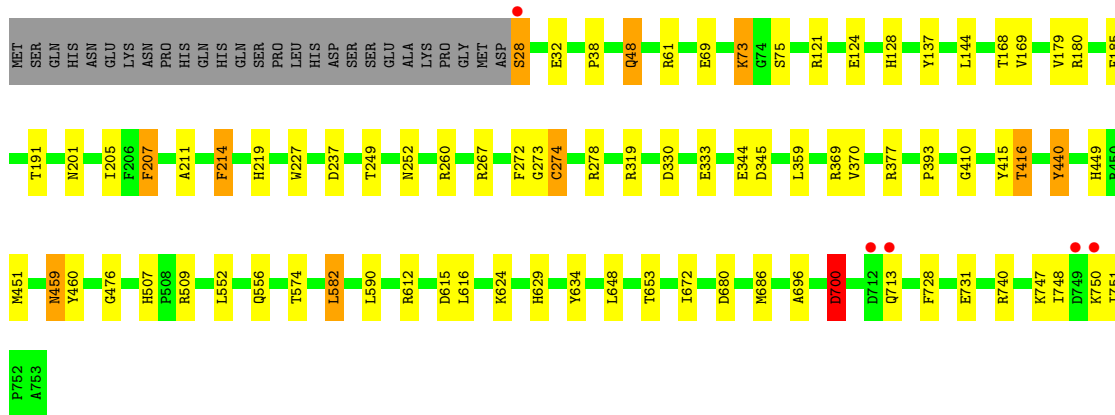
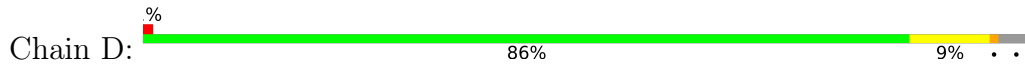
- Molecule 1: Catalase HPII







• Molecule 1: Catalase HPII



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.50Å 133.02Å 122.67Å 90.00° 109.40° 90.00°	Depositor
Resolution (Å)	31.96 – 1.80 31.68 – 1.80	Depositor EDS
% Data completeness (in resolution range)	92.7 (31.96-1.80) 92.7 (31.68-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 1.79Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.143 , 0.190 0.143 , 0.190	Depositor DCC
$R_{free}$ test set	12210 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.5	Xtrriage
Anisotropy	0.011	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 47.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	26829	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: HDE, H2S, 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	1.20	11/5932 (0.2%)	0.99	16/8064 (0.2%)
1	B	1.14	8/5931 (0.1%)	0.96	10/8062 (0.1%)
1	C	1.14	7/5908 (0.1%)	0.95	13/8033 (0.2%)
1	D	1.20	11/5966 (0.2%)	0.98	14/8109 (0.2%)
All	All	1.17	37/23737 (0.2%)	0.97	53/32268 (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	C	0	2

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	440	TYR	CE1-CZ	7.47	1.48	1.38
1	A	255	TRP	CE3-CZ3	7.23	1.50	1.38
1	A	227	TRP	CE3-CZ3	7.02	1.50	1.38
1	B	137	TYR	CD1-CE1	6.92	1.49	1.39
1	D	272	PHE	CE2-CZ	6.87	1.50	1.37
1	A	240	TRP	CE3-CZ3	6.70	1.49	1.38
1	A	440	TYR	CE1-CZ	6.63	1.47	1.38
1	B	196	PHE	CE1-CZ	6.59	1.49	1.37
1	B	69	GLU	CB-CG	6.45	1.64	1.52
1	A	684	TYR	CD2-CE2	6.17	1.48	1.39
1	B	391	PHE	CE2-CZ	6.00	1.48	1.37
1	C	495	ARG	CZ-NH1	5.96	1.40	1.33
1	A	121	ARG	CG-CD	5.92	1.66	1.51
1	D	333	GLU	CD-OE2	-5.91	1.19	1.25

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	327	GLU	CB-CG	5.86	1.63	1.52
1	D	28	SER	CB-OG	5.78	1.49	1.42
1	A	501	PHE	CE2-CZ	5.71	1.48	1.37
1	D	460	TYR	CD1-CE1	5.68	1.47	1.39
1	A	108	PHE	CE2-CZ	5.67	1.48	1.37
1	D	69	GLU	CG-CD	5.52	1.60	1.51
1	D	124	GLU	CB-CG	5.51	1.62	1.52
1	C	217	PHE	CG-CD1	5.42	1.46	1.38
1	A	196	PHE	CE1-CZ	5.38	1.47	1.37
1	D	179	VAL	CB-CG2	5.36	1.64	1.52
1	C	59	ASP	CB-CG	5.34	1.62	1.51
1	C	214	PHE	CE1-CZ	5.32	1.47	1.37
1	D	214	PHE	CE2-CZ	5.24	1.47	1.37
1	C	382	PHE	CD2-CE2	5.22	1.49	1.39
1	D	207	PHE	CE1-CZ	5.13	1.47	1.37
1	C	207	PHE	CE1-CZ	5.13	1.47	1.37
1	A	137	TYR	CD2-CE2	5.12	1.47	1.39
1	D	440	TYR	CE1-CZ	5.11	1.45	1.38
1	B	112	GLU	CB-CG	5.10	1.61	1.52
1	B	402	PHE	CD2-CE2	5.07	1.49	1.39
1	C	402	PHE	CE1-CZ	5.05	1.47	1.37
1	A	440	TYR	CD2-CE2	5.03	1.46	1.39
1	D	137	TYR	CD2-CE2	5.01	1.46	1.39

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	495	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	A	495	ARG	NE-CZ-NH2	-9.41	115.60	120.30
1	A	479	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	D	509	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	C	636	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	C	636	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	B	350	ASP	CB-CG-OD1	-6.51	112.44	118.30
1	A	740	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	D	615	ASP	CB-CG-OD2	6.47	124.12	118.30
1	B	377	ARG	NE-CZ-NH1	-6.27	117.17	120.30
1	D	377	ARG	NE-CZ-NH1	-6.21	117.20	120.30
1	B	369	ARG	NE-CZ-NH1	-6.17	117.21	120.30
1	C	495	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	D	180	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	A	155	ASP	CB-CG-OD2	6.08	123.78	118.30

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	488	ARG	NE-CZ-NH1	-5.83	117.38	120.30
1	A	479	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	D	740	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	338	PHE	CB-CG-CD1	-5.80	116.74	120.80
1	B	435	ARG	NE-CZ-NH1	-5.73	117.43	120.30
1	D	582	LEU	CB-CG-CD1	5.72	120.72	111.00
1	D	700	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	294	LYS	CD-CE-NZ	-5.66	98.68	111.70
1	A	121	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	422	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	D	686	MET	CG-SD-CE	5.62	109.20	100.20
1	D	680	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	740	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	D	61	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	D	345	ASP	CB-CG-OD2	-5.56	113.29	118.30
1	D	278	ARG	NE-CZ-NH1	-5.53	117.54	120.30
1	A	497	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	497	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	609	ASP	CB-CG-OD2	5.46	123.22	118.30
1	C	313	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	C	725	ASP	N-CA-C	5.42	125.64	111.00
1	B	509	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	C	740	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	C	59	ASP	CB-CG-OD1	5.30	123.07	118.30
1	C	197	ASP	CB-CG-OD2	5.28	123.05	118.30
1	C	310	LEU	CB-CG-CD1	5.28	119.98	111.00
1	D	121	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	A	130	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	B	33	ASP	CB-CG-OD1	5.18	122.96	118.30
1	D	612	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	B	107	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	686	MET	CG-SD-CE	5.10	108.36	100.20
1	B	259	ASP	CB-CG-OD2	5.10	122.89	118.30
1	C	159	ILE	CB-CG1-CD1	-5.09	99.64	113.90
1	C	96	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	C	355	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	685	LEU	CB-CG-CD1	-5.02	102.46	111.00
1	C	260	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	724	ALA	Peptide
1	C	725	ASP	Peptide

## 5.2 Too-close contacts [i](#)

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	5755	0	5582	61	0
1	B	5757	0	5587	60	0
1	C	5747	0	5577	71	1
1	D	5771	0	5598	46	0
2	A	44	0	31	11	0
2	B	44	0	31	17	0
2	C	44	0	31	15	0
2	D	44	0	31	10	0
3	A	44	0	36	12	0
3	B	44	0	36	11	0
3	C	44	0	36	13	0
3	D	44	0	36	7	0
4	A	1	0	0	7	0
4	B	1	0	0	7	0
4	C	1	0	0	6	0
4	D	1	0	0	7	0
5	A	893	0	0	14	2
5	B	790	0	0	11	0
5	C	850	0	0	24	0
5	D	910	0	0	18	2
All	All	26829	0	22612	280	3

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 6.

All (280) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:CYS:HB3	4:C:754:H2S:S	1.32	1.65
1:D:274:CYS:HB3	4:D:754:H2S:S	1.35	1.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:CYS:HB3	4:A:754:H2S:S	1.38	1.63
1:B:274:CYS:HB3	4:B:754:H2S:S	1.41	1.60
2:C:760[A]:HDD:HBB2	4:C:754:H2S:S	1.40	1.58
2:B:760[A]:HDD:HBB2	4:B:754:H2S:S	1.38	1.57
3:B:761[B]:HDE:HMC	3:B:761[B]:HDE:CBC	1.59	1.33
2:C:760[A]:HDD:CBB	4:C:754:H2S:S	2.17	1.30
2:D:760[A]:HDD:HBB2	4:D:754:H2S:S	1.72	1.30
1:A:449[A]:HIS:CE1	5:A:3608:HOH:O	1.72	1.29
1:C:274:CYS:CB	4:C:754:H2S:S	2.22	1.27
1:C:449[B]:HIS:CE1	5:C:3610:HOH:O	1.75	1.27
2:B:760[A]:HDD:CBB	4:B:754:H2S:S	2.22	1.26
1:B:274:CYS:CB	4:B:754:H2S:S	2.27	1.23
1:D:274:CYS:CB	4:D:754:H2S:S	2.25	1.22
1:D:451:MET:SD	5:D:3617:HOH:O	1.99	1.19
1:A:716:GLU:HG2	5:A:3090:HOH:O	1.43	1.18
1:A:274:CYS:CB	4:A:754:H2S:S	2.32	1.17
3:C:761[B]:HDE:HMC	3:C:761[B]:HDE:CBC	1.74	1.17
3:C:761[B]:HDE:CMC	3:C:761[B]:HDE:HBCB	1.70	1.15
1:C:578:ASP:HB3	5:C:2919:HOH:O	1.46	1.13
2:D:760[A]:HDD:CBB	4:D:754:H2S:S	2.36	1.12
1:C:267:ARG:HG3	5:C:2916:HOH:O	1.49	1.10
1:B:416:THR:HG21	5:D:2464:HOH:O	1.52	1.08
2:A:760[A]:HDD:HBB2	4:A:754:H2S:S	1.94	1.07
3:B:761[B]:HDE:HMC	3:B:761[B]:HDE:HBCA	1.14	1.07
1:C:451:MET:SD	5:C:3612:HOH:O	2.12	1.06
1:B:201:ASN:CG	2:B:760[A]:HDD:HMB2	1.75	1.05
1:A:416[A]:THR:HG21	5:A:3313:HOH:O	1.54	1.04
3:B:761[B]:HDE:HBCA	3:B:761[B]:HDE:CMC	1.84	1.04
1:A:201:ASN:CG	2:A:760[A]:HDD:HMB2	1.77	1.01
3:B:761[B]:HDE:CBC	3:B:761[B]:HDE:CMC	2.34	1.01
1:A:541:GLU:OE2	5:A:2550:HOH:O	1.79	1.00
1:D:201:ASN:CG	2:D:760[A]:HDD:HMB2	1.82	0.99
3:A:761[B]:HDE:HBCB	3:A:761[B]:HDE:HMC	1.44	0.99
1:A:274:CYS:SG	2:A:760[A]:HDD:CMB	2.49	0.99
1:C:201:ASN:CG	2:C:760[A]:HDD:HMB2	1.84	0.98
1:A:274:CYS:SG	2:A:760[A]:HDD:HMB1	2.05	0.97
3:B:761[B]:HDE:HMC	3:B:761[B]:HDE:HBCB	1.46	0.94
1:A:451:MET:SD	5:A:3609:HOH:O	2.25	0.94
1:B:533[A]:LYS:HE2	5:B:3100:HOH:O	1.67	0.94
1:A:28:SER:O	1:A:28:SER:OG	1.78	0.93
1:A:29:LEU:HD22	5:C:2405:HOH:O	1.69	0.92

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:760[A]:HDD:CBB	4:A:754:H2S:S	2.57	0.92
1:B:451:MET:SD	5:B:3614:HOH:O	2.27	0.91
1:C:449[B]:HIS:NE2	5:C:3610:HOH:O	1.83	0.91
3:A:761[B]:HDE:HMC	3:A:761[B]:HDE:CBC	2.01	0.90
3:D:761[B]:HDE:HBCB	3:D:761[B]:HDE:HMC	1.55	0.89
1:A:274:CYS:SG	2:A:760[A]:HDD:HMB3	2.13	0.88
3:C:761[B]:HDE:HMC	3:C:761[B]:HDE:HBCB	0.89	0.86
1:A:751:ILE:HD13	1:A:751:ILE:O	1.78	0.84
1:A:639:GLU:HG3	5:A:2414:HOH:O	1.75	0.84
3:C:761[B]:HDE:CBC	3:C:761[B]:HDE:CMC	2.42	0.84
1:B:201:ASN:ND2	2:B:760[A]:HDD:HMB2	1.94	0.82
1:A:449[A]:HIS:NE2	5:A:3608:HOH:O	1.90	0.80
1:D:274:CYS:SG	2:D:760[A]:HDD:CMB	2.68	0.80
3:C:761[B]:HDE:HMB	3:C:761[B]:HDE:CBB	2.12	0.79
1:D:201:ASN:ND2	2:D:760[A]:HDD:HMB2	1.96	0.79
1:C:440:TYR:HD1	5:C:3454:HOH:O	1.63	0.79
3:D:761[B]:HDE:HMB	3:D:761[B]:HDE:HBBB	1.65	0.79
1:A:29:LEU:HD23	5:C:3144:HOH:O	1.82	0.78
1:A:201:ASN:ND2	2:A:760[A]:HDD:HMB2	1.99	0.78
1:D:274:CYS:SG	2:D:760[A]:HDD:HMB3	2.25	0.77
3:D:761[B]:HDE:HMB	3:D:761[B]:HDE:CBB	2.15	0.76
3:A:761[B]:HDE:HMB	3:A:761[B]:HDE:HBBB	1.67	0.76
2:B:760[A]:HDD:HBB1	2:B:760[A]:HDD:HMB1	1.66	0.75
1:D:731:GLU:OE2	5:D:3028:HOH:O	2.03	0.75
1:C:274:CYS:SG	2:C:760[A]:HDD:HMB3	2.27	0.75
1:B:440:TYR:O	1:D:73[B]:LYS:HE3	1.87	0.74
1:D:748:ILE:O	1:D:751:ILE:HG22	1.86	0.74
3:A:761[B]:HDE:HMB	3:A:761[B]:HDE:CBB	2.16	0.74
3:C:761[B]:HDE:HMB	3:C:761[B]:HDE:HBBA	1.68	0.74
3:B:761[B]:HDE:CMC	3:B:761[B]:HDE:HBCB	2.09	0.73
1:C:201:ASN:ND2	2:C:760[A]:HDD:HMB2	2.04	0.73
1:D:274:CYS:SG	2:D:760[A]:HDD:HMB1	2.29	0.73
1:B:449[B]:HIS:HD2	5:B:3613:HOH:O	1.69	0.73
2:B:760[A]:HDD:HBC1	2:B:760[A]:HDD:HMC1	1.68	0.72
3:B:761[B]:HDE:HMB	3:B:761[B]:HDE:HBBB	1.70	0.72
1:C:28:SER:HA	5:C:2523:HOH:O	1.88	0.72
1:C:274:CYS:SG	2:C:760[A]:HDD:CMB	2.78	0.72
3:D:761[B]:HDE:HMC	4:D:754:H2S:S	2.29	0.71
3:B:761[B]:HDE:HMB	3:B:761[B]:HDE:CBB	2.22	0.70
1:B:700:ASP:HB2	5:B:3595:HOH:O	1.91	0.69
1:C:556:GLN:NE2	5:C:2533:HOH:O	2.26	0.68

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:760[A]:HDD:CBB	2:B:760[A]:HDD:HMB1	2.23	0.68
1:D:672:ILE:HG12	1:D:700:ASP:OD2	1.93	0.68
1:C:725:ASP:O	5:C:2403:HOH:O	2.11	0.68
1:C:274:CYS:HB3	2:C:760[A]:HDD:CBB	2.23	0.68
1:B:440:TYR:O	1:D:73[B]:LYS:CE	2.41	0.68
1:C:629:HIS:HD2	5:C:1129:HOH:O	1.76	0.67
1:B:748:ILE:O	1:B:751:ILE:HG22	1.94	0.67
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.79	0.66
1:C:449[A]:HIS:HD2	5:C:3611:HOH:O	1.80	0.65
1:B:724:ALA:O	1:B:725:ASP:O	2.15	0.65
2:A:760[A]:HDD:CAB	4:A:754:H2S:S	2.87	0.62
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.79	0.62
1:B:73:LYS:HE3	5:D:3517:HOH:O	1.99	0.62
1:B:274:CYS:SG	2:B:760[A]:HDD:HMB3	2.38	0.62
2:B:760[A]:HDD:HBB1	2:B:760[A]:HDD:CMB	2.30	0.62
1:A:416[B]:THR:HG22	5:A:904:HOH:O	2.00	0.61
1:D:629:HIS:HD2	5:D:1554:HOH:O	1.82	0.61
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.82	0.61
1:B:214:PHE:CD2	2:B:760[A]:HDD:HMC2	2.36	0.61
1:B:37:ARG:HD3	5:B:2886:HOH:O	1.99	0.61
1:C:609:ASP:O	5:C:1764:HOH:O	2.16	0.60
1:C:636:ARG:HD3	5:C:2717:HOH:O	2.00	0.60
1:D:28:SER:HA	5:D:2467:HOH:O	2.00	0.60
1:B:274:CYS:SG	2:B:760[A]:HDD:CMB	2.89	0.60
1:B:274:CYS:SG	2:B:760[A]:HDD:HBB1	2.42	0.60
1:D:267:ARG:HG3	5:D:1920:HOH:O	2.02	0.60
1:B:115:THR:HG21	5:B:3420:HOH:O	2.02	0.59
1:C:274:CYS:CA	4:C:754:H2S:S	2.91	0.59
1:C:274:CYS:CB	2:C:760[A]:HDD:HBB1	2.33	0.59
1:C:368:GLN:NE2	5:C:1787:HOH:O	2.16	0.59
1:A:244:SER:HA	1:A:546[B]:GLN:NE2	2.17	0.59
1:B:73:LYS:CE	5:D:3517:HOH:O	2.51	0.59
1:C:634:TYR:O	1:C:653:THR:HA	2.03	0.59
1:C:713:GLN:HB3	5:C:3004:HOH:O	2.03	0.58
1:B:201:ASN:ND2	2:B:760[A]:HDD:CMB	2.67	0.58
1:D:449[A]:HIS:HD2	5:D:3615:HOH:O	1.86	0.58
3:A:761[B]:HDE:HBCB	3:A:761[B]:HDE:CMC	2.26	0.57
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.88	0.57
2:B:760[A]:HDD:HBC1	2:B:760[A]:HDD:CMC	2.36	0.56
3:C:761[B]:HDE:HMC	4:C:754:H2S:S	2.44	0.56
2:B:760[A]:HDD:HMC1	2:B:760[A]:HDD:CBC	2.34	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:761[B]:HDE:HMB	3:C:761[B]:HDE:HBBB	1.87	0.56
1:C:59:ASP:OD2	5:C:3406:HOH:O	2.18	0.56
3:A:761[B]:HDE:CBC	3:A:761[B]:HDE:CMC	2.75	0.56
1:C:578:ASP:HB2	1:C:582:LEU:O	2.06	0.56
1:C:28:SER:N	5:C:2523:HOH:O	2.39	0.55
1:D:449[A]:HIS:HE1	5:D:1789:HOH:O	1.89	0.55
1:B:629:HIS:HD2	5:B:1055:HOH:O	1.90	0.55
1:C:274:CYS:SG	2:C:760[A]:HDD:HMB1	2.46	0.54
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.10	0.54
1:D:359:LEU:H	1:D:507:HIS:HD2	1.56	0.54
1:A:29:LEU:HB2	5:C:2405:HOH:O	2.08	0.53
1:C:28:SER:CA	5:C:2523:HOH:O	2.52	0.53
1:D:556:GLN:NE2	5:D:2773:HOH:O	2.41	0.53
1:A:748:ILE:O	1:A:751:ILE:HD12	2.09	0.53
1:A:690:LYS:HG3	1:A:751:ILE:HD11	1.91	0.52
1:B:449[B]:HIS:HE1	5:D:1789:HOH:O	1.92	0.52
1:B:411:ARG:HG2	3:B:761[B]:HDE:C3B	2.39	0.52
1:C:359:LEU:H	1:C:507:HIS:HD2	1.58	0.52
1:B:521:ARG:HG3	5:B:3553:HOH:O	2.10	0.52
3:A:761[B]:HDE:HMC	3:A:761[B]:HDE:HBCA	1.89	0.52
1:C:610:GLU:HG2	5:C:3224:HOH:O	2.09	0.52
1:C:583:LYS:HG2	5:C:2919:HOH:O	2.10	0.52
1:B:73:LYS:CD	5:D:3517:HOH:O	2.58	0.52
1:B:583:LYS:O	1:B:584:LYS:HB3	2.11	0.51
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.26	0.51
1:A:392:HIS:CD2	1:A:394:GLY:H	2.29	0.51
5:B:3557:HOH:O	1:C:686:MET:HE1	2.10	0.51
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.41	0.51
1:B:144:LEU:HD11	1:B:370:VAL:HG13	1.93	0.50
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.26	0.50
1:A:36:HIS:HE1	5:A:1872:HOH:O	1.95	0.50
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.94	0.50
3:D:761[B]:HDE:HBCB	4:D:754:H2S:S	2.52	0.50
1:A:61:ARG:HD2	5:A:3208:HOH:O	2.10	0.50
1:A:125:ARG:HG2	3:A:761[B]:HDE:HBA	1.94	0.50
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.27	0.50
1:D:273:GLY:C	1:D:274:CYS:SG	2.90	0.50
1:A:184:GLY:HA3	2:A:760[A]:HDD:HMA2	1.94	0.49
1:A:700:ASP:HB2	5:A:3594:HOH:O	2.11	0.49
3:B:761[B]:HDE:HMC	4:B:754:H2S:S	2.53	0.49
1:B:359:LEU:H	1:B:507:HIS:HD2	1.60	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:725:ASP:H	1:A:728:PHE:HB3	1.78	0.49
1:B:369:ARG:HG2	5:B:1639:HOH:O	2.12	0.48
3:D:761[B]:HDE:HMAA	3:D:761[B]:HDE:HAAA	1.71	0.48
1:A:201:ASN:ND2	2:A:760[A]:HDD:CMB	2.73	0.48
1:A:469:TRP:CE3	1:A:471:ARG:HG3	2.48	0.48
1:A:543:VAL:HA	1:A:546[B]:GLN:HE21	1.78	0.48
5:A:1788:HOH:O	1:C:449[A]:HIS:HE1	1.96	0.48
1:D:416[B]:THR:HG22	5:D:1415:HOH:O	2.14	0.48
1:D:207:PHE:O	1:D:249:THR:HA	2.13	0.48
1:D:214:PHE:CD1	2:D:760[A]:HDD:HAC	2.49	0.47
1:A:144:LEU:HD11	1:A:370:VAL:HG13	1.97	0.47
1:C:274:CYS:SG	2:C:760[A]:HDD:HBB1	2.54	0.47
1:C:211:ALA:CB	3:C:761[B]:HDE:HBB	2.44	0.47
1:C:610:GLU:OE1	1:C:643:ASP:HA	2.15	0.47
1:B:274:CYS:SG	2:B:760[A]:HDD:HMB1	2.55	0.47
1:C:274:CYS:CB	2:C:760[A]:HDD:CBB	2.88	0.47
1:B:274:CYS:HB2	4:B:754:H2S:S	2.42	0.47
1:A:199:VAL:HG12	3:A:761[B]:HDE:HHDA	1.97	0.47
1:B:157:ASN:C	1:B:157:ASN:HD22	2.19	0.47
1:B:552:LEU:HD22	1:B:556:GLN:HG3	1.97	0.47
1:A:274:CYS:CA	4:A:754:H2S:S	3.03	0.47
1:B:596:GLY:HA3	1:B:737:ALA:O	2.15	0.47
1:B:634:TYR:O	1:B:653:THR:HA	2.14	0.47
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.30	0.46
1:C:748:ILE:O	1:C:751:ILE:HG22	2.15	0.46
1:D:672:ILE:CG1	1:D:700:ASP:OD2	2.61	0.46
1:D:128:HIS:CE1	1:D:169:VAL:HG22	2.50	0.46
1:B:38:PRO:HG2	1:B:51:ALA:HB2	1.98	0.46
1:B:207:PHE:O	1:B:249:THR:HA	2.15	0.46
1:B:440:TYR:O	1:D:73[B]:LYS:HE2	2.12	0.46
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.46	0.46
3:D:761[B]:HDE:HMB	3:D:761[B]:HDE:HBBA	1.94	0.46
1:C:214:PHE:CD2	2:C:760[A]:HDD:HMC2	2.51	0.46
1:D:476:GLY:HA3	5:D:1112:HOH:O	2.14	0.46
2:C:760[A]:HDD:CBB	2:C:760[A]:HDD:HMB1	2.46	0.46
1:C:583:LYS:O	1:C:584:LYS:HB3	2.15	0.45
1:C:440:TYR:CD1	5:C:3454:HOH:O	2.51	0.45
2:C:760[A]:HDD:HMC1	2:C:760[A]:HDD:CBC	2.46	0.45
3:C:761[B]:HDE:CMC	3:C:761[B]:HDE:HBCA	2.42	0.45
1:B:128:HIS:CE1	1:B:169:VAL:HG22	2.52	0.45
1:B:319:ARG:HD3	1:C:227:TRP:O	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:LEU:H	1:C:507:HIS:CD2	2.36	0.45
1:B:309:LYS:HD2	1:B:660:LEU:HD11	1.98	0.44
1:C:411:ARG:HG2	3:C:761[B]:HDE:C3B	2.46	0.44
1:B:583:LYS:NZ	1:B:583:LYS:H	2.15	0.44
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.48	0.44
1:C:273:GLY:C	1:C:274:CYS:SG	2.96	0.44
1:B:115:THR:CG2	5:B:3420:HOH:O	2.62	0.43
1:B:393:PRO:HD2	1:B:415:TYR:CG	2.53	0.43
1:B:732:LEU:C	1:B:732:LEU:HD13	2.39	0.43
1:A:393:PRO:HD2	1:A:415:TYR:CG	2.53	0.43
1:D:359:LEU:H	1:D:507:HIS:CD2	2.33	0.43
1:C:393:PRO:HD2	1:C:415:TYR:CG	2.52	0.43
1:D:48:GLN:HE21	1:D:48:GLN:HB3	1.63	0.43
1:A:36:HIS:CD2	1:A:36:HIS:H	2.37	0.43
1:B:273:GLY:C	1:B:274:CYS:SG	2.97	0.43
1:D:369:ARG:CG	5:D:3574:HOH:O	2.67	0.43
1:A:146:ASP:HB2	5:A:2592:HOH:O	2.19	0.43
1:D:144:LEU:HD11	1:D:370:VAL:HG13	2.00	0.43
3:B:761[B]:HDE:CBC	4:B:754:H2S:S	3.07	0.43
1:B:451:MET:HE1	1:D:451:MET:HE2	2.01	0.43
1:C:704:PHE:O	1:C:707:THR:HG22	2.18	0.43
1:A:192:GLU:OE1	1:A:479:ARG:NH2	2.52	0.42
5:A:1016:HOH:O	1:C:104:LEU:HB3	2.19	0.42
1:D:38:PRO:HA	1:D:48:GLN:HE21	1.84	0.42
1:D:128:HIS:HA	1:D:168:THR:O	2.18	0.42
1:A:205:ILE:HD13	1:A:205:ILE:H	1.84	0.42
2:A:760[A]:HDD:HAB	4:A:754:H2S:S	2.59	0.42
1:C:309:LYS:HD2	1:C:660:LEU:HD11	2.01	0.42
1:D:214:PHE:CD1	2:D:760[A]:HDD:CAC	3.02	0.42
1:A:414:SER:OG	3:A:761[B]:HDE:HHB	2.19	0.42
1:C:509:ARG:HD2	1:C:576:PRO:HD2	2.02	0.42
1:D:260:ARG:HD3	1:D:590:LEU:HD21	2.02	0.42
1:B:211:ALA:CB	1:B:410:GLY:HA3	2.49	0.42
1:A:227:TRP:O	1:D:319:ARG:HD3	2.19	0.42
3:A:761[B]:HDE:HMB	3:A:761[B]:HDE:HBBA	1.97	0.42
1:C:128:HIS:HA	1:C:168:THR:O	2.19	0.42
1:B:73:LYS:HD2	5:D:3517:HOH:O	2.17	0.42
1:B:602:VAL:HG22	1:B:629:HIS:HB2	2.02	0.42
1:A:356:PRO:HG3	1:A:407:LEU:HB2	2.02	0.42
1:B:201:ASN:OD1	2:B:760[A]:HDD:HMB2	2.15	0.41
1:C:155:ASP:HB3	1:C:158:LYS:HB2	2.02	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:760[A]:HDD:HMC1	2:C:760[A]:HDD:HBC1	2.00	0.41
1:C:535:VAL:O	1:C:537:PRO:HD3	2.21	0.41
1:A:128:HIS:CE1	1:A:169:VAL:HG22	2.55	0.41
1:C:224:GLU:HB3	5:D:3120:HOH:O	2.21	0.41
1:A:91:ASP:OD1	1:C:461:GLU:OE1	2.38	0.41
3:C:761[B]:HDE:HMAA	3:C:761[B]:HDE:HAAA	1.70	0.41
1:D:696:ALA:HB1	1:D:728:PHE:CZ	2.56	0.41
1:A:751:ILE:HD13	1:A:751:ILE:C	2.38	0.41
1:C:313:ARG:HG3	1:C:660:LEU:HD12	2.03	0.41
1:C:317:PHE:O	1:C:321:GLU:HB2	2.20	0.41
1:A:38:PRO:HG2	1:A:51:ALA:HB2	2.02	0.41
1:A:413:PHE:HB2	1:C:105:LEU:HD11	2.03	0.41
3:A:761[B]:HDE:HMAB	3:A:761[B]:HDE:HAAA	1.97	0.41
1:B:50:THR:HG21	1:C:227:TRP:CZ3	2.56	0.41
1:D:393:PRO:HD2	1:D:415:TYR:CG	2.55	0.41
1:A:461:GLU:HB2	1:A:462:PRO:HA	2.04	0.41
1:B:157:ASN:HD22	1:B:158:LYS:N	2.19	0.41
1:A:73:LYS:HE3	1:C:440:TYR:O	2.21	0.40
1:C:64:LYS:HE2	1:C:190:TYR:CE1	2.55	0.40
1:D:634:TYR:O	1:D:653:THR:HA	2.20	0.40
1:C:199:VAL:HG12	3:C:761[B]:HDE:HHDA	2.03	0.40
1:A:448:MET:HG3	1:A:449[B]:HIS:CD2	2.57	0.40
1:B:359:LEU:H	1:B:507:HIS:CD2	2.37	0.40
2:D:760[A]:HDD:CAB	4:D:754:H2S:S	3.00	0.40
1:C:249:THR:O	1:C:253:VAL:HG23	2.21	0.40
1:C:440:TYR:CD2	1:C:440:TYR:C	2.94	0.40

All (3) 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:C:584:LYS:NZ	5:A:1624:HOH:O[1_554]	2.13	0.07
5:A:3241:HOH:O	5:D:2457:HOH:O[2_646]	2.14	0.06
5:D:2178:HOH:O	5:D:2976:HOH:O[1_655]	2.18	0.02

## 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	729/753 (97%)	707 (97%)	21 (3%)	1 (0%)	51	36
1	B	729/753 (97%)	705 (97%)	22 (3%)	2 (0%)	41	27
1	C	726/753 (96%)	702 (97%)	22 (3%)	2 (0%)	41	27
1	D	733/753 (97%)	713 (97%)	19 (3%)	1 (0%)	51	36
All	All	2917/3012 (97%)	2827 (97%)	84 (3%)	6 (0%)	47	33

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	725	ASP
1	A	75	SER
1	C	75	SER
1	B	75	SER
1	D	75	SER
1	C	725	ASP

### 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	614/634 (97%)	598 (97%)	16 (3%)	46	32
1	B	614/634 (97%)	589 (96%)	25 (4%)	30	16
1	C	611/634 (96%)	580 (95%)	31 (5%)	24	10
1	D	618/634 (98%)	592 (96%)	26 (4%)	30	15

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2457/2536 (97%)	2359 (96%)	98 (4%)	32 16

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	29	LEU
1	A	185	PHE
1	A	191	THR
1	A	205	ILE
1	A	227	TRP
1	A	252	ASN
1	A	369	ARG
1	A	432	PRO
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	707	THR
1	A	713	GLN
1	A	732	LEU
1	A	751	ILE
1	B	157	ASN
1	B	158	LYS
1	B	185	PHE
1	B	205	ILE
1	B	227	TRP
1	B	237	ASP
1	B	252	ASN
1	B	274	CYS
1	B	398	PRO
1	B	432	PRO
1	B	440	TYR
1	B	459	ASN
1	B	552	LEU
1	B	562	LEU
1	B	565	GLU
1	B	566	LEU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	616	LEU
1	B	633	LEU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	703	LYS
1	B	713	GLN
1	B	725	ASP
1	B	750	LYS
1	C	32	GLU
1	C	61	ARG
1	C	159	ILE
1	C	185	PHE
1	C	191	THR
1	C	205	ILE
1	C	227	TRP
1	C	230	PRO
1	C	252	ASN
1	C	274	CYS
1	C	285	LYS
1	C	377	ARG
1	C	432	PRO
1	C	440	TYR
1	C	459	ASN
1	C	488	ARG
1	C	521	ARG
1	C	537	PRO
1	C	552	LEU
1	C	571	LEU
1	C	584	LYS
1	C	606	LEU
1	C	616	LEU
1	C	633	LEU
1	C	636	ARG
1	C	648	LEU
1	C	709	LYS
1	C	713	GLN
1	C	725	ASP
1	C	733	LEU
1	C	750	LYS
1	D	32	GLU
1	D	48	GLN
1	D	73[A]	LYS
1	D	73[B]	LYS
1	D	185	PHE
1	D	191	THR
1	D	205	ILE

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	D	227	TRP
1	D	237	ASP
1	D	252	ASN
1	D	274	CYS
1	D	344	GLU
1	D	416[A]	THR
1	D	416[B]	THR
1	D	440	TYR
1	D	459	ASN
1	D	552	LEU
1	D	574	THR
1	D	582	LEU
1	D	616	LEU
1	D	624	LYS
1	D	648	LEU
1	D	700	ASP
1	D	713	GLN
1	D	747	LYS
1	D	750	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	252	ASN
1	A	459	ASN
1	A	515	GLN
1	B	157	ASN
1	B	252	ASN
1	B	368	GLN
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	C	252	ASN
1	C	459	ASN
1	C	507	HIS
1	C	556	GLN
1	C	629	HIS
1	C	671	ASN
1	D	48	GLN
1	D	252	ASN
1	D	459	ASN

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type
1	D	507	HIS
1	D	556	GLN
1	D	629	HIS
1	D	671	ASN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are modelled with single atom - leaving 8 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	760[A]	5,1	41,52,52	2.10	13 (31%)	31,89,89	2.42	11 (35%)
2	HDD	B	760[A]	5,1	41,52,52	2.04	14 (34%)	31,89,89	2.45	9 (29%)
2	HDD	A	760[A]	5,1	41,52,52	2.36	13 (31%)	31,89,89	2.06	9 (29%)
3	HDE	D	761[B]	5,1	44,52,52	2.59	13 (29%)	41,89,89	2.71	22 (53%)
3	HDE	C	761[B]	5,1	44,52,52	2.41	14 (31%)	41,89,89	2.74	17 (41%)
3	HDE	A	761[B]	5,1	44,52,52	2.72	16 (36%)	41,89,89	2.54	18 (43%)
2	HDD	D	760[A]	5,1	41,52,52	2.40	16 (39%)	31,89,89	2.05	11 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HDE	B	761[B]	5,1	44,52,52	2.69	15 (34%)	41,89,89	2.62	17 (41%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HDD	C	760[A]	5,1	-	2/5/89/89	0/1/9/9
2	HDD	B	760[A]	5,1	-	2/5/89/89	0/1/9/9
2	HDD	A	760[A]	5,1	-	2/5/89/89	0/1/9/9
3	HDE	D	761[B]	5,1	-	6/9/89/89	0/1/9/9
3	HDE	C	761[B]	5,1	-	6/9/89/89	0/1/9/9
3	HDE	A	761[B]	5,1	-	6/9/89/89	0/1/9/9
2	HDD	D	760[A]	5,1	-	2/5/89/89	0/1/9/9
3	HDE	B	761[B]	5,1	-	6/9/89/89	0/1/9/9

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	760[A]	HDD	FE-ND	8.02	2.26	1.95
3	B	761[B]	HDE	CHC-C4B	-7.82	1.43	1.51
3	A	761[B]	HDE	C4C-C3C	7.53	1.48	1.38
3	B	761[B]	HDE	C4C-C3C	7.14	1.47	1.38
2	C	760[A]	HDD	FE-ND	7.12	2.23	1.95
3	D	761[B]	HDE	CHC-C4B	-6.83	1.44	1.51
3	D	761[B]	HDE	C4C-C3C	6.63	1.47	1.38
3	C	761[B]	HDE	C4C-C3C	6.32	1.46	1.38
3	A	761[B]	HDE	CHC-C1C	-6.28	1.44	1.51
2	A	760[A]	HDD	O1D-C3D	-6.19	1.36	1.46
3	D	761[B]	HDE	CHD-C1D	-6.13	1.44	1.51
3	C	761[B]	HDE	CHC-C4B	-6.06	1.44	1.51
2	A	760[A]	HDD	FE-ND	5.96	2.18	1.95
3	A	761[B]	HDE	CHC-C4B	-5.81	1.45	1.51
2	A	760[A]	HDD	C3B-C2B	-5.78	1.32	1.40
3	B	761[B]	HDE	O1A-CGA	5.76	1.45	1.35
3	A	761[B]	HDE	O1A-CGA	5.72	1.45	1.35
2	D	760[A]	HDD	C3B-C2B	-5.30	1.33	1.40
3	B	761[B]	HDE	CHD-C4C	-5.05	1.46	1.51
3	C	761[B]	HDE	CHD-C1D	-4.90	1.46	1.51

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	761[B]	HDE	O1A-CGA	4.88	1.43	1.35
3	C	761[B]	HDE	CHD-C4C	-4.86	1.46	1.51
3	A	761[B]	HDE	CHD-C1D	-4.85	1.46	1.51
3	B	761[B]	HDE	CHD-C1D	-4.84	1.46	1.51
3	D	761[B]	HDE	CHD-C4C	-4.83	1.46	1.51
2	B	760[A]	HDD	C3C-C2C	-4.67	1.33	1.40
3	D	761[B]	HDE	O1A-CGA	4.63	1.43	1.35
2	D	760[A]	HDD	O1D-C3D	-4.50	1.39	1.46
2	C	760[A]	HDD	C3B-C2B	-4.44	1.34	1.40
3	B	761[B]	HDE	CHC-C1C	-4.40	1.46	1.51
3	D	761[B]	HDE	CHC-C1C	-4.34	1.46	1.51
3	A	761[B]	HDE	C1A-NA	4.11	1.44	1.37
3	D	761[B]	HDE	C3B-C2B	4.10	1.49	1.37
2	D	760[A]	HDD	CHD-C1D	4.07	1.42	1.36
2	A	760[A]	HDD	C3C-C2C	-4.02	1.34	1.40
3	C	761[B]	HDE	C3B-C2B	3.92	1.49	1.37
2	B	760[A]	HDD	C3B-C2B	-3.89	1.35	1.40
3	D	761[B]	HDE	C1A-NA	3.89	1.44	1.37
3	A	761[B]	HDE	C3C-C2C	3.77	1.48	1.37
3	D	761[B]	HDE	C4A-NA	3.77	1.44	1.37
3	B	761[B]	HDE	C1A-NA	3.74	1.44	1.37
3	B	761[B]	HDE	C3B-C2B	3.70	1.48	1.37
2	B	760[A]	HDD	FE-ND	3.67	2.10	1.95
2	C	760[A]	HDD	C3C-C2C	-3.67	1.35	1.40
3	B	761[B]	HDE	C3C-C2C	3.64	1.48	1.37
3	A	761[B]	HDE	C4A-NA	3.61	1.43	1.37
3	A	761[B]	HDE	C3B-C2B	3.56	1.48	1.37
3	C	761[B]	HDE	C3D-C2D	3.49	1.48	1.37
2	B	760[A]	HDD	CMD-C2D	3.47	1.58	1.53
2	A	760[A]	HDD	C3B-CAB	3.45	1.54	1.47
2	D	760[A]	HDD	C3C-CAC	3.43	1.54	1.47
3	D	761[B]	HDE	C3C-C2C	3.43	1.47	1.37
2	B	760[A]	HDD	O1D-C3D	-3.42	1.41	1.46
3	A	761[B]	HDE	C1C-C2C	3.42	1.42	1.38
3	C	761[B]	HDE	CHC-C1C	-3.42	1.47	1.51
2	B	760[A]	HDD	C3C-CAC	3.36	1.54	1.47
3	A	761[B]	HDE	CHD-C4C	-3.31	1.47	1.51
3	A	761[B]	HDE	C3D-C2D	3.30	1.47	1.37
2	B	760[A]	HDD	CHD-C1D	3.23	1.41	1.36
3	A	761[B]	HDE	C1B-CHB	3.23	1.50	1.41
2	D	760[A]	HDD	C3B-CAB	3.20	1.54	1.47
2	C	760[A]	HDD	CHD-C1D	3.17	1.41	1.36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	760[A]	HDD	CHD-C1D	3.11	1.41	1.36
2	C	760[A]	HDD	C3B-CAB	3.11	1.54	1.47
2	B	760[A]	HDD	C3B-CAB	3.10	1.54	1.47
2	C	760[A]	HDD	O1D-C3D	-3.09	1.41	1.46
3	B	761[B]	HDE	C1C-C2C	3.04	1.42	1.38
3	C	761[B]	HDE	C1A-NA	3.04	1.42	1.37
3	A	761[B]	HDE	C1B-NB	3.03	1.42	1.36
3	C	761[B]	HDE	C1C-C2C	3.03	1.42	1.38
2	C	760[A]	HDD	CHA-C4D	2.97	1.40	1.36
3	D	761[B]	HDE	C4D-CHA	2.87	1.49	1.41
2	D	760[A]	HDD	CMD-C2D	2.82	1.57	1.53
2	A	760[A]	HDD	C3C-CAC	2.78	1.53	1.47
2	A	760[A]	HDD	CAA-C2A	2.78	1.56	1.52
2	A	760[A]	HDD	CMC-C2C	2.78	1.57	1.51
3	D	761[B]	HDE	C1B-NB	2.78	1.41	1.36
2	B	760[A]	HDD	C4D-ND	2.72	1.42	1.37
3	C	761[B]	HDE	C3C-C2C	2.72	1.45	1.37
3	D	761[B]	HDE	C3D-C2D	2.67	1.45	1.37
3	C	761[B]	HDE	C4A-NA	2.61	1.42	1.37
2	C	760[A]	HDD	C1A-NA	2.60	1.41	1.36
3	B	761[B]	HDE	C4A-NA	2.60	1.42	1.37
2	D	760[A]	HDD	CAA-C2A	2.56	1.55	1.52
3	B	761[B]	HDE	C3D-C2D	2.54	1.45	1.37
2	D	760[A]	HDD	C3C-C2C	-2.53	1.36	1.40
3	B	761[B]	HDE	C4D-CHA	2.52	1.48	1.41
2	D	760[A]	HDD	CHA-C4D	2.52	1.40	1.36
3	A	761[B]	HDE	C4D-CHA	2.49	1.47	1.41
2	B	760[A]	HDD	CMA-C3A	2.44	1.56	1.51
2	B	760[A]	HDD	C1A-NA	2.44	1.41	1.36
2	C	760[A]	HDD	C3C-CAC	2.42	1.52	1.47
2	D	760[A]	HDD	C4C-NC	2.41	1.41	1.36
3	B	761[B]	HDE	C1B-NB	2.40	1.41	1.36
3	C	761[B]	HDE	C1B-NB	2.39	1.41	1.36
2	A	760[A]	HDD	C4A-NA	2.33	1.41	1.36
2	D	760[A]	HDD	CMC-C2C	2.33	1.56	1.51
2	A	760[A]	HDD	O2D-CGD	2.32	1.29	1.22
3	A	761[B]	HDE	CHA-C1A	-2.27	1.32	1.36
2	D	760[A]	HDD	C4D-ND	2.26	1.41	1.37
2	D	760[A]	HDD	C1A-NA	2.21	1.40	1.36
2	C	760[A]	HDD	CAA-C2A	2.21	1.55	1.52
2	A	760[A]	HDD	CMA-C3A	2.20	1.56	1.51
2	C	760[A]	HDD	C4D-ND	2.19	1.41	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	760[A]	HDD	OND-C2D	2.17	1.47	1.42
2	C	760[A]	HDD	CMC-C2C	2.16	1.56	1.51
2	D	760[A]	HDD	O1D-CGD	-2.13	1.32	1.35
2	A	760[A]	HDD	C1A-NA	2.13	1.40	1.36
2	B	760[A]	HDD	C2A-C3A	-2.12	1.31	1.37
2	B	760[A]	HDD	CHA-C4D	2.09	1.39	1.36
2	C	760[A]	HDD	CMD-C2D	2.08	1.56	1.53
3	C	761[B]	HDE	C1B-CHB	2.08	1.46	1.41
3	B	761[B]	HDE	CHB-C4A	-2.03	1.32	1.36
2	B	760[A]	HDD	C1D-ND	2.00	1.41	1.37

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	760[A]	HDD	O1D-CGD-O2D	8.28	128.19	120.80
2	C	760[A]	HDD	O1D-CGD-O2D	7.56	127.55	120.80
2	A	760[A]	HDD	O1D-CGD-CBD	-6.97	103.16	110.19
3	A	761[B]	HDE	CHC-C4B-C3B	-6.73	121.56	129.68
3	A	761[B]	HDE	CHD-C1D-C2D	-6.58	118.53	129.53
3	C	761[B]	HDE	CBC-CAC-C3C	-5.91	97.21	112.27
2	D	760[A]	HDD	O1D-CGD-CBD	-5.83	104.31	110.19
3	A	761[B]	HDE	CHD-C4C-C3C	-5.47	123.07	129.68
3	C	761[B]	HDE	CHC-C4B-C3B	-5.44	123.11	129.68
3	C	761[B]	HDE	CHD-C1D-C2D	-5.43	120.45	129.53
3	B	761[B]	HDE	CBC-CAC-C3C	-5.21	98.99	112.27
3	D	761[B]	HDE	CHC-C4B-C3B	-5.15	123.46	129.68
3	B	761[B]	HDE	CHC-C4B-C3B	-5.11	123.51	129.68
2	B	760[A]	HDD	O1D-CGD-CBD	-5.07	105.07	110.19
3	C	761[B]	HDE	CHD-C4C-C3C	-4.97	123.68	129.68
3	B	761[B]	HDE	C1B-C2B-C3B	-4.91	103.58	107.00
3	D	761[B]	HDE	CHD-C1D-C2D	-4.90	121.34	129.53
3	B	761[B]	HDE	CHD-C1D-C2D	-4.89	121.35	129.53
3	D	761[B]	HDE	C1B-CHB-C4A	-4.85	120.52	130.12
3	B	761[B]	HDE	C1C-C2C-C3C	-4.70	100.81	105.81
3	B	761[B]	HDE	C4C-CHD-C1D	4.56	123.98	112.87
3	C	761[B]	HDE	C1B-CHB-C4A	-4.44	121.32	130.12
3	D	761[B]	HDE	CHD-C4C-C3C	-4.34	124.44	129.68
3	D	761[B]	HDE	C4C-CHD-C1D	4.26	123.27	112.87
3	D	761[B]	HDE	CHC-C1C-C2C	-4.22	122.47	129.53
2	C	760[A]	HDD	O1D-CGD-CBD	-4.20	105.95	110.19
3	D	761[B]	HDE	C3A-C4A-CHB	-4.07	117.55	124.28
3	D	761[B]	HDE	C1B-C2B-C3B	-3.99	104.22	107.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	761[B]	HDE	C1C-C2C-C3C	-3.98	101.58	105.81
3	D	761[B]	HDE	CAD-CBD-CGD	-3.94	102.73	113.76
3	A	761[B]	HDE	CAD-CBD-CGD	-3.88	102.89	113.76
3	B	761[B]	HDE	O1A-CGA-O2A	3.83	124.22	120.80
3	C	761[B]	HDE	C4C-CHD-C1D	3.81	122.16	112.87
3	A	761[B]	HDE	C1B-CHB-C4A	-3.79	122.61	130.12
2	C	760[A]	HDD	OND-C2D-CMD	-3.79	102.61	109.59
2	D	760[A]	HDD	O1D-CGD-O2D	3.79	124.18	120.80
3	C	761[B]	HDE	C4D-CHA-C1A	-3.74	122.72	130.12
2	B	760[A]	HDD	CMC-C2C-C1C	-3.66	122.84	128.46
3	C	761[B]	HDE	CAD-CBD-CGD	-3.65	103.52	113.76
2	B	760[A]	HDD	C1A-CHA-C4D	-3.62	122.94	130.12
3	B	761[B]	HDE	C1B-CHB-C4A	-3.62	122.95	130.12
3	D	761[B]	HDE	C4D-CHA-C1A	-3.56	123.08	130.12
3	B	761[B]	HDE	CHC-C1C-C2C	-3.51	123.65	129.53
3	B	761[B]	HDE	CAD-CBD-CGD	-3.45	104.09	113.76
3	D	761[B]	HDE	CMA-C3A-C4A	-3.43	106.53	112.63
3	A	761[B]	HDE	O1A-CGA-O2A	3.40	123.83	120.80
3	C	761[B]	HDE	CMA-C3A-C4A	-3.38	106.62	112.63
2	D	760[A]	HDD	C2B-C3B-C4B	3.37	109.25	106.90
3	D	761[B]	HDE	CMC-C2C-C3C	3.27	131.11	124.94
2	A	760[A]	HDD	C2B-C3B-C4B	3.24	109.16	106.90
3	A	761[B]	HDE	C4B-CHC-C1C	3.23	120.75	112.87
3	C	761[B]	HDE	CHC-C1C-C2C	-3.22	124.14	129.53
2	C	760[A]	HDD	OND-C2D-C1D	-3.22	105.39	111.92
3	C	761[B]	HDE	C3A-C4A-CHB	-3.22	118.96	124.28
3	D	761[B]	HDE	CAC-C3C-C4C	-3.21	123.33	127.19
2	B	760[A]	HDD	CAA-CBA-CGA	-3.19	104.80	113.76
3	A	761[B]	HDE	CMD-C2D-C3D	3.18	130.94	124.94
2	C	760[A]	HDD	C2B-C3B-C4B	3.16	109.11	106.90
3	B	761[B]	HDE	C4D-CHA-C1A	-3.12	123.95	130.12
3	B	761[B]	HDE	CHD-C4C-C3C	-3.11	125.92	129.68
2	A	760[A]	HDD	CAD-CBD-CGD	-3.10	99.78	104.56
2	A	760[A]	HDD	OND-C2D-CMD	-3.07	103.93	109.59
3	A	761[B]	HDE	C4C-CHD-C1D	3.03	120.26	112.87
3	D	761[B]	HDE	C1C-C2C-C3C	-3.03	102.59	105.81
3	A	761[B]	HDE	CHC-C1C-C2C	-3.03	124.47	129.53
3	C	761[B]	HDE	C4B-CHC-C1C	3.02	120.25	112.87
3	B	761[B]	HDE	CMB-C2B-C3B	2.99	130.58	124.94
3	D	761[B]	HDE	CMB-C2B-C3B	2.93	130.47	124.94
2	C	760[A]	HDD	CMC-C2C-C1C	-2.93	123.96	128.46
3	D	761[B]	HDE	C4B-CHC-C1C	2.91	119.97	112.87

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	761[B]	HDE	C4B-CHC-C1C	2.91	119.97	112.87
3	D	761[B]	HDE	CHB-C4A-NA	2.90	128.46	124.20
3	C	761[B]	HDE	CMD-C2D-C3D	2.89	130.39	124.94
2	A	760[A]	HDD	C3B-C4B-NB	-2.85	105.56	110.94
3	C	761[B]	HDE	C4C-C3C-C2C	2.84	110.16	105.93
2	D	760[A]	HDD	C4A-C3A-C2A	2.77	108.92	107.00
3	D	761[B]	HDE	O1A-CGA-O2A	2.77	123.27	120.80
2	D	760[A]	HDD	CMC-C2C-C1C	-2.74	124.25	128.46
2	D	760[A]	HDD	CAA-CBA-CGA	-2.74	106.08	113.76
3	A	761[B]	HDE	C1C-C2C-C3C	-2.70	102.94	105.81
3	B	761[B]	HDE	C3A-C4A-CHB	-2.69	119.84	124.28
2	A	760[A]	HDD	CAA-CBA-CGA	-2.64	106.35	113.76
3	D	761[B]	HDE	CBC-CAC-C3C	-2.64	105.55	112.27
2	C	760[A]	HDD	C3C-C4C-NC	-2.63	105.81	109.21
2	B	760[A]	HDD	CMC-C2C-C3C	2.62	129.59	124.68
3	D	761[B]	HDE	O1A-C2A-C1A	2.59	113.51	108.25
2	C	760[A]	HDD	CHA-C4D-ND	-2.58	120.42	124.20
2	D	760[A]	HDD	CMA-C3A-C4A	-2.57	124.51	128.46
3	A	761[B]	HDE	C4D-CHA-C1A	-2.54	125.09	130.12
3	A	761[B]	HDE	CBC-CAC-C3C	-2.52	105.85	112.27
3	A	761[B]	HDE	C1D-C2D-C3D	-2.49	103.16	105.81
3	C	761[B]	HDE	O1A-C2A-CAA	2.48	107.68	103.01
2	D	760[A]	HDD	C2D-C1D-CHD	2.39	128.22	124.28
3	B	761[B]	HDE	C4C-C3C-C2C	2.31	109.38	105.93
2	D	760[A]	HDD	O2A-CGA-CBA	2.31	121.45	114.03
2	A	760[A]	HDD	C3C-C4C-NC	-2.27	106.27	109.21
3	A	761[B]	HDE	O1A-C2A-C1A	2.26	112.85	108.25
3	A	761[B]	HDE	CAB-C3B-C4B	-2.26	124.47	127.19
2	C	760[A]	HDD	CAA-CBA-CGA	-2.25	107.45	113.76
2	B	760[A]	HDD	OND-C2D-CMD	-2.22	105.50	109.59
3	C	761[B]	HDE	C1D-C2D-C3D	-2.21	103.46	105.81
2	B	760[A]	HDD	C4A-C3A-C2A	2.20	108.53	107.00
2	D	760[A]	HDD	OND-C2D-CMD	-2.19	105.57	109.59
2	C	760[A]	HDD	CMC-C2C-C3C	2.18	128.75	124.68
2	A	760[A]	HDD	C4A-C3A-C2A	2.08	108.44	107.00
2	D	760[A]	HDD	C3B-C4B-NB	-2.08	107.02	110.94
3	D	761[B]	HDE	CMB-C2B-C1B	-2.06	125.30	128.46
3	D	761[B]	HDE	O1A-C2A-CAA	2.05	106.87	103.01
3	B	761[B]	HDE	CMA-C3A-C4A	-2.05	108.99	112.63
2	C	760[A]	HDD	CMA-C3A-C4A	-2.04	125.32	128.46
2	A	760[A]	HDD	CMA-C3A-C4A	-2.04	125.33	128.46
3	A	761[B]	HDE	ONA-C3A-C4A	-2.04	107.78	111.92

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	760[A]	HDD	CMA-C3A-C4A	-2.01	125.37	128.46
3	A	761[B]	HDE	CMC-C2C-C3C	2.01	128.73	124.94

There are no chirality outliers.

All (32) torsion outliers are listed below:

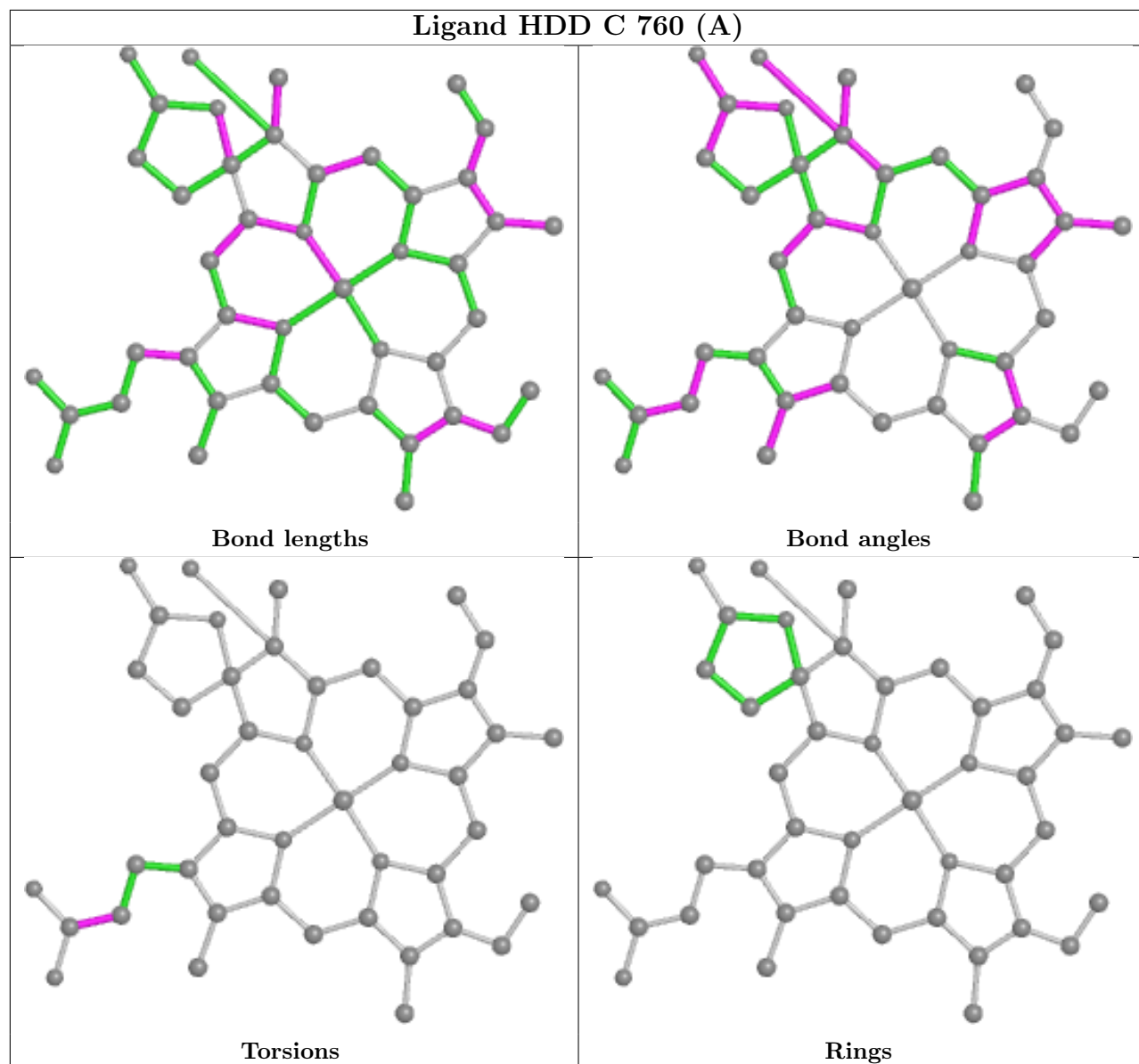
Mol	Chain	Res	Type	Atoms
3	A	761[B]	HDE	C2B-C3B-CAB-CBB
3	A	761[B]	HDE	C4B-C3B-CAB-CBB
3	A	761[B]	HDE	C2C-C3C-CAC-CBC
3	A	761[B]	HDE	C4C-C3C-CAC-CBC
3	B	761[B]	HDE	C2B-C3B-CAB-CBB
3	B	761[B]	HDE	C4B-C3B-CAB-CBB
3	B	761[B]	HDE	C2C-C3C-CAC-CBC
3	B	761[B]	HDE	C4C-C3C-CAC-CBC
3	C	761[B]	HDE	C2B-C3B-CAB-CBB
3	C	761[B]	HDE	C4B-C3B-CAB-CBB
3	C	761[B]	HDE	C2C-C3C-CAC-CBC
3	C	761[B]	HDE	C4C-C3C-CAC-CBC
3	D	761[B]	HDE	C2B-C3B-CAB-CBB
3	D	761[B]	HDE	C4B-C3B-CAB-CBB
3	D	761[B]	HDE	C2C-C3C-CAC-CBC
3	D	761[B]	HDE	C4C-C3C-CAC-CBC
2	D	760[A]	HDD	CAA-CBA-CGA-O2A
2	B	760[A]	HDD	CAA-CBA-CGA-O1A
3	A	761[B]	HDE	CAD-CBD-CGD-O2D
2	A	760[A]	HDD	CAA-CBA-CGA-O1A
2	C	760[A]	HDD	CAA-CBA-CGA-O1A
3	C	761[B]	HDE	CAD-CBD-CGD-O2D
3	D	761[B]	HDE	CAD-CBD-CGD-O2D
3	D	761[B]	HDE	CAD-CBD-CGD-O1D
2	A	760[A]	HDD	CAA-CBA-CGA-O2A
2	D	760[A]	HDD	CAA-CBA-CGA-O1A
2	B	760[A]	HDD	CAA-CBA-CGA-O2A
2	C	760[A]	HDD	CAA-CBA-CGA-O2A
3	A	761[B]	HDE	CAD-CBD-CGD-O1D
3	B	761[B]	HDE	CAD-CBD-CGD-O2D
3	C	761[B]	HDE	CAD-CBD-CGD-O1D
3	B	761[B]	HDE	CAD-CBD-CGD-O1D

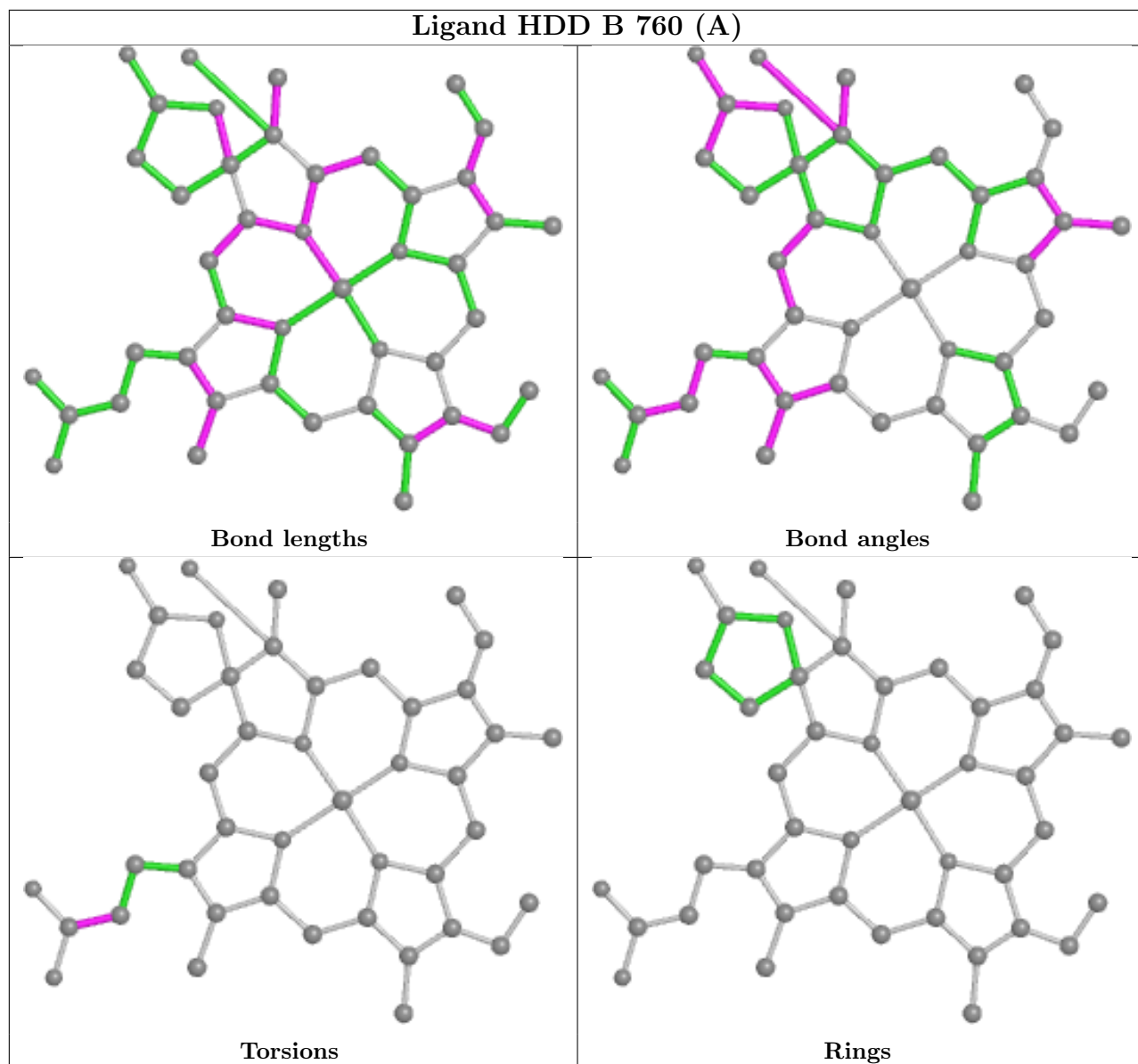
There are no ring outliers.

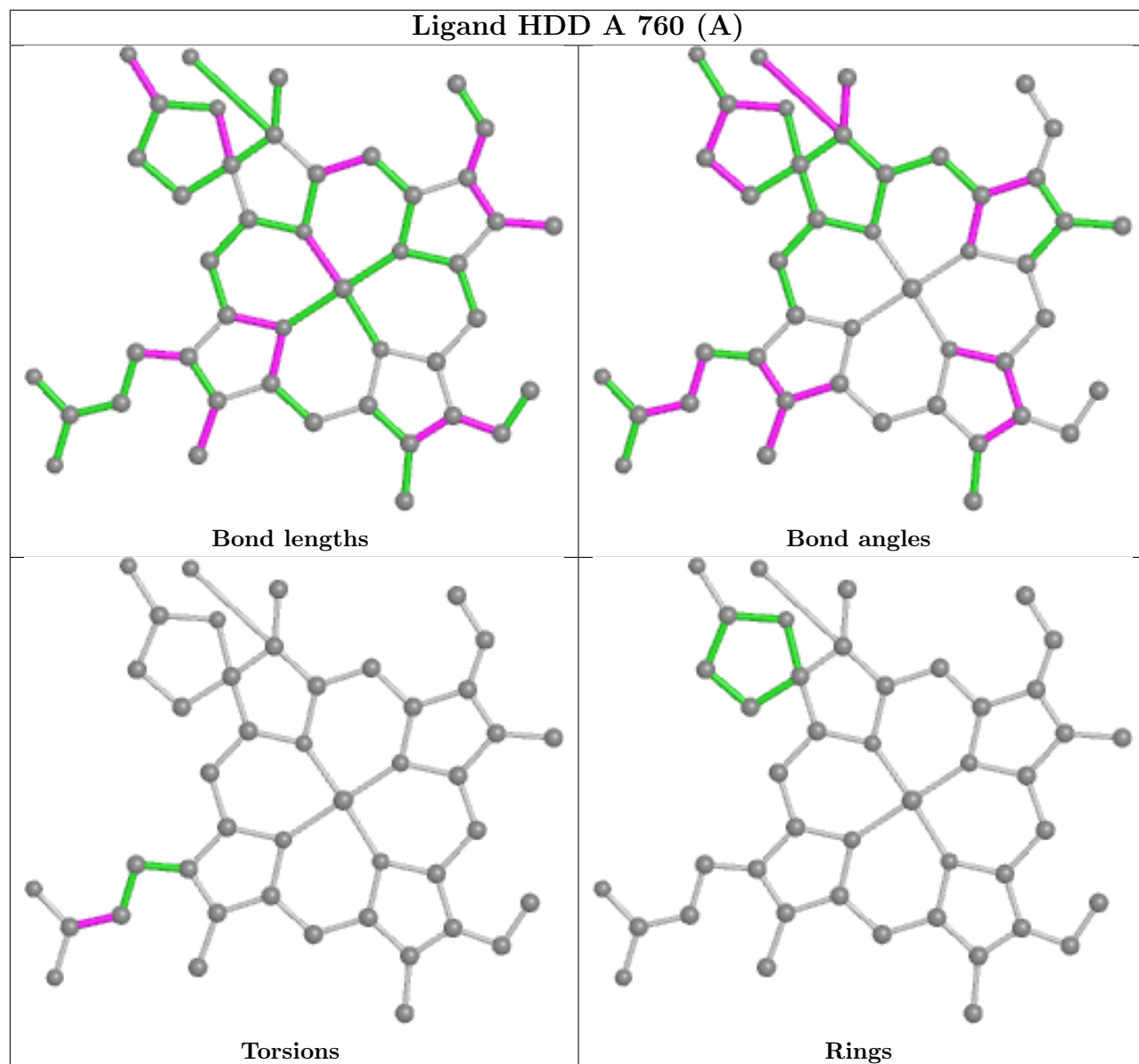
8 monomers are involved in 96 short contacts:

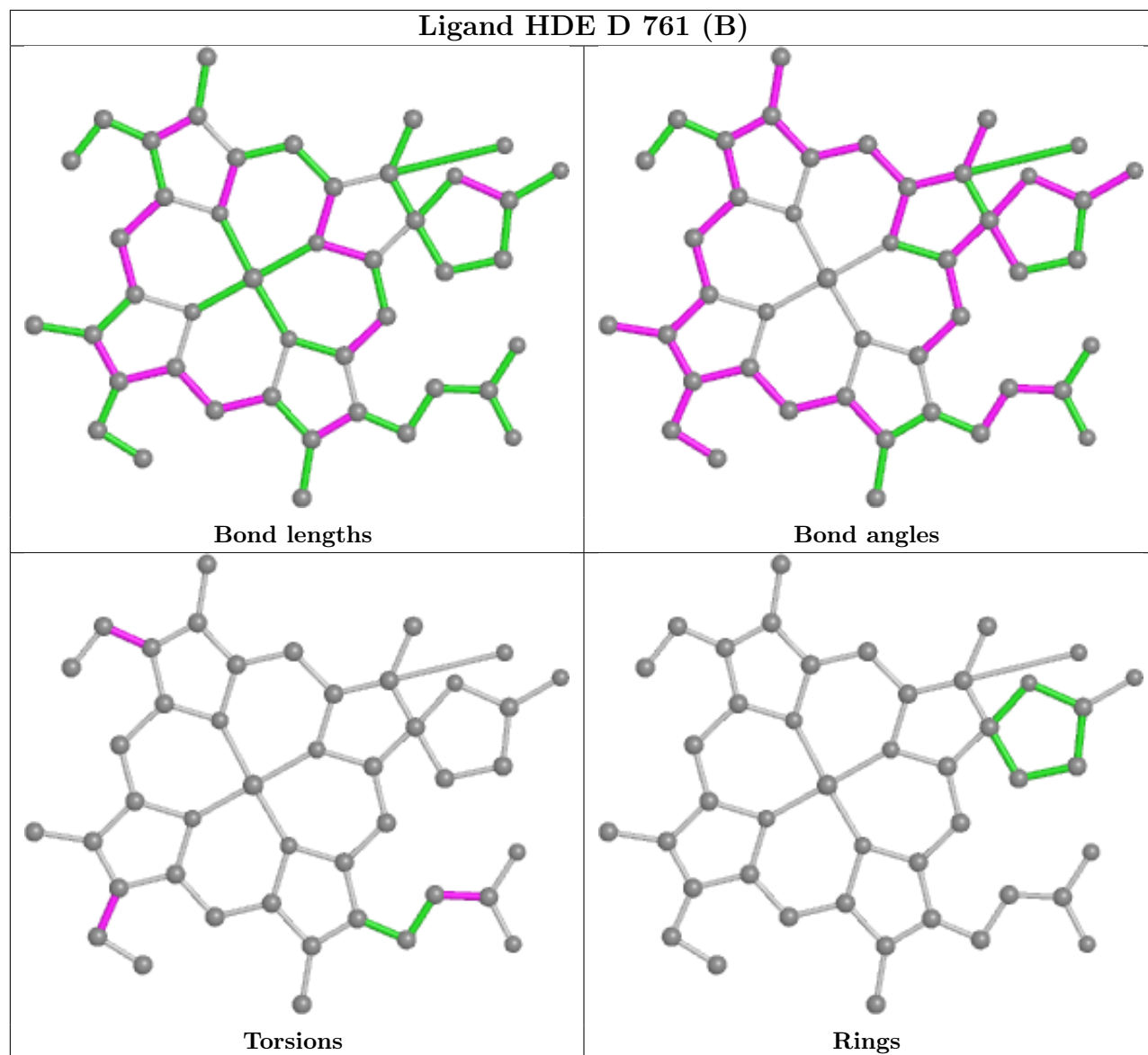
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	760[A]	HDD	15	0
2	B	760[A]	HDD	17	0
2	A	760[A]	HDD	11	0
3	D	761[B]	HDE	7	0
3	C	761[B]	HDE	13	0
3	A	761[B]	HDE	12	0
2	D	760[A]	HDD	10	0
3	B	761[B]	HDE	11	0

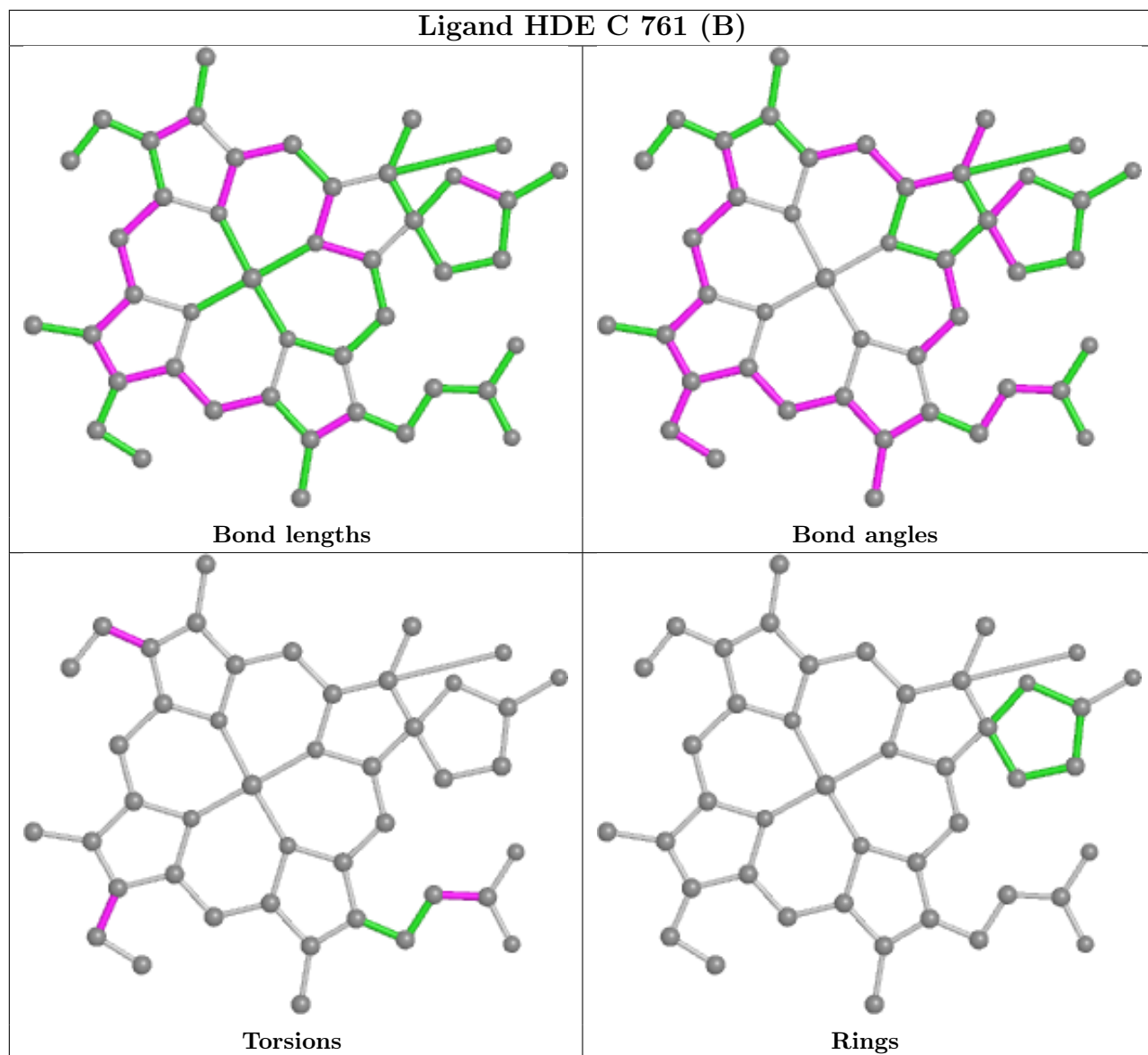
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

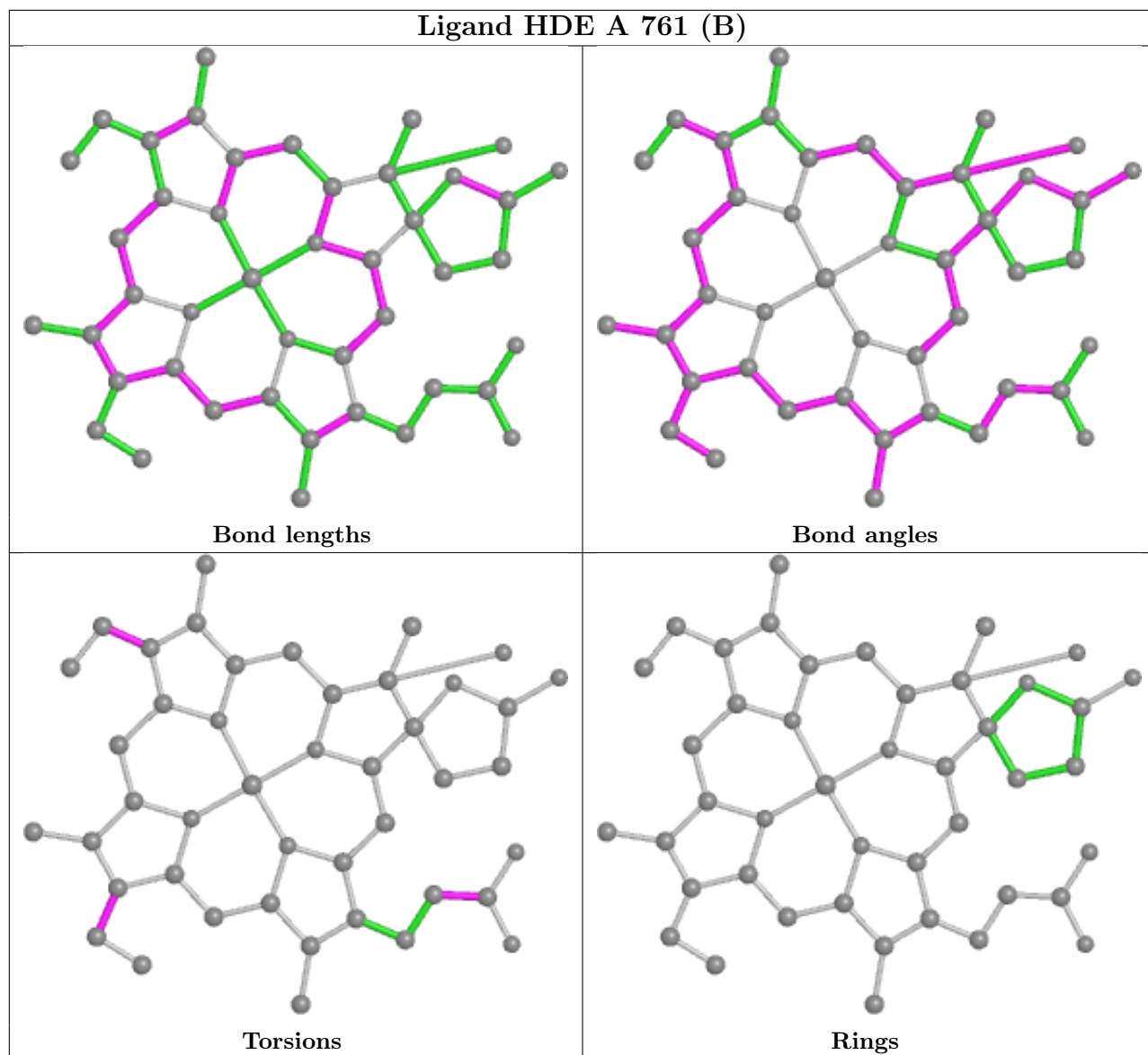




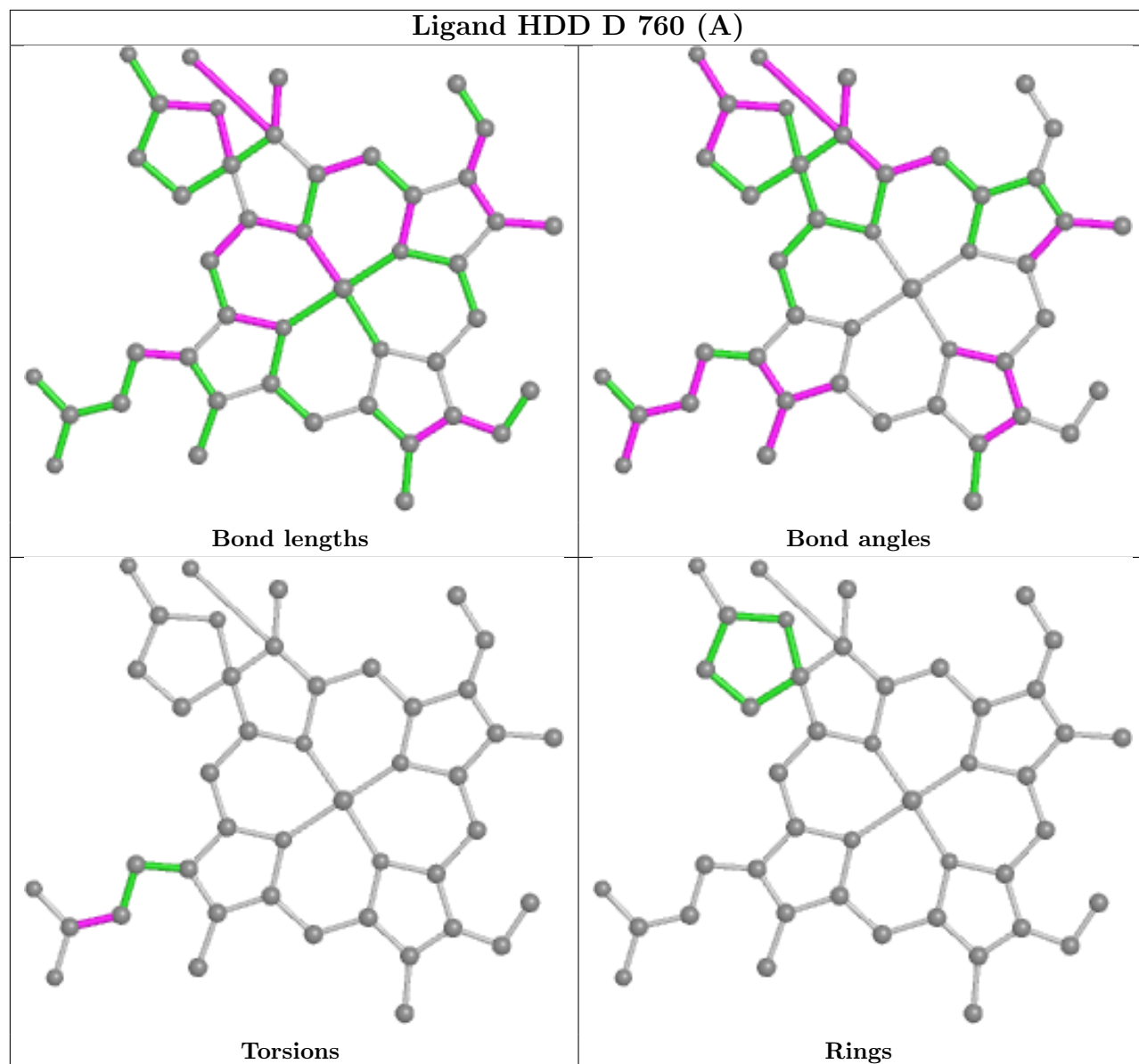


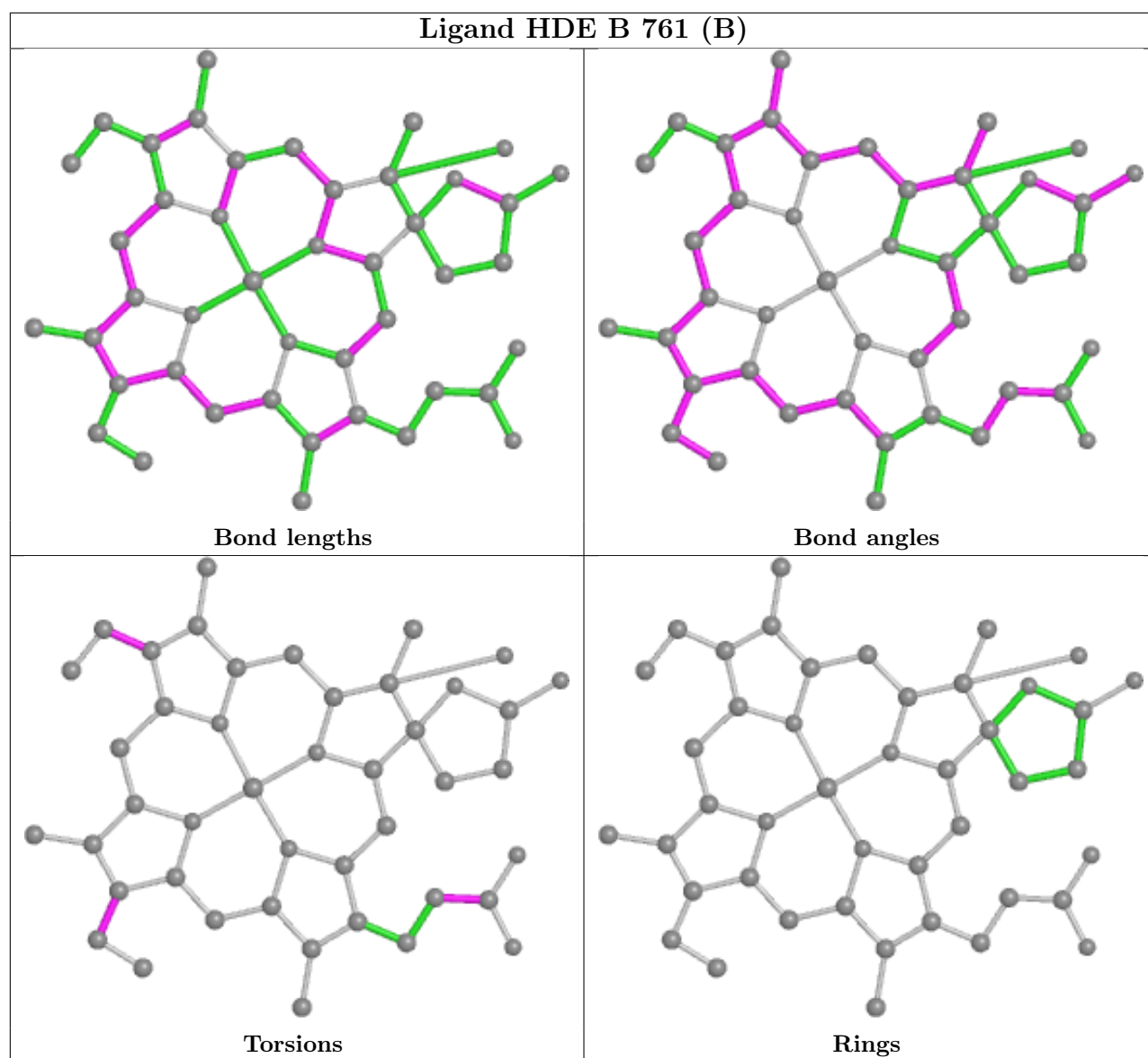












## 5.7 Other polymers [i](#)

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, 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	726/753 (96%)	-0.78	3 (0%) 92 90	3, 10, 27, 44	2 (0%)
1	B	726/753 (96%)	-0.63	10 (1%) 75 72	4, 12, 32, 45	2 (0%)
1	C	726/753 (96%)	-0.67	6 (0%) 86 84	4, 12, 31, 45	2 (0%)
1	D	726/753 (96%)	-0.78	5 (0%) 87 86	3, 10, 28, 45	1 (0%)
All	All	2904/3012 (96%)	-0.72	24 (0%) 86 84	3, 11, 30, 45	7 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	726	GLY	4.3
1	D	28	SER	3.6
1	B	32	GLU	3.5
1	B	713	GLN	3.1
1	C	726	GLY	3.0
1	B	725	ASP	2.8
1	B	28	SER	2.7
1	D	749	ASP	2.6
1	B	712	ASP	2.6
1	C	750	LYS	2.6
1	B	647	VAL	2.6
1	B	568	ASP	2.5
1	A	32	GLU	2.5
1	D	750	LYS	2.5
1	A	750	LYS	2.4
1	C	711	ALA	2.3
1	C	594	PRO	2.3
1	D	713	GLN	2.2
1	D	712	ASP	2.2
1	B	677	ASP	2.1
1	C	28	SER	2.1

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	583	LYS	2.1
1	A	713	GLN	2.0
1	C	583	LYS	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

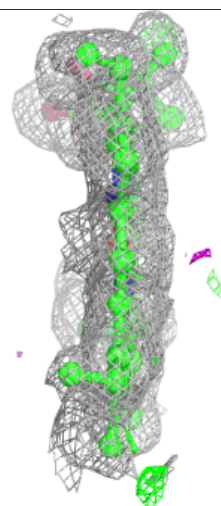
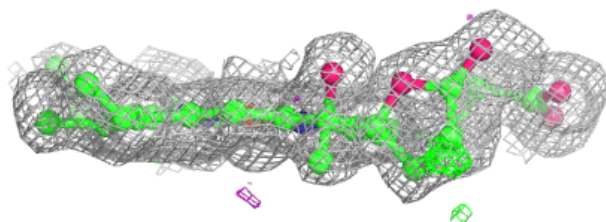
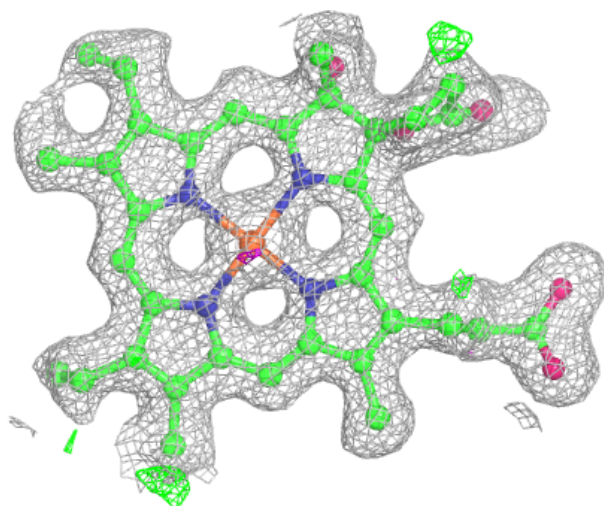
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	H2S	D	754	1/1	0.93	0.33	25,25,25,25	1
4	H2S	C	754	1/1	0.94	0.24	19,19,19,19	1
4	H2S	A	754	1/1	0.95	0.34	29,29,29,29	1
2	HDD	A	760[A]	44/44	0.98	0.07	2,3,8,10	44
4	H2S	B	754	1/1	0.98	0.27	20,20,20,20	1
2	HDD	B	760[A]	44/44	0.98	0.07	3,4,8,8	44
3	HDE	B	761[B]	44/44	0.98	0.07	3,9,13,15	44
3	HDE	D	761[B]	44/44	0.99	0.06	2,8,13,17	44
2	HDD	D	760[A]	44/44	0.99	0.06	2,3,7,14	44
3	HDE	A	761[B]	44/44	0.99	0.07	2,7,11,15	44
2	HDD	C	760[A]	44/44	0.99	0.07	3,4,9,15	44
3	HDE	C	761[B]	44/44	0.99	0.07	3,11,13,13	44

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.

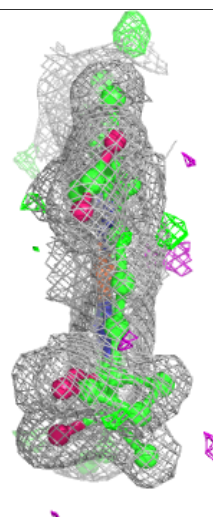
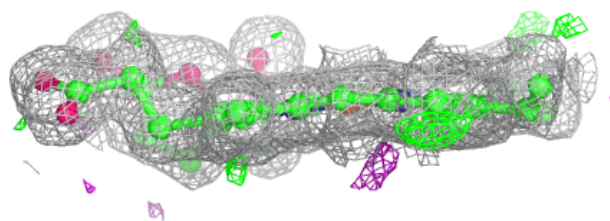
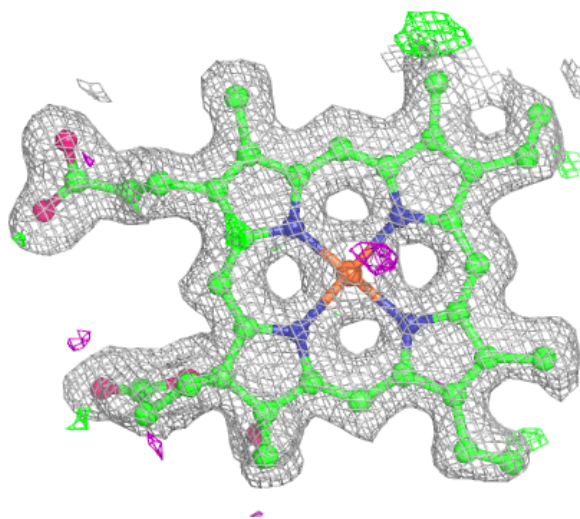
**Electron density around HDD A 760 (A):**

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



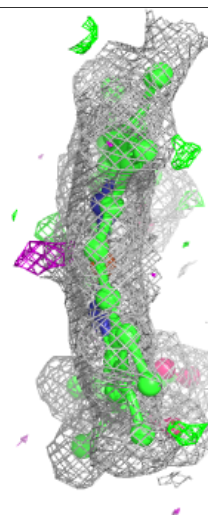
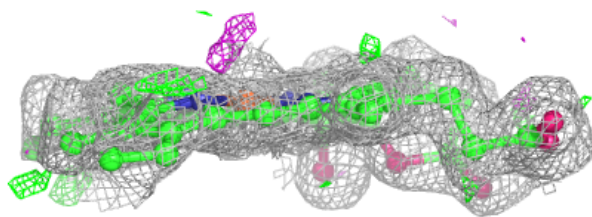
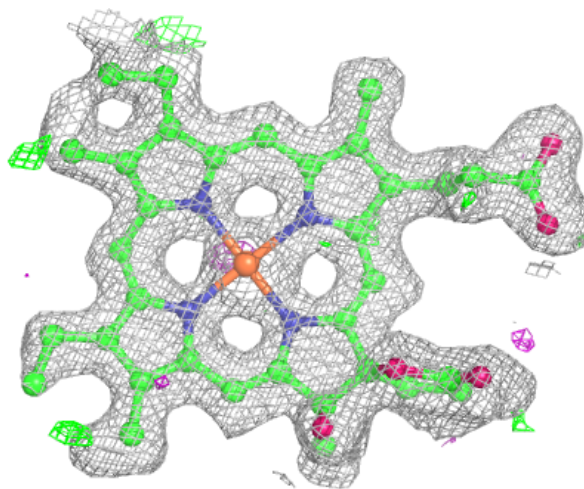
**Electron density around HDD B 760 (A):**

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



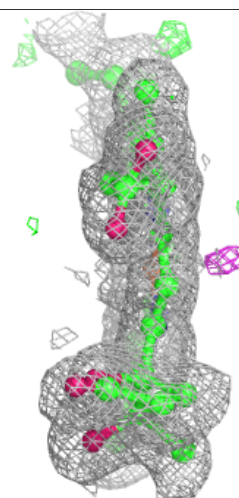
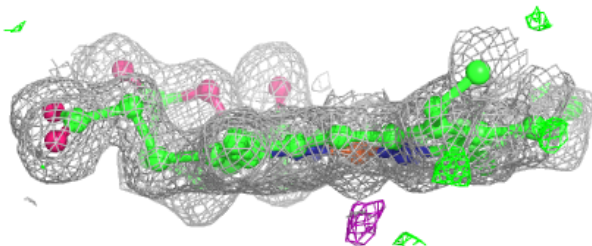
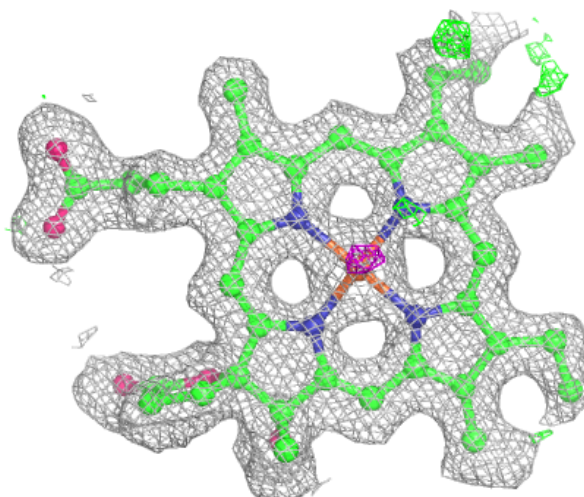
**Electron density around HDE B 761 (B):**

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



**Electron density around HDE D 761 (B):**

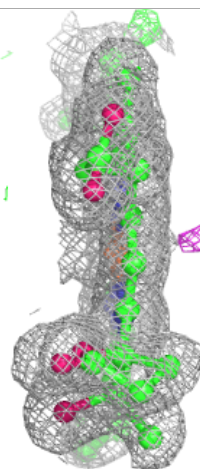
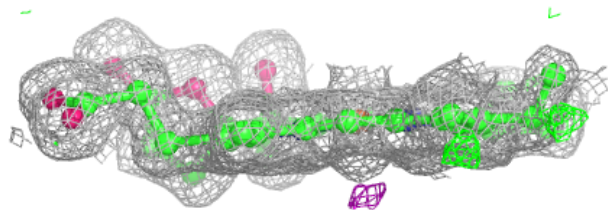
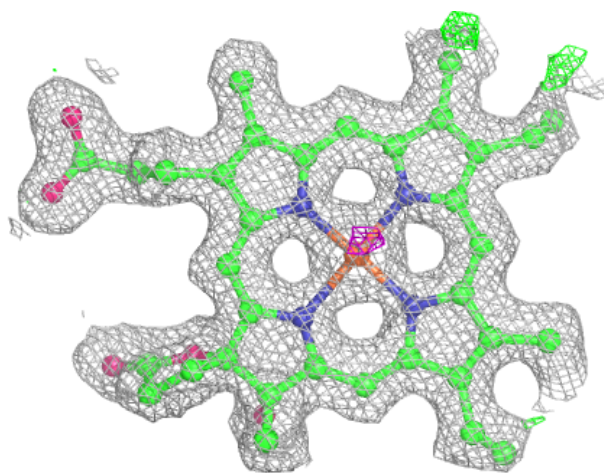
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





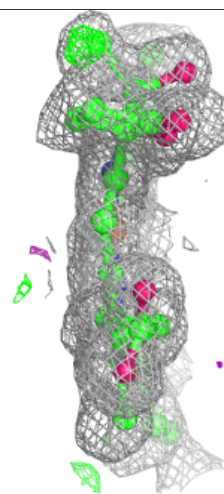
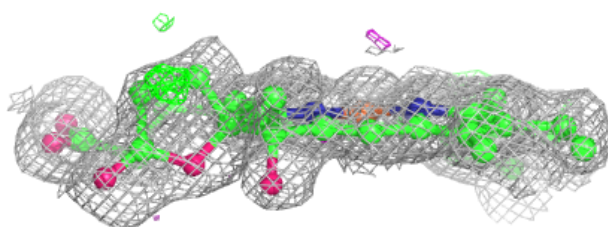
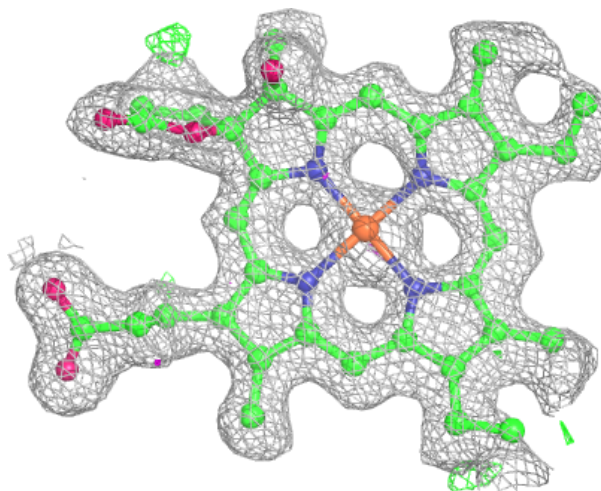
**Electron density around HDD D 760 (A):**

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



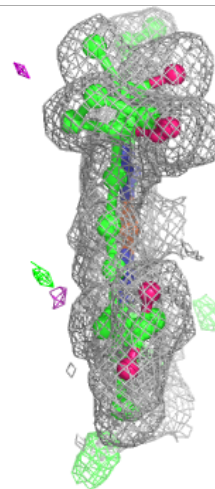
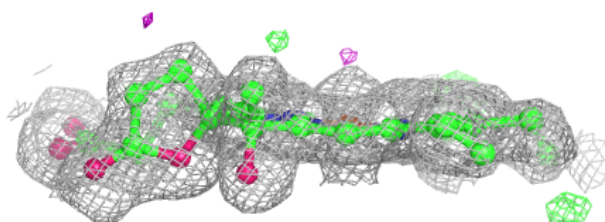
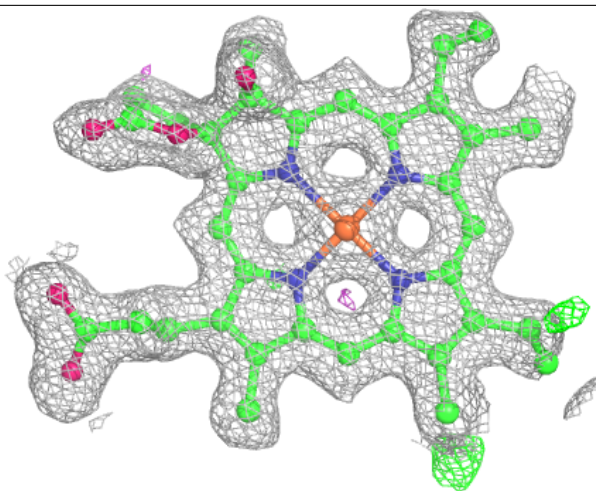
**Electron density around HDE A 761 (B):**

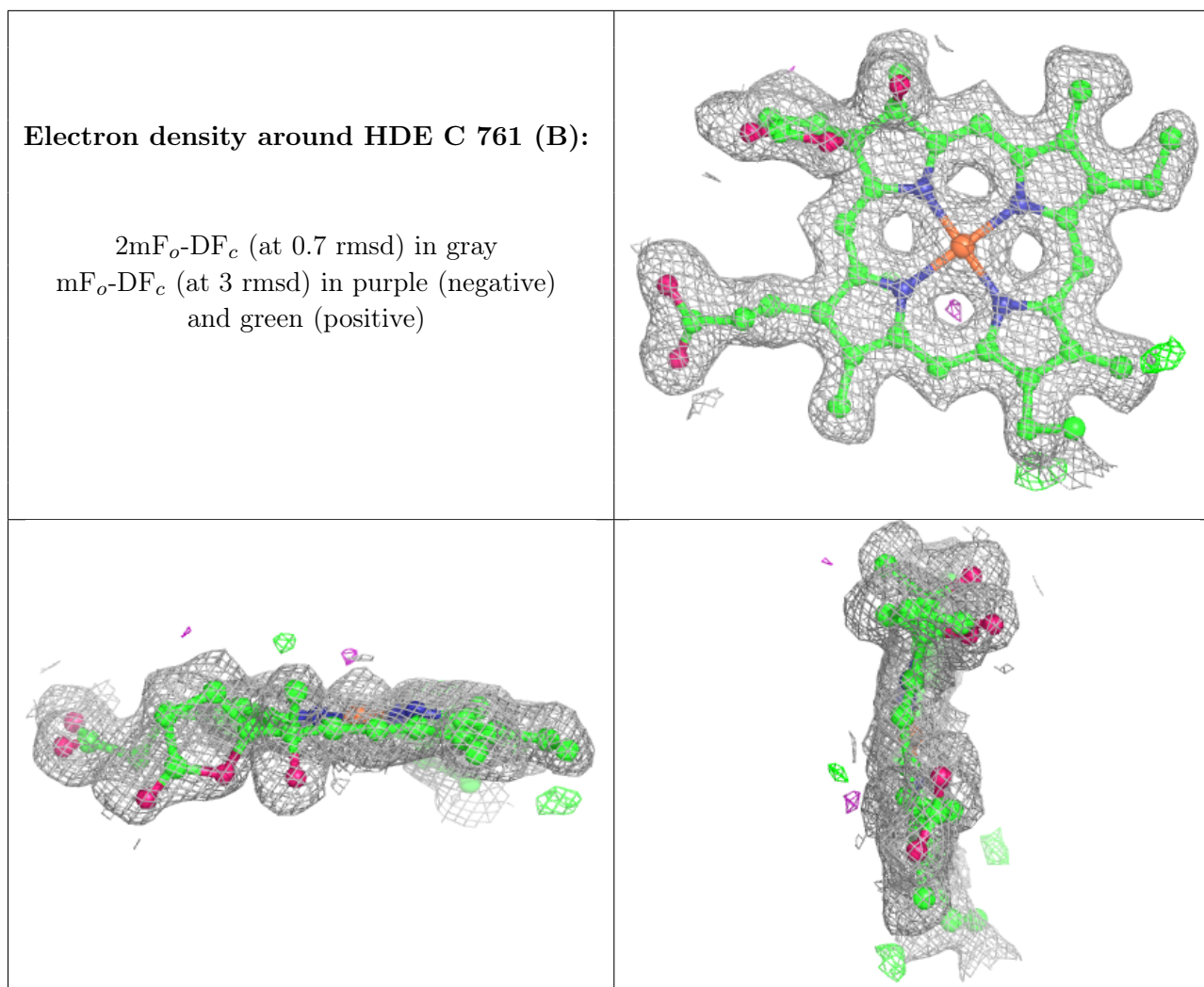
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HDD C 760 (A):**

$2mF_o-DF_c$  (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.