Full wwPDB X-ray Structure Validation Report (i)

Aug 30, 2023 – 07:54 AM EDT

PDB ID	:	3PQ3
Title	:	Structure of I274C variant of E. coli KatE[] - Images 7-12
Authors	:	Loewen, P.C.; Jha, V.; Louis, S.; Chelikani, P.; Carpena, X.; Fita, I.
Deposited on	:	2010-11-25
Resolution	:	1.79 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

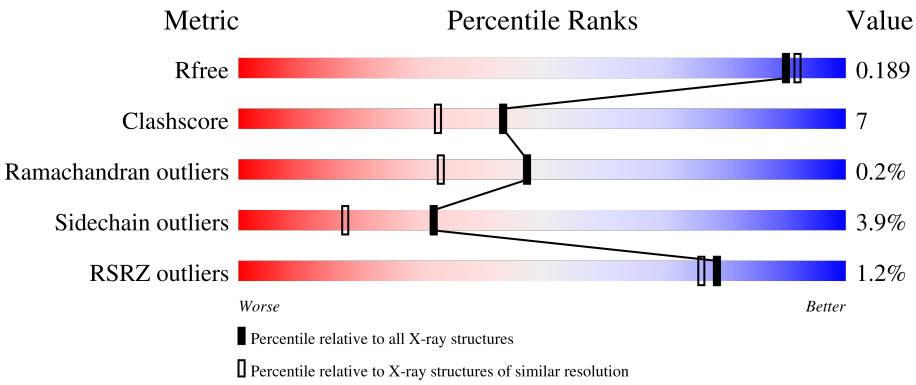
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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 >=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 <=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	2% 84% 11%
1	C	753	% 86% 9%
1	D	753	% 84% 11%

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 (i)

There are 5 unique types of molecules in this entry. The entry contains 26828 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.

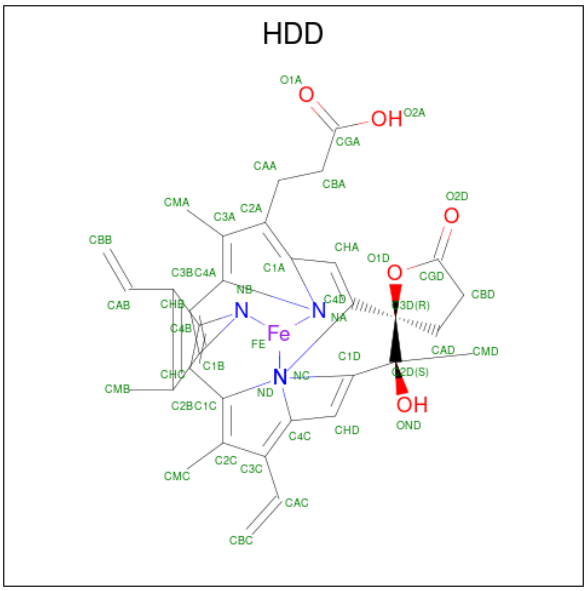
- Molecule 1 is a protein called Catalase HPII.

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:

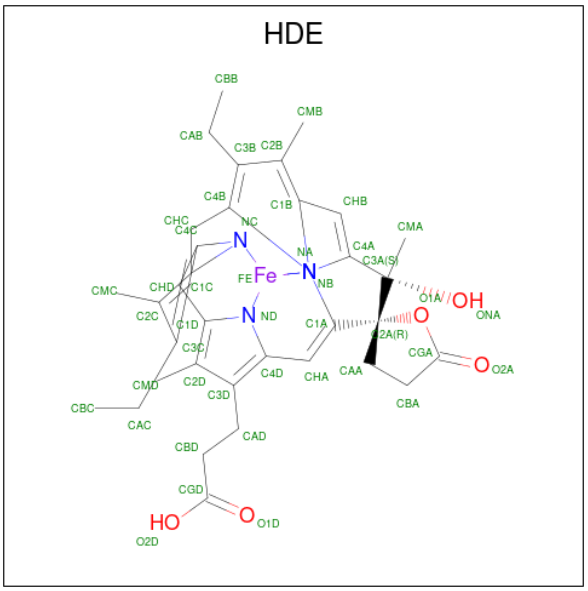
Chain	Residue	Modelled	Actual	Comment	Reference
A	274	CYS	ILE	engineered mutation	UNP P21179
A	438	ALA	CYS	engineered mutation	UNP P21179
A	669	ALA	CYS	engineered mutation	UNP P21179
B	274	CYS	ILE	engineered mutation	UNP P21179
B	438	ALA	CYS	engineered mutation	UNP P21179
B	669	ALA	CYS	engineered mutation	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: $C_{34}H_{32}FeN_4O_5$).



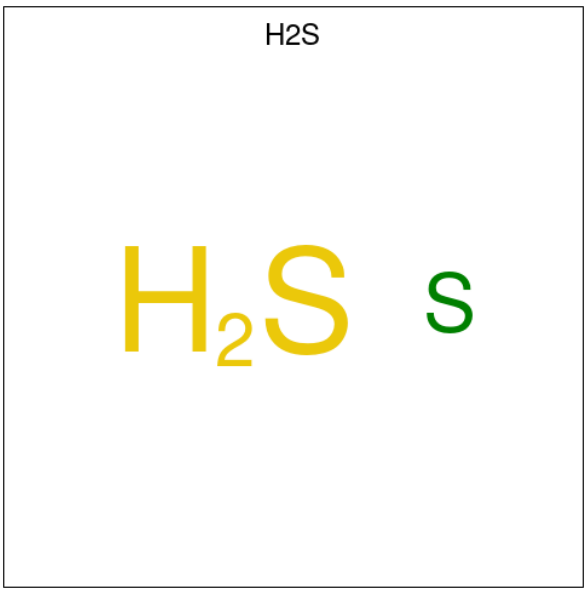
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	44	34	1	4	5	0	1
			Total	C	Fe	N	O		
2	B	1	44	34	1	4	5	0	1
			Total	C	Fe	N	O		
2	C	1	44	34	1	4	5	0	1
			Total	C	Fe	N	O		
2	D	1	44	34	1	4	5	0	1

- 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
			Total	C	Fe	N	O		
3	A	1	44	34	1	4	5	0	1
3	B	1	44	34	1	4	5	0	1
3	C	1	44	34	1	4	5	0	1
3	D	1	44	34	1	4	5	0	1

- Molecule 4 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H_2S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	895	895	895	0	0
5	B	791	791	791	0	0

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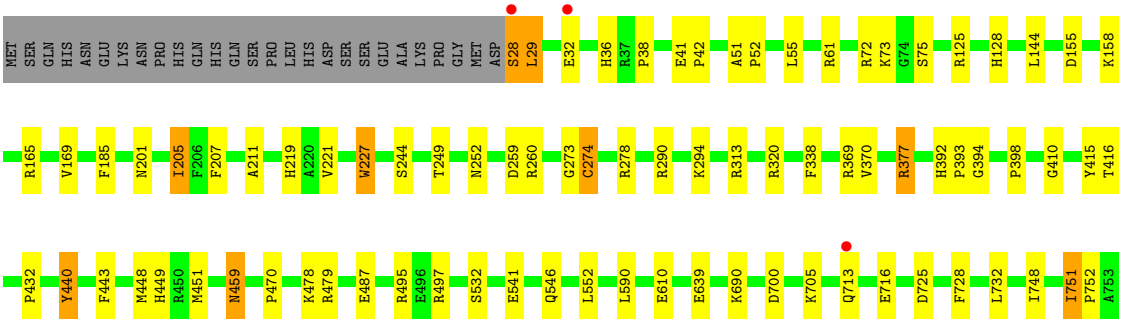
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	C	842	842	842	0	0
			Total	O		
5	D	914	914	914	0	0

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.

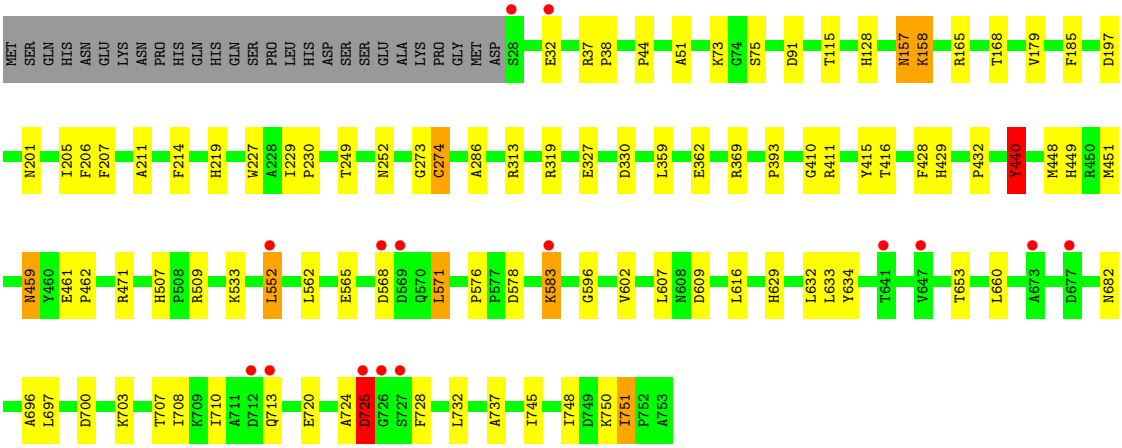
- Molecule 1: Catalase HPII

Chain A:



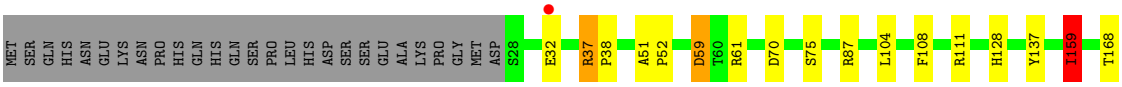
- Molecule 1: Catalase HPII

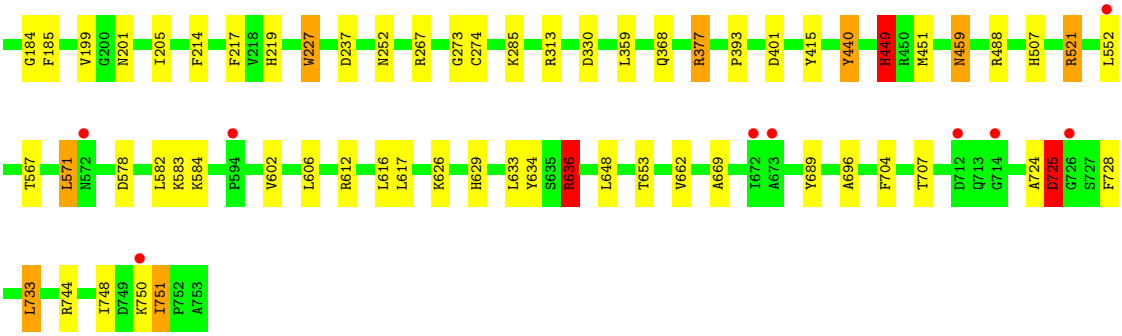
Chain B:



- Molecule 1: Catalase HPII

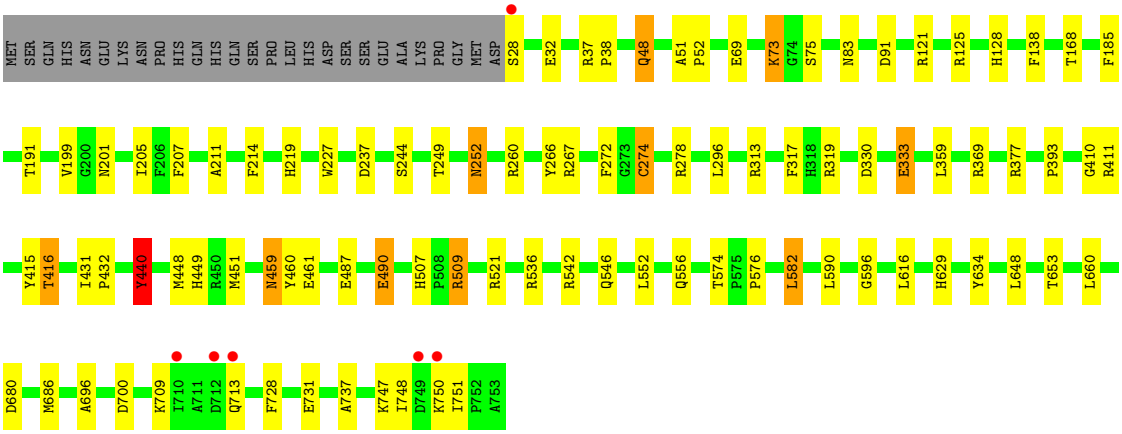
Chain C:





- Molecule 1: Catalase HPII

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.51Å 133.03Å 122.65Å 90.00° 109.39° 90.00°	Depositor
Resolution (Å)	35.23 – 1.79 35.23 – 1.79	Depositor EDS
% Data completeness (in resolution range)	92.3 (35.23-1.79) 92.3 (35.23-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 1.79Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.142 , 0.189 0.142 , 0.189	Depositor DCC
R_{free} test set	12198 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	11.4	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	26828	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: H2S, HDE, 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	1.17	5/5932 (0.1%)	0.97	11/8064 (0.1%)
1	B	1.12	6/5931 (0.1%)	0.94	4/8062 (0.0%)
1	C	1.13	2/5908 (0.0%)	0.96	16/8033 (0.2%)
1	D	1.19	11/5966 (0.2%)	0.96	11/8109 (0.1%)
All	All	1.15	24/23737 (0.1%)	0.96	42/32268 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	440	TYR	CE1-CZ	7.19	1.47	1.38
1	B	440	TYR	CE1-CZ	6.39	1.46	1.38
1	B	362	GLU	CB-CG	6.08	1.63	1.52
1	B	327	GLU	CB-CG	5.98	1.63	1.52
1	D	138	PHE	CD1-CE1	5.89	1.51	1.39
1	C	108	PHE	CE2-CZ	5.75	1.48	1.37
1	B	428	PHE	CE2-CZ	5.66	1.48	1.37
1	D	272	PHE	CE2-CZ	5.65	1.48	1.37
1	A	440	TYR	CE1-CZ	5.64	1.45	1.38
1	D	266	TYR	CD2-CE2	5.63	1.47	1.39
1	D	214	PHE	CE2-CZ	5.62	1.48	1.37
1	D	199	VAL	CB-CG1	5.59	1.64	1.52
1	B	179	VAL	CB-CG2	5.58	1.64	1.52
1	D	333	GLU	CD-OE2	-5.54	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	317	PHE	CE2-CZ	5.46	1.47	1.37
1	D	69	GLU	CG-CD	5.29	1.59	1.51
1	B	286	ALA	CA-CB	5.28	1.63	1.52
1	D	460	TYR	CD1-CE1	5.11	1.47	1.39
1	A	221	VAL	CB-CG2	5.09	1.63	1.52
1	C	217	PHE	CB-CG	-5.09	1.42	1.51
1	A	338	PHE	CE2-CZ	5.08	1.47	1.37
1	D	440	TYR	CD2-CE2	5.06	1.47	1.39
1	A	377	ARG	CZ-NH2	5.02	1.39	1.33
1	A	41	GLU	CG-CD	5.01	1.59	1.51

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	636	ARG	NE-CZ-NH2	-8.87	115.87	120.30
1	C	636	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	A	495	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	A	495	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	C	377	ARG	NE-CZ-NH1	-7.51	116.55	120.30
1	B	609	ASP	CB-CG-OD2	6.88	124.50	118.30
1	C	111	ARG	NE-CZ-NH1	-6.87	116.86	120.30
1	D	686	MET	CG-SD-CE	6.82	111.10	100.20
1	A	320	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	A	294	LYS	CD-CE-NZ	-6.35	97.09	111.70
1	A	479	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	C	401	ASP	CB-CG-OD2	6.27	123.94	118.30
1	C	733	LEU	CA-CB-CG	6.19	129.53	115.30
1	C	449[A]	HIS	CA-C-O	-6.12	107.26	120.10
1	C	449[B]	HIS	CA-C-O	-6.12	107.26	120.10
1	D	377	ARG	NE-CZ-NH1	-6.05	117.28	120.30
1	C	87	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	C	37	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	D	125	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	D	121	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	C	59	ASP	CB-CG-OD1	5.79	123.51	118.30
1	D	582	LEU	CB-CG-CD1	5.75	120.78	111.00
1	C	159	ILE	CB-CG1-CD1	-5.54	98.38	113.90
1	C	70	ASP	CB-CG-OD2	5.54	123.29	118.30
1	D	125	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	D	536	ARG	NE-CZ-NH1	-5.49	117.56	120.30
1	A	497	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	D	509	ARG	NE-CZ-NH1	5.48	123.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	197	ASP	CB-CG-OD2	5.44	123.19	118.30
1	C	313	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C	725	ASP	N-CA-C	5.37	125.51	111.00
1	A	290	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	D	521	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	471	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	C	313	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	A	72	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	A	313	ARG	NE-CZ-NH1	-5.27	117.67	120.30
1	A	479	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	D	680	ASP	CB-CG-OD2	5.21	122.99	118.30
1	D	542	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	A	259	ASP	CB-CG-OD2	5.16	122.95	118.30
1	B	609	ASP	CB-CG-OD1	-5.16	113.65	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	449[A]	HIS	Mainchain
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	74	0
1	B	5757	0	5587	82	0
1	C	5747	0	5577	61	1
1	D	5771	0	5598	52	0
2	A	44	0	31	9	0
2	B	44	0	31	20	0
2	C	44	0	30	15	0
2	D	44	0	31	8	0
3	A	44	0	36	7	0
3	B	44	0	36	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	44	0	36	12	0
3	D	44	0	36	11	0
4	A	1	0	0	6	0
4	B	1	0	0	8	0
4	C	1	0	0	3	0
4	D	1	0	0	8	0
5	A	895	0	0	20	2
5	B	791	0	0	16	1
5	C	842	0	0	20	0
5	D	914	0	0	18	0
All	All	26828	0	22611	308	2

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 7.

All (308) 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:D:274:CYS:HB3	4:D:754:H2S:S	1.27	1.70
1:A:274:CYS:HB3	4:A:754:H2S:S	1.32	1.69
2:B:760[A]:HDD:HBB2	4:B:754:H2S:S	1.33	1.67
1:C:274:CYS:HB3	4:C:754:H2S:S	1.41	1.57
1:B:274:CYS:HB3	4:B:754:H2S:S	1.54	1.47
1:D:274:CYS:CB	4:D:754:H2S:S	2.15	1.33
2:B:760[A]:HDD:CBB	4:B:754:H2S:S	2.17	1.31
1:B:449[A]:HIS:CE1	5:B:3618:HOH:O	1.65	1.28
3:B:761[B]:HDE:HMC	3:B:761[B]:HDE:CBC	1.61	1.27
2:D:760[A]:HDD:HBB2	4:D:754:H2S:S	1.75	1.27
1:B:274:CYS:CB	4:B:754:H2S:S	2.23	1.26
1:A:274:CYS:CB	4:A:754:H2S:S	2.25	1.23
3:B:761[B]:HDE:CMC	3:B:761[B]:HDE:HBCA	1.65	1.22
1:A:716:GLU:HG2	5:A:3090:HOH:O	1.40	1.20
3:C:761[B]:HDE:CBC	3:C:761[B]:HDE:HMC	1.75	1.15
1:D:451:MET:SD	5:D:3617:HOH:O	2.05	1.14
1:C:274:CYS:CB	4:C:754:H2S:S	2.36	1.13
1:C:578:ASP:HB3	5:C:2919:HOH:O	1.48	1.12
1:C:451:MET:SD	5:C:3612:HOH:O	2.07	1.11
3:D:761[B]:HDE:HBCB	3:D:761[B]:HDE:HMC	1.32	1.10
1:B:73:LYS:HE3	5:D:3517:HOH:O	1.51	1.10
2:D:760[A]:HDD:CBB	4:D:754:H2S:S	2.40	1.09
1:B:416:THR:HG21	5:D:2464:HOH:O	1.51	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:761[B]:HDE:HMC	3:C:761[B]:HDE:HBCB	1.06	1.06
1:C:267:ARG:HG3	5:C:2916:HOH:O	1.54	1.05
3:C:761[B]:HDE:HBCB	3:C:761[B]:HDE:CMC	1.82	1.05
1:A:201:ASN:CG	2:A:760[A]:HDD:HMB2	1.77	1.04
1:B:451:MET:SD	5:B:3614:HOH:O	2.16	1.03
1:B:201:ASN:CG	2:B:760[A]:HDD:HMB2	1.82	1.00
1:D:201:ASN:CG	2:D:760[A]:HDD:HMB2	1.81	0.99
1:C:201:ASN:CG	2:C:760[A]:HDD:HMB2	1.84	0.97
2:A:760[A]:HDD:HBB2	4:A:754:H2S:S	2.05	0.97
1:A:274:CYS:SG	2:A:760[A]:HDD:CMB	2.53	0.95
1:A:28:SER:O	1:A:28:SER:OG	1.82	0.94
1:A:416[A]:THR:HG21	5:C:3313:HOH:O	1.68	0.93
1:A:274:CYS:SG	2:A:760[A]:HDD:HMB3	2.09	0.92
3:A:761[B]:HDE:HBCB	3:A:761[B]:HDE:HMC	1.52	0.91
1:B:449[A]:HIS:NE2	5:B:3618:HOH:O	1.82	0.91
3:B:761[B]:HDE:HMC	3:B:761[B]:HDE:HBCA	0.90	0.90
2:A:760[A]:HDD:CBB	4:A:754:H2S:S	2.61	0.89
1:C:748:ILE:O	1:C:751:ILE:HG22	1.74	0.88
1:C:274:CYS:SG	2:C:760[A]:HDD:HMB3	2.14	0.88
1:A:751:ILE:HD13	1:A:751:ILE:O	1.75	0.87
1:D:274:CYS:SG	2:D:760[A]:HDD:HMB3	2.15	0.87
2:B:760[A]:HDD:HBB1	2:B:760[A]:HDD:HMB1	1.57	0.87
1:D:274:CYS:SG	2:D:760[A]:HDD:CMB	2.62	0.87
3:C:761[B]:HDE:CBC	3:C:761[B]:HDE:CMC	2.44	0.86
3:B:761[B]:HDE:CBC	3:B:761[B]:HDE:CMC	2.33	0.84
1:A:274:CYS:SG	2:A:760[A]:HDD:HMB1	2.17	0.84
1:B:274:CYS:HB2	4:B:754:H2S:S	2.17	0.84
2:C:760[A]:HDD:HMB1	2:C:760[A]:HDD:HBB1	1.57	0.83
1:A:29:LEU:HD23	5:C:3144:HOH:O	1.80	0.82
1:A:29:LEU:HD22	5:C:2405:HOH:O	1.80	0.81
3:B:761[B]:HDE:HMB	3:B:761[B]:HDE:HBBB	1.61	0.81
1:A:201:ASN:ND2	2:A:760[A]:HDD:HMB2	1.96	0.81
1:C:201:ASN:ND2	2:C:760[A]:HDD:HMB2	1.96	0.81
3:D:761[B]:HDE:HBCB	3:D:761[B]:HDE:CMC	2.11	0.80
1:B:201:ASN:ND2	2:B:760[A]:HDD:HMB2	1.97	0.80
1:C:274:CYS:SG	2:C:760[A]:HDD:CMB	2.70	0.80
1:C:440:TYR:HD1	5:C:3454:HOH:O	1.65	0.80
1:B:533[A]:LYS:HE2	5:B:3100:HOH:O	1.81	0.80
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.65	0.79
2:C:760[A]:HDD:HMB1	2:C:760[A]:HDD:CBB	2.12	0.78
1:D:731:GLU:OE2	5:D:3028:HOH:O	2.02	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:761[B]:HDE:HMB	3:B:761[B]:HDE:CBB	2.16	0.76
1:C:274:CYS:HB3	2:C:760[A]:HDD:CBB	2.16	0.76
1:A:610:GLU:HG2	5:A:3555:HOH:O	1.86	0.75
1:D:274:CYS:SG	2:D:760[A]:HDD:HMB1	2.27	0.75
3:D:761[B]:HDE:HMB	3:D:761[B]:HDE:CBB	2.17	0.74
1:A:748:ILE:O	1:A:751:ILE:HD12	1.90	0.72
1:D:748:ILE:O	1:D:751:ILE:HG22	1.90	0.72
1:A:451:MET:SD	5:A:3609:HOH:O	2.47	0.72
1:C:725:ASP:O	5:C:2403:HOH:O	2.08	0.72
1:B:440:TYR:O	1:D:73[B]:LYS:HE3	1.90	0.72
1:B:578:ASP:HB2	5:B:2590:HOH:O	1.90	0.71
2:C:760[A]:HDD:HBB1	2:C:760[A]:HDD:CMB	2.22	0.70
3:D:761[B]:HDE:HMC	4:D:754:H2S:S	2.31	0.70
1:D:201:ASN:ND2	2:D:760[A]:HDD:HMB2	2.07	0.69
1:D:629:HIS:HD2	5:D:1554:HOH:O	1.75	0.69
1:C:59:ASP:OD2	5:C:2529:HOH:O	2.11	0.69
1:A:532:SER:OG	5:A:2410:HOH:O	2.09	0.68
1:C:578:ASP:HB2	1:C:582:LEU:O	1.96	0.66
3:D:761[B]:HDE:HMB	3:D:761[B]:HDE:HBBA	1.78	0.66
1:A:751:ILE:O	1:A:751:ILE:CD1	2.45	0.65
2:B:760[A]:HDD:CBB	2:B:760[A]:HDD:HMB1	2.25	0.65
1:B:700:ASP:HB2	5:B:3595:HOH:O	1.97	0.65
1:C:274:CYS:SG	2:C:760[A]:HDD:HBB1	2.35	0.65
1:B:748:ILE:O	1:B:751:ILE:HG22	1.97	0.65
3:A:761[B]:HDE:HMB	3:A:761[B]:HDE:HBBB	1.77	0.65
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.80	0.64
1:B:115:THR:HG21	5:B:3420:HOH:O	1.97	0.64
1:D:28:SER:HA	5:D:2467:HOH:O	1.98	0.64
3:C:761[B]:HDE:HMB	3:C:761[B]:HDE:CBB	2.28	0.63
3:B:761[B]:HDE:HMC	3:B:761[B]:HDE:HBCB	1.74	0.63
1:D:274:CYS:HB2	4:D:754:H2S:S	2.35	0.63
1:C:59:ASP:OD2	5:C:3406:HOH:O	2.15	0.63
2:B:760[A]:HDD:HBC1	2:B:760[A]:HDD:HMC1	1.80	0.62
3:B:761[B]:HDE:CMC	3:B:761[B]:HDE:HBCB	2.28	0.62
1:A:705:LYS:HE2	5:A:3467:HOH:O	1.99	0.62
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.82	0.62
2:B:760[A]:HDD:HBB1	2:B:760[A]:HDD:CMB	2.29	0.62
1:B:274:CYS:SG	2:B:760[A]:HDD:HBB1	2.39	0.61
3:C:761[B]:HDE:HMC	4:C:754:H2S:S	2.41	0.61
3:B:761[B]:HDE:HMC	4:B:754:H2S:S	2.39	0.61
1:A:73:LYS:HE3	1:C:440:TYR:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:CYS:SG	2:B:760[A]:HDD:CMB	2.89	0.61
1:A:610:GLU:OE1	5:A:2394:HOH:O	2.16	0.61
1:B:629:HIS:HD2	5:B:1056:HOH:O	1.84	0.60
1:D:556:GLN:NE2	5:D:2773:HOH:O	2.33	0.60
1:A:61:ARG:HG2	1:A:61:ARG:HH11	1.66	0.60
1:C:629:HIS:HD2	5:C:1129:HOH:O	1.83	0.60
1:C:449[A]:HIS:HD2	5:C:3611:HOH:O	1.85	0.60
1:D:449[A]:HIS:HD2	5:D:3615:HOH:O	1.85	0.59
1:A:752:PRO:HG3	5:A:2478:HOH:O	2.01	0.59
1:C:274:CYS:CB	2:C:760[A]:HDD:HBB1	2.33	0.59
1:C:359:LEU:H	1:C:507:HIS:HD2	1.50	0.59
1:B:449[B]:HIS:HE1	5:D:1789:HOH:O	1.85	0.59
3:C:761[B]:HDE:CMC	3:C:761[B]:HDE:HBCA	2.31	0.59
1:D:267:ARG:HG3	5:D:1920:HOH:O	2.01	0.59
1:C:751:ILE:HB	5:C:2367:HOH:O	2.04	0.58
1:A:29:LEU:HB2	5:C:2405:HOH:O	2.03	0.58
1:B:274:CYS:SG	2:B:760[A]:HDD:HMB3	2.43	0.58
3:D:761[B]:HDE:HMB	3:D:761[B]:HDE:HBBB	1.84	0.58
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.87	0.58
1:A:610:GLU:CG	5:A:3555:HOH:O	2.49	0.58
1:B:583:LYS:NZ	1:B:583:LYS:H	2.03	0.57
1:B:73:LYS:CD	5:D:3517:HOH:O	2.49	0.57
1:A:61:ARG:HD2	5:A:3208:HOH:O	2.04	0.57
1:A:416[B]:THR:HG22	5:A:908:HOH:O	2.04	0.57
1:C:583:LYS:HG2	5:C:2919:HOH:O	2.03	0.57
1:A:443:PHE:CZ	1:A:470:PRO:HD2	2.40	0.57
1:B:201:ASN:ND2	2:B:760[A]:HDD:CMB	2.67	0.57
2:C:760[A]:HDD:HMD1	2:C:760[A]:HDD:HBD2	1.87	0.57
1:A:244:SER:HA	1:A:546[B]:GLN:NE2	2.21	0.56
1:B:369:ARG:HG2	5:B:1639:HOH:O	2.04	0.55
1:A:541:GLU:OE2	5:A:2550:HOH:O	2.17	0.55
1:A:751:ILE:HD13	1:A:751:ILE:C	2.27	0.55
1:B:32:GLU:HB2	5:B:2850:HOH:O	2.07	0.55
1:B:607:LEU:HD11	1:B:632:LEU:HB3	1.89	0.54
1:A:36:HIS:CD2	1:A:36:HIS:H	2.26	0.54
1:B:533[A]:LYS:CE	5:B:3100:HOH:O	2.47	0.54
1:B:37:ARG:HD3	5:B:2886:HOH:O	2.08	0.54
1:C:521:ARG:NH1	1:C:521:ARG:HG2	2.23	0.54
1:C:567:THR:O	1:C:571:LEU:HD22	2.08	0.53
1:B:393:PRO:HD2	1:B:415:TYR:CG	2.44	0.53
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:760[A]:HDD:CAB	4:A:754:H2S:S	2.97	0.53
3:A:761[B]:HDE:HMB	3:A:761[B]:HDE:CBB	2.37	0.53
1:B:274:CYS:SG	2:B:760[A]:HDD:HMB1	2.49	0.53
3:D:761[B]:HDE:HBCB	4:D:754:H2S:S	2.49	0.53
1:B:552:LEU:HD21	1:B:571:LEU:CD1	2.36	0.53
1:D:260:ARG:HD3	1:D:590:LEU:HD21	1.89	0.53
3:C:761[B]:HDE:HMB	3:C:761[B]:HDE:HBBB	1.90	0.53
2:B:760[A]:HDD:HBC1	2:B:760[A]:HDD:CMC	2.39	0.53
1:A:273:GLY:C	1:A:274:CYS:SG	2.87	0.53
1:A:639:GLU:HG3	5:A:2414:HOH:O	2.09	0.52
1:C:634:TYR:O	1:C:653:THR:HA	2.10	0.52
1:C:274:CYS:SG	2:C:760[A]:HDD:HMB1	2.44	0.52
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.13	0.52
1:C:636:ARG:HD3	5:C:2717:HOH:O	2.10	0.52
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.25	0.52
1:A:725:ASP:H	1:A:728:PHE:HB3	1.74	0.52
1:B:157:ASN:C	1:B:157:ASN:HD22	2.13	0.51
1:B:440:TYR:CE1	1:D:73[B]:LYS:HE2	2.45	0.51
3:C:761[B]:HDE:HMB	3:C:761[B]:HDE:HBBA	1.92	0.51
1:A:125:ARG:HB3	3:A:761[B]:HDE:HBA	1.93	0.51
1:C:612:ARG:HH11	1:C:669:ALA:HB3	1.76	0.51
1:C:359:LEU:H	1:C:507:HIS:CD2	2.29	0.51
1:B:229:ILE:HG23	1:B:230:PRO:HA	1.93	0.50
1:B:745:ILE:O	1:B:748:ILE:HG12	2.12	0.50
2:D:760[A]:HDD:CAB	4:D:754:H2S:S	2.95	0.50
1:A:690:LYS:HG3	1:A:751:ILE:HD11	1.92	0.50
5:A:1016:HOH:O	1:C:104:LEU:HB3	2.11	0.50
1:B:634:TYR:O	1:B:653:THR:HA	2.11	0.50
1:A:61:ARG:HG2	1:A:61:ARG:NH1	2.25	0.50
1:A:201:ASN:ND2	2:A:760[A]:HDD:CMB	2.74	0.49
1:C:583:LYS:O	1:C:584:LYS:HB3	2.12	0.49
1:D:313:ARG:HG3	1:D:660:LEU:HD12	1.94	0.49
1:B:273:GLY:C	1:B:274:CYS:SG	2.90	0.49
1:B:411:ARG:HG2	3:B:761[B]:HDE:C3B	2.42	0.49
1:D:393:PRO:HD2	1:D:415:TYR:CG	2.47	0.49
1:A:700:ASP:HB2	5:A:3594:HOH:O	2.11	0.49
1:B:73:LYS:CE	5:D:3517:HOH:O	2.25	0.49
3:B:761[B]:HDE:CMC	4:B:754:H2S:S	3.01	0.49
1:B:449[B]:HIS:HD2	5:B:3613:HOH:O	1.94	0.49
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.28	0.48
2:B:760[A]:HDD:HMC1	2:B:760[A]:HDD:CBC	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:2368:HOH:O	1:D:416[B]:THR:HG21	2.13	0.48
3:A:761[B]:HDE:HMC	3:A:761[B]:HDE:CBC	2.35	0.48
1:A:451:MET:HE2	1:C:451:MET:HE1	1.94	0.48
1:A:700:ASP:HB2	5:A:2575:HOH:O	2.13	0.48
1:B:724:ALA:O	1:B:725:ASP:O	2.31	0.48
1:D:440:TYR:CZ	5:D:3517:HOH:O	2.55	0.48
1:A:36:HIS:HE1	5:A:1872:HOH:O	1.97	0.48
1:B:115:THR:CG2	5:B:3420:HOH:O	2.56	0.48
3:D:761[B]:HDE:CMC	3:D:761[B]:HDE:CBC	2.85	0.48
1:B:359:LEU:H	1:B:507:HIS:HD2	1.60	0.48
1:B:157:ASN:HD22	1:B:158:LYS:N	2.12	0.48
1:D:37:ARG:HD2	5:D:2157:HOH:O	2.14	0.47
1:B:602:VAL:HG22	1:B:629:HIS:HB2	1.96	0.47
1:C:38:PRO:HG2	1:C:51:ALA:HB2	1.97	0.47
1:A:451:MET:HE1	1:C:451:MET:HE2	1.95	0.47
1:D:411:ARG:HG2	3:D:761[B]:HDE:C3B	2.45	0.47
3:B:761[B]:HDE:HMAA	3:B:761[B]:HDE:HAAA	1.75	0.47
1:D:490:GLU:OE1	5:D:2308:HOH:O	2.20	0.47
1:B:319:ARG:HD3	1:C:227:TRP:O	2.14	0.47
1:B:697:LEU:O	1:B:720:GLU:HA	2.15	0.47
1:B:583:LYS:H	1:B:583:LYS:HZ2	1.61	0.46
1:C:748:ILE:O	1:C:751:ILE:CG2	2.55	0.46
1:B:207:PHE:O	1:B:249:THR:HA	2.15	0.46
1:B:211:ALA:CB	1:B:410:GLY:HA3	2.46	0.46
3:C:761[B]:HDE:HMAA	3:C:761[B]:HDE:HAAA	1.76	0.46
3:D:761[B]:HDE:HMC	3:D:761[B]:HDE:CBC	2.22	0.46
1:B:274:CYS:CB	2:B:760[A]:HDD:HBB1	2.45	0.46
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.31	0.46
3:D:761[B]:HDE:HMAA	3:D:761[B]:HDE:HAAA	1.70	0.46
1:D:696:ALA:HB1	1:D:728:PHE:CZ	2.51	0.46
1:C:696:ALA:HB1	1:C:728:PHE:CZ	2.51	0.45
1:A:393:PRO:HD2	1:A:415:TYR:CG	2.51	0.45
1:A:451:MET:CE	1:C:451:MET:CE	2.94	0.45
1:D:709:LYS:HD3	5:D:3333:HOH:O	2.16	0.45
1:A:751:ILE:CD1	1:A:751:ILE:C	2.85	0.45
1:B:596:GLY:HA3	1:B:737:ALA:O	2.17	0.45
1:A:274:CYS:CA	4:A:754:H2S:S	3.00	0.45
1:B:509:ARG:HD2	1:B:576:PRO:HD2	1.99	0.45
1:C:201:ASN:ND2	2:C:760[A]:HDD:CMB	2.76	0.45
1:B:274:CYS:CB	2:B:760[A]:HDD:CBB	2.95	0.45
5:A:943:HOH:O	1:C:52:PRO:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:PHE:CE2	1:A:470:PRO:HD2	2.52	0.44
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.99	0.44
1:C:184:GLY:HA3	2:C:760[A]:HDD:HMA2	2.00	0.44
1:C:689:TYR:CE1	1:C:744:ARG:HD3	2.53	0.44
1:C:488:ARG:NH1	5:C:2379:HOH:O	2.40	0.44
1:D:449[A]:HIS:HE1	5:D:1789:HOH:O	2.01	0.44
1:B:157:ASN:C	1:B:157:ASN:ND2	2.71	0.44
1:C:273:GLY:C	1:C:274:CYS:SG	2.96	0.44
1:A:205:ILE:HD13	1:A:205:ILE:H	1.82	0.43
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.49	0.43
3:C:761[B]:HDE:HMC	3:C:761[B]:HDE:HBCA	1.82	0.43
1:D:207:PHE:O	1:D:249:THR:HA	2.17	0.43
1:A:155:ASP:CG	5:A:3378:HOH:O	2.56	0.43
1:B:73:LYS:NZ	5:B:1110:HOH:O	2.51	0.43
1:C:368:GLN:NE2	5:C:1787:HOH:O	2.33	0.43
1:C:612:ARG:HH11	1:C:669:ALA:CB	2.31	0.43
1:B:274:CYS:HB3	2:B:760[A]:HDD:CBB	2.46	0.43
1:B:313:ARG:HG3	1:B:660:LEU:HD12	2.00	0.43
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.49	0.43
1:D:48:GLN:HE21	1:D:48:GLN:HB3	1.69	0.43
1:D:448:MET:O	1:D:449[A]:HIS:HB2	2.19	0.43
1:A:459:ASN:HD22	1:A:459:ASN:C	2.21	0.42
3:B:761[B]:HDE:CBC	4:B:754:H2S:S	3.07	0.42
1:A:128:HIS:CE1	1:A:169:VAL:HG22	2.55	0.42
5:A:1788:HOH:O	1:C:449[A]:HIS:HE1	2.00	0.42
1:C:214:PHE:CD2	2:C:760[A]:HDD:HMC2	2.54	0.42
1:D:244:SER:HA	1:D:546[B]:GLN:NE2	2.34	0.42
1:D:634:TYR:O	1:D:653:THR:HA	2.19	0.42
1:B:214:PHE:CD2	2:B:760[A]:HDD:HMC2	2.55	0.42
1:B:429:HIS:CG	1:D:83:ASN:HB3	2.53	0.42
1:A:165:ARG:HD3	3:A:761[B]:HDE:O2D	2.19	0.42
1:B:461:GLU:OE1	1:D:91:ASP:OD1	2.37	0.42
1:B:725:ASP:C	1:B:725:ASP:OD2	2.57	0.42
1:C:37:ARG:HD3	5:C:2621:HOH:O	2.19	0.42
1:C:488:ARG:HD2	5:C:2379:HOH:O	2.20	0.42
1:D:359:LEU:H	1:D:507:HIS:HD2	1.67	0.42
1:A:448:MET:HG3	1:A:449[B]:HIS:CD2	2.55	0.42
1:B:165:ARG:HD3	3:B:761[B]:HDE:O2D	2.20	0.42
1:D:596:GLY:HA3	1:D:737:ALA:O	2.20	0.42
1:C:602[B]:VAL:HG13	1:C:662:VAL:HA	2.01	0.41
1:A:478:LYS:HG2	5:A:3259:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:PRO:HD2	1:B:415:TYR:CD2	2.55	0.41
1:D:278:ARG:HH12	1:D:487:GLU:CD	2.24	0.41
1:A:144:LEU:HD11	1:A:370:VAL:HG13	2.02	0.41
1:B:91:ASP:OD1	1:D:461:GLU:OE1	2.39	0.41
1:D:51:ALA:HB1	1:D:52:PRO:HD2	2.01	0.41
1:A:52:PRO:HG2	1:A:55:LEU:HD12	2.01	0.41
1:A:207:PHE:O	1:A:249:THR:HA	2.20	0.41
1:D:252:ASN:HD22	1:D:252:ASN:HA	1.69	0.41
1:B:206:PHE:CG	1:B:207:PHE:N	2.89	0.41
1:B:128:HIS:HA	1:B:168:THR:O	2.21	0.41
1:B:461:GLU:HA	1:B:462:PRO:C	2.41	0.41
1:B:708:ILE:HG13	1:B:710:ILE:HG12	2.02	0.41
1:A:38:PRO:HG2	1:A:51:ALA:HB2	2.02	0.41
1:A:201:ASN:CG	3:A:761[B]:HDE:HAC	2.40	0.41
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.51	0.41
1:A:227:TRP:O	1:D:319:ARG:HD3	2.20	0.41
1:A:392:HIS:CD2	1:A:394:GLY:H	2.39	0.41
1:C:128:HIS:HA	1:C:168:THR:O	2.20	0.41
1:C:393:PRO:HD2	1:C:415:TYR:CG	2.55	0.41
1:D:128:HIS:HA	1:D:168:THR:O	2.21	0.41
1:C:199:VAL:HG12	3:C:761[B]:HDE:HHDA	2.03	0.41
1:A:448:MET:O	1:A:449[B]:HIS:HB2	2.21	0.40
1:B:214:PHE:CD2	2:B:760[A]:HDD:CMC	3.04	0.40
1:B:696:ALA:HB1	1:B:728:PHE:CZ	2.56	0.40
1:C:704:PHE:O	1:C:707:THR:HG22	2.22	0.40
1:D:509:ARG:HD2	1:D:576:PRO:HD2	2.03	0.40
1:A:260:ARG:HD3	1:A:590:LEU:HD21	2.03	0.40
1:B:38:PRO:HG2	1:B:51:ALA:HB2	2.04	0.40
1:D:296:LEU:HD12	1:D:333:GLU:HB3	2.04	0.40
1:B:44:PRO:HB3	1:B:629:HIS:CD2	2.57	0.40
1:B:448:MET:O	1:B:449[B]:HIS:HB2	2.22	0.40
1:B:449[A]:HIS:CE1	1:D:431:ILE:HG13	2.55	0.40
1:B:449[B]:HIS:CE1	5:D:1789:HOH:O	2.67	0.40

All (2) 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)
5:A:3348:HOH:O	5:B:2822:HOH:O[2_545]	2.13	0.07
1:C:584:LYS:NZ	5:A:1624:HOH:O[1_554]	2.19	0.01

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%)	708 (97%)	19 (3%)	2 (0%)	41	27
1	C	726/753 (96%)	700 (96%)	25 (3%)	1 (0%)	51	36
1	D	733/753 (97%)	710 (97%)	22 (3%)	1 (0%)	51	36
All	All	2917/3012 (97%)	2825 (97%)	87 (3%)	5 (0%)	47	33

All (5) 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

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%)	595 (97%)	19 (3%)	40	25
1	B	614/634 (97%)	590 (96%)	24 (4%)	32	17
1	C	611/634 (96%)	585 (96%)	26 (4%)	29	14
1	D	618/634 (98%)	590 (96%)	28 (4%)	27	13
All	All	2457/2536 (97%)	2360 (96%)	97 (4%)	32	17

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	29	LEU
1	A	32	GLU
1	A	42	PRO
1	A	185	PHE
1	A	205	ILE
1	A	227	TRP
1	A	252	ASN
1	A	274	CYS
1	A	369	ARG
1	A	377	ARG
1	A	398	PRO
1	A	432	PRO
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
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	252	ASN
1	B	274	CYS
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	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	616	LEU
1	B	633	LEU
1	B	703	LYS
1	B	713	GLN
1	B	725	ASP
1	B	732	LEU
1	B	750	LYS

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Mol	Chain	Res	Type
1	B	751	ILE
1	C	32	GLU
1	C	61	ARG
1	C	159	ILE
1	C	185	PHE
1	C	205	ILE
1	C	227	TRP
1	C	237	ASP
1	C	252	ASN
1	C	285	LYS
1	C	377	ARG
1	C	440	TYR
1	C	459	ASN
1	C	521	ARG
1	C	552	LEU
1	C	571	LEU
1	C	606	LEU
1	C	616	LEU
1	C	617	LEU
1	C	626	LYS
1	C	633	LEU
1	C	636	ARG
1	C	648	LEU
1	C	725	ASP
1	C	733	LEU
1	C	750	LYS
1	C	751	ILE
1	D	32	GLU
1	D	38	PRO
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
1	D	227	TRP
1	D	237	ASP
1	D	252	ASN
1	D	274	CYS
1	D	369	ARG
1	D	416[A]	THR
1	D	416[B]	THR

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Mol	Chain	Res	Type
1	D	432	PRO
1	D	440	TYR
1	D	459	ASN
1	D	490	GLU
1	D	552	LEU
1	D	574	THR
1	D	582	LEU
1	D	616	LEU
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 (24) 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	459	ASN
1	B	507	HIS
1	B	629	HIS
1	B	713	GLN
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	157	ASN
1	D	252	ASN
1	D	459	ASN
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	2.17	13 (31%)	31,89,89	2.34	17 (54%)
3	HDE	B	761[B]	5,1	44,52,52	2.77	15 (34%)	41,89,89	2.74	20 (48%)
3	HDE	A	761[B]	5,1	44,52,52	2.60	15 (34%)	41,89,89	2.71	19 (46%)
2	HDD	B	760[A]	5,1	41,52,52	1.98	12 (29%)	31,89,89	2.23	9 (29%)
3	HDE	D	761[B]	5,1	44,52,52	2.53	14 (31%)	41,89,89	2.74	22 (53%)
2	HDD	A	760[A]	5,1	41,52,52	2.23	12 (29%)	31,89,89	2.65	8 (25%)
3	HDE	C	761[B]	5,1	44,52,52	2.48	14 (31%)	41,89,89	2.96	21 (51%)
2	HDD	D	760[A]	5,1	41,52,52	2.33	10 (24%)	31,89,89	2.19	10 (32%)

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
3	HDE	B	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	B	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
2	HDD	A	760[A]	5,1	-	2/5/89/89	0/1/9/9
3	HDE	C	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

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	761[B]	HDE	C4C-C3C	8.38	1.49	1.38
3	A	761[B]	HDE	C4C-C3C	7.52	1.48	1.38
3	C	761[B]	HDE	C4C-C3C	7.08	1.47	1.38
2	D	760[A]	HDD	FE-ND	7.02	2.23	1.95
3	B	761[B]	HDE	CHC-C4B	-6.97	1.44	1.51
2	C	760[A]	HDD	FE-ND	6.66	2.21	1.95
3	D	761[B]	HDE	CHC-C4B	-6.51	1.44	1.51
3	A	761[B]	HDE	CHC-C4B	-6.32	1.44	1.51
3	D	761[B]	HDE	C4C-C3C	6.29	1.46	1.38
2	A	760[A]	HDD	O1D-C3D	-6.19	1.36	1.46
3	A	761[B]	HDE	CHC-C1C	-6.09	1.44	1.51
3	C	761[B]	HDE	CHD-C4C	-5.79	1.45	1.51
3	D	761[B]	HDE	CHD-C1D	-5.71	1.45	1.51
3	B	761[B]	HDE	O1A-CGA	5.51	1.44	1.35
3	B	761[B]	HDE	CHD-C1D	-5.50	1.45	1.51
3	C	761[B]	HDE	CHC-C4B	-5.49	1.45	1.51
2	A	760[A]	HDD	FE-ND	5.47	2.17	1.95
3	A	761[B]	HDE	O1A-CGA	5.41	1.44	1.35
2	D	760[A]	HDD	O1D-C3D	-5.40	1.38	1.46
2	A	760[A]	HDD	C3B-C2B	-5.31	1.33	1.40
3	D	761[B]	HDE	CHD-C4C	-5.29	1.45	1.51
3	C	761[B]	HDE	O1A-CGA	5.14	1.44	1.35
3	D	761[B]	HDE	CHC-C1C	-5.05	1.46	1.51
2	C	760[A]	HDD	C3B-C2B	-5.00	1.33	1.40
2	D	760[A]	HDD	C3B-C2B	-4.91	1.33	1.40
2	A	760[A]	HDD	C3C-C2C	-4.88	1.33	1.40
2	B	760[A]	HDD	C3C-C2C	-4.72	1.33	1.40
3	D	761[B]	HDE	O1A-CGA	4.31	1.42	1.35
3	B	761[B]	HDE	C4A-NA	4.19	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	761[B]	HDE	C1A-NA	4.08	1.44	1.37
3	B	761[B]	HDE	CHD-C4C	-4.08	1.46	1.51
3	C	761[B]	HDE	CHD-C1D	-4.07	1.46	1.51
2	C	760[A]	HDD	O1D-C3D	-4.04	1.40	1.46
3	C	761[B]	HDE	C3B-C2B	4.00	1.49	1.37
3	D	761[B]	HDE	C3B-C2B	3.96	1.49	1.37
3	C	761[B]	HDE	CHC-C1C	-3.92	1.47	1.51
2	D	760[A]	HDD	CHD-C1D	3.88	1.42	1.36
2	D	760[A]	HDD	C3B-CAB	3.87	1.55	1.47
2	D	760[A]	HDD	C3C-C2C	-3.86	1.35	1.40
3	B	761[B]	HDE	C1A-NA	3.83	1.44	1.37
3	B	761[B]	HDE	C1C-C2C	3.82	1.43	1.38
3	A	761[B]	HDE	C3B-C2B	3.80	1.48	1.37
3	A	761[B]	HDE	C3C-C2C	3.79	1.48	1.37
3	C	761[B]	HDE	C3D-C2D	3.73	1.48	1.37
2	D	760[A]	HDD	C3C-CAC	3.72	1.55	1.47
3	B	761[B]	HDE	C3C-C2C	3.68	1.48	1.37
3	A	761[B]	HDE	C3D-C2D	3.66	1.48	1.37
3	B	761[B]	HDE	C3B-C2B	3.65	1.48	1.37
2	B	760[A]	HDD	C3B-C2B	-3.65	1.35	1.40
2	B	760[A]	HDD	O1D-C3D	-3.63	1.40	1.46
2	C	760[A]	HDD	C3C-C2C	-3.60	1.35	1.40
2	C	760[A]	HDD	CHD-C1D	3.52	1.41	1.36
3	D	761[B]	HDE	C1A-NA	3.49	1.43	1.37
3	C	761[B]	HDE	C1A-NA	3.44	1.43	1.37
3	A	761[B]	HDE	CHD-C1D	-3.44	1.47	1.51
3	A	761[B]	HDE	CHD-C4C	-3.39	1.47	1.51
3	B	761[B]	HDE	CHC-C1C	-3.33	1.47	1.51
2	C	760[A]	HDD	CHA-C4D	3.32	1.41	1.36
2	B	760[A]	HDD	C1D-ND	3.30	1.43	1.37
2	B	760[A]	HDD	C3C-CAC	3.28	1.54	1.47
3	D	761[B]	HDE	C3C-C2C	3.27	1.47	1.37
2	B	760[A]	HDD	CMD-C2D	3.25	1.57	1.53
3	C	761[B]	HDE	C3C-C2C	3.21	1.47	1.37
2	C	760[A]	HDD	C3B-CAB	3.19	1.54	1.47
2	B	760[A]	HDD	C3B-CAB	3.19	1.54	1.47
3	D	761[B]	HDE	C3D-C2D	2.92	1.46	1.37
3	A	761[B]	HDE	C4A-NA	2.90	1.42	1.37
3	D	761[B]	HDE	C4D-CHA	2.89	1.49	1.41
3	C	761[B]	HDE	C1C-C2C	2.87	1.42	1.38
3	D	761[B]	HDE	C4A-NA	2.85	1.42	1.37
2	A	760[A]	HDD	C3C-CAC	2.84	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	761[B]	HDE	C1B-NB	2.83	1.42	1.36
2	D	760[A]	HDD	CMD-C2D	2.83	1.57	1.53
2	C	760[A]	HDD	CMD-C2D	2.79	1.57	1.53
3	B	761[B]	HDE	C3D-C2D	2.79	1.45	1.37
2	B	760[A]	HDD	FE-ND	2.77	2.06	1.95
2	A	760[A]	HDD	C4A-NA	2.72	1.41	1.36
3	A	761[B]	HDE	C1C-C2C	2.71	1.41	1.38
3	A	761[B]	HDE	C1B-CHB	2.69	1.48	1.41
3	B	761[B]	HDE	C4D-CHA	2.68	1.48	1.41
2	A	760[A]	HDD	C3B-CAB	2.68	1.53	1.47
2	A	760[A]	HDD	CAA-C2A	2.67	1.56	1.52
3	A	761[B]	HDE	C1B-NB	2.64	1.41	1.36
2	A	760[A]	HDD	OND-C2D	2.62	1.47	1.42
2	C	760[A]	HDD	CMC-C2C	2.58	1.57	1.51
3	C	761[B]	HDE	C4D-CHA	2.57	1.48	1.41
3	C	761[B]	HDE	C4A-NA	2.51	1.42	1.37
2	B	760[A]	HDD	C1A-NA	2.48	1.41	1.36
2	A	760[A]	HDD	CHD-C1D	2.43	1.39	1.36
3	B	761[B]	HDE	CHB-C4A	-2.40	1.32	1.36
2	D	760[A]	HDD	CMB-C2B	2.39	1.57	1.51
3	A	761[B]	HDE	C4D-CHA	2.38	1.47	1.41
2	C	760[A]	HDD	C3C-CAC	2.37	1.52	1.47
2	D	760[A]	HDD	C1A-NA	2.35	1.41	1.36
3	D	761[B]	HDE	C1B-NB	2.35	1.41	1.36
2	A	760[A]	HDD	CMC-C2C	2.31	1.56	1.51
2	B	760[A]	HDD	CMA-C3A	2.30	1.56	1.51
2	A	760[A]	HDD	C1A-NA	2.21	1.40	1.36
2	B	760[A]	HDD	OND-C2D	2.17	1.47	1.42
3	C	761[B]	HDE	C1B-NB	2.15	1.40	1.36
3	D	761[B]	HDE	O1A-C2A	-2.14	1.43	1.46
2	C	760[A]	HDD	C1C-NC	2.10	1.40	1.36
2	C	760[A]	HDD	C1A-NA	2.08	1.40	1.36
2	C	760[A]	HDD	C4D-ND	2.02	1.41	1.37
2	B	760[A]	HDD	CMC-C2C	2.01	1.55	1.51

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	760[A]	HDD	O1D-CGD-CBD	-8.27	101.85	110.19
2	B	760[A]	HDD	O1D-CGD-O2D	6.83	126.89	120.80
3	C	761[B]	HDE	CBC-CAC-C3C	-6.29	96.24	112.27
3	C	761[B]	HDE	CHD-C1D-C2D	-6.19	119.17	129.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	761[B]	HDE	CBC-CAC-C3C	-6.19	96.51	112.27
3	A	761[B]	HDE	CHD-C4C-C3C	-5.92	122.54	129.68
3	A	761[B]	HDE	CHD-C1D-C2D	-5.78	119.86	129.53
3	D	761[B]	HDE	CHD-C1D-C2D	-5.71	119.99	129.53
2	A	760[A]	HDD	CAD-CBD-CGD	-5.67	95.79	104.56
3	D	761[B]	HDE	CHC-C4B-C3B	-5.52	123.02	129.68
3	A	761[B]	HDE	CHC-C4B-C3B	-5.51	123.03	129.68
3	B	761[B]	HDE	C1C-C2C-C3C	-5.38	100.08	105.81
2	D	760[A]	HDD	C2B-C3B-C4B	5.30	110.60	106.90
3	B	761[B]	HDE	CHC-C4B-C3B	-5.24	123.36	129.68
2	A	760[A]	HDD	C4A-C3A-C2A	5.22	110.63	107.00
2	D	760[A]	HDD	O1D-CGD-CBD	-5.09	105.06	110.19
3	C	761[B]	HDE	CHC-C4B-C3B	-5.07	123.57	129.68
3	C	761[B]	HDE	C1B-CHB-C4A	-5.06	120.09	130.12
3	B	761[B]	HDE	CHD-C1D-C2D	-5.01	121.15	129.53
3	C	761[B]	HDE	CHD-C4C-C3C	-4.97	123.68	129.68
3	B	761[B]	HDE	C4C-CHD-C1D	4.87	124.74	112.87
3	B	761[B]	HDE	CAD-CBD-CGD	-4.84	100.19	113.76
3	A	761[B]	HDE	CAD-CBD-CGD	-4.66	100.69	113.76
3	A	761[B]	HDE	O1A-CGA-O2A	4.63	124.93	120.80
3	D	761[B]	HDE	CHD-C4C-C3C	-4.61	124.11	129.68
2	B	760[A]	HDD	O1D-CGD-CBD	-4.51	105.64	110.19
2	A	760[A]	HDD	C2B-C3B-C4B	4.49	110.03	106.90
2	B	760[A]	HDD	CMC-C2C-C1C	-4.49	121.57	128.46
2	C	760[A]	HDD	O1D-CGD-O2D	4.47	124.79	120.80
3	C	761[B]	HDE	CMB-C2B-C3B	4.41	133.26	124.94
3	D	761[B]	HDE	C1B-CHB-C4A	-4.40	121.41	130.12
3	D	761[B]	HDE	CAD-CBD-CGD	-4.36	101.52	113.76
3	C	761[B]	HDE	CHC-C1C-C2C	-4.33	122.28	129.53
2	A	760[A]	HDD	CMA-C3A-C4A	-4.20	122.01	128.46
3	D	761[B]	HDE	C1B-C2B-C3B	-4.13	104.12	107.00
3	B	761[B]	HDE	C1B-CHB-C4A	-4.08	122.04	130.12
3	D	761[B]	HDE	CBC-CAC-C3C	-4.05	101.94	112.27
2	D	760[A]	HDD	O1D-CGD-O2D	4.04	124.40	120.80
2	D	760[A]	HDD	CAA-CBA-CGA	-4.04	102.45	113.76
2	C	760[A]	HDD	C2B-C3B-C4B	4.02	109.71	106.90
3	C	761[B]	HDE	CMB-C2B-C1B	-4.01	122.31	128.46
3	A	761[B]	HDE	C1C-C2C-C3C	-3.97	101.58	105.81
2	C	760[A]	HDD	OND-C2D-CMD	-3.95	102.32	109.59
3	A	761[B]	HDE	C4B-CHC-C1C	3.87	122.32	112.87
3	D	761[B]	HDE	CHC-C1C-C2C	-3.78	123.20	129.53
3	C	761[B]	HDE	C1B-C2B-C3B	-3.76	104.38	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	760[A]	HDD	O1D-CGD-CBD	-3.75	106.41	110.19
3	C	761[B]	HDE	C1C-C2C-C3C	-3.73	101.84	105.81
3	C	761[B]	HDE	CMD-C2D-C3D	3.73	131.97	124.94
3	B	761[B]	HDE	CHC-C1C-C2C	-3.67	123.39	129.53
2	B	760[A]	HDD	CAA-CBA-CGA	-3.67	103.48	113.76
3	B	761[B]	HDE	C1B-C2B-C3B	-3.63	104.47	107.00
3	C	761[B]	HDE	C4C-CHD-C1D	3.61	121.67	112.87
3	D	761[B]	HDE	C4C-CHD-C1D	3.61	121.67	112.87
3	A	761[B]	HDE	CHC-C1C-C2C	-3.60	123.51	129.53
3	A	761[B]	HDE	CAC-C3C-C4C	-3.58	122.88	127.19
3	D	761[B]	HDE	C1C-C2C-C3C	-3.40	102.19	105.81
3	A	761[B]	HDE	C1B-CHB-C4A	-3.40	123.38	130.12
2	C	760[A]	HDD	CMC-C2C-C1C	-3.40	123.24	128.46
3	C	761[B]	HDE	CAD-CBD-CGD	-3.33	104.42	113.76
3	D	761[B]	HDE	C4D-CHA-C1A	-3.28	123.63	130.12
3	C	761[B]	HDE	C4B-CHC-C1C	3.19	120.65	112.87
3	A	761[B]	HDE	CAB-C3B-C4B	-3.19	123.35	127.19
2	B	760[A]	HDD	OND-C2D-CMD	-3.19	103.72	109.59
2	C	760[A]	HDD	CMD-C2D-C1D	3.17	118.27	112.63
3	D	761[B]	HDE	CMB-C2B-C3B	3.16	130.90	124.94
3	C	761[B]	HDE	C3A-C4A-CHB	-3.15	119.08	124.28
3	C	761[B]	HDE	C4D-CHA-C1A	-3.06	124.05	130.12
3	A	761[B]	HDE	C4D-CHA-C1A	-3.06	124.06	130.12
3	A	761[B]	HDE	CMC-C2C-C3C	3.05	130.70	124.94
2	C	760[A]	HDD	C3C-C4C-NC	-3.05	105.26	109.21
3	B	761[B]	HDE	C4D-CHA-C1A	-3.04	124.10	130.12
3	D	761[B]	HDE	CMD-C2D-C3D	3.02	130.64	124.94
3	B	761[B]	HDE	CHD-C4C-C3C	-3.02	126.03	129.68
2	D	760[A]	HDD	C4A-C3A-C2A	3.00	109.08	107.00
2	C	760[A]	HDD	C2D-C1D-CHD	2.98	129.21	124.28
3	D	761[B]	HDE	CMC-C2C-C3C	2.98	130.56	124.94
2	C	760[A]	HDD	CMA-C3A-C4A	-2.98	123.89	128.46
2	A	760[A]	HDD	CMD-C2D-C1D	-2.86	107.53	112.63
2	B	760[A]	HDD	C1A-CHA-C4D	-2.86	124.45	130.12
3	B	761[B]	HDE	C4C-C3C-C2C	2.85	110.18	105.93
3	B	761[B]	HDE	O1A-CGA-O2A	2.84	123.33	120.80
3	C	761[B]	HDE	CMC-C2C-C3C	2.82	130.26	124.94
3	D	761[B]	HDE	C3A-C4A-CHB	-2.82	119.63	124.28
2	D	760[A]	HDD	CMC-C2C-C1C	-2.81	124.14	128.46
3	B	761[B]	HDE	C4B-CHC-C1C	2.79	119.67	112.87
3	A	761[B]	HDE	C4C-CHD-C1D	2.75	119.59	112.87
3	D	761[B]	HDE	CMA-C3A-C4A	-2.74	107.75	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	760[A]	HDD	OND-C2D-CMD	-2.73	104.57	109.59
3	C	761[B]	HDE	O1A-CGA-O2A	2.72	123.22	120.80
3	B	761[B]	HDE	C3A-C4A-CHB	-2.70	119.82	124.28
3	D	761[B]	HDE	C4B-CHC-C1C	2.67	119.38	112.87
2	A	760[A]	HDD	CAA-CBA-CGA	-2.63	106.39	113.76
3	D	761[B]	HDE	O1A-CGA-O2A	2.61	123.13	120.80
3	A	761[B]	HDE	C1B-C2B-C3B	-2.61	105.18	107.00
2	D	760[A]	HDD	CMA-C3A-C4A	-2.60	124.47	128.46
3	D	761[B]	HDE	CAC-C3C-C4C	-2.59	124.07	127.19
2	D	760[A]	HDD	C3B-C4B-NB	-2.55	106.12	110.94
3	A	761[B]	HDE	O1A-C2A-C1A	2.50	113.33	108.25
3	C	761[B]	HDE	C1D-C2D-C3D	-2.49	103.16	105.81
3	D	761[B]	HDE	CBB-CAB-C3B	-2.48	105.95	112.27
3	B	761[B]	HDE	CMB-C2B-C3B	2.48	129.62	124.94
2	A	760[A]	HDD	C3B-C4B-NB	-2.47	106.28	110.94
3	B	761[B]	HDE	O1A-C2A-C1A	2.43	113.19	108.25
2	C	760[A]	HDD	CAD-CBD-CGD	-2.40	100.85	104.56
2	D	760[A]	HDD	C1A-CHA-C4D	-2.40	125.37	130.12
2	C	760[A]	HDD	O1A-CGA-CBA	-2.36	115.51	123.08
2	C	760[A]	HDD	CMC-C2C-C3C	2.35	129.07	124.68
3	D	761[B]	HDE	C1D-C2D-C3D	-2.30	103.36	105.81
3	A	761[B]	HDE	CMD-C2D-C3D	2.30	129.27	124.94
3	D	761[B]	HDE	CMB-C2B-C1B	-2.29	124.94	128.46
2	C	760[A]	HDD	C4A-C3A-C2A	2.27	108.58	107.00
3	C	761[B]	HDE	CMA-C3A-C4A	-2.27	108.59	112.63
3	A	761[B]	HDE	CMB-C2B-C3B	2.22	129.13	124.94
2	C	760[A]	HDD	CAA-CBA-CGA	-2.22	107.54	113.76
3	B	761[B]	HDE	CMA-C3A-C4A	-2.19	108.74	112.63
2	C	760[A]	HDD	C3B-C4B-NB	-2.17	106.86	110.94
2	C	760[A]	HDD	OND-C2D-C3D	-2.15	105.10	110.45
2	C	760[A]	HDD	O2A-CGA-CBA	2.14	120.90	114.03
3	B	761[B]	HDE	ONA-C3A-C4A	2.12	116.22	111.92
2	B	760[A]	HDD	C3C-C4C-NC	-2.08	106.53	109.21
2	B	760[A]	HDD	CAD-CBD-CGD	-2.06	101.38	104.56
3	B	761[B]	HDE	C1D-C2D-C3D	-2.04	103.63	105.81
3	A	761[B]	HDE	CBC-CAC-C3C	-2.03	107.11	112.27
3	C	761[B]	HDE	C4C-C3C-C2C	2.03	108.95	105.93
2	B	760[A]	HDD	CMC-C2C-C3C	2.01	128.43	124.68

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	A	760[A]	HDD	CAA-CBA-CGA-O2A
3	C	761[B]	HDE	CAD-CBD-CGD-O1D
3	C	761[B]	HDE	CAD-CBD-CGD-O2D
3	D	761[B]	HDE	CAD-CBD-CGD-O1D
3	D	761[B]	HDE	CAD-CBD-CGD-O2D
2	B	760[A]	HDD	CAA-CBA-CGA-O1A
2	C	760[A]	HDD	CAA-CBA-CGA-O1A
2	D	760[A]	HDD	CAA-CBA-CGA-O1A
2	D	760[A]	HDD	CAA-CBA-CGA-O2A
2	C	760[A]	HDD	CAA-CBA-CGA-O2A
3	A	761[B]	HDE	CAD-CBD-CGD-O2D
2	A	760[A]	HDD	CAA-CBA-CGA-O1A
3	A	761[B]	HDE	CAD-CBD-CGD-O1D
2	B	760[A]	HDD	CAA-CBA-CGA-O2A
3	B	761[B]	HDE	CAD-CBD-CGD-O1D
3	B	761[B]	HDE	CAD-CBD-CGD-O2D

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
3	B	761[B]	HDE	14	0
3	A	761[B]	HDE	7	0
2	B	760[A]	HDD	20	0
3	D	761[B]	HDE	11	0
2	A	760[A]	HDD	9	0

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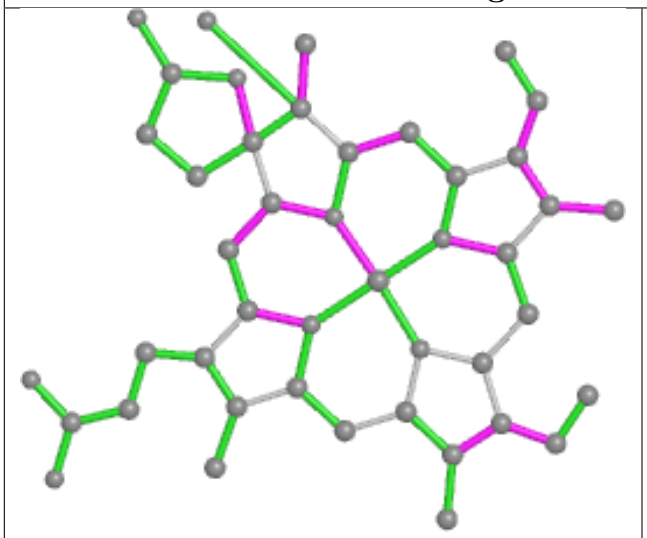
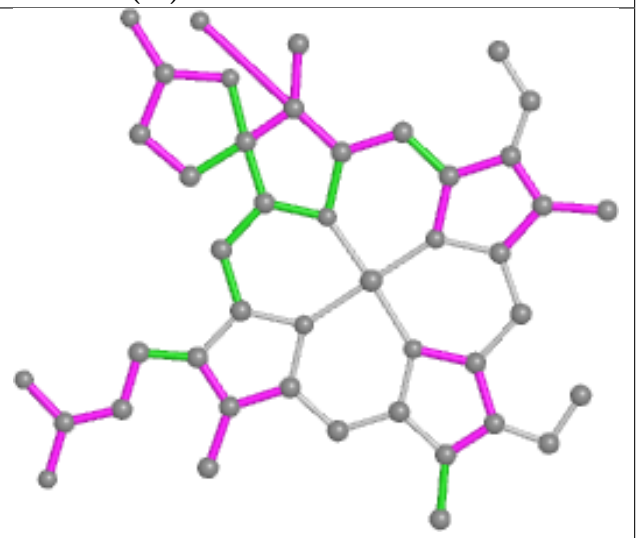
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	761[B]	HDE	12	0
2	D	760[A]	HDD	8	0

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 then 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.

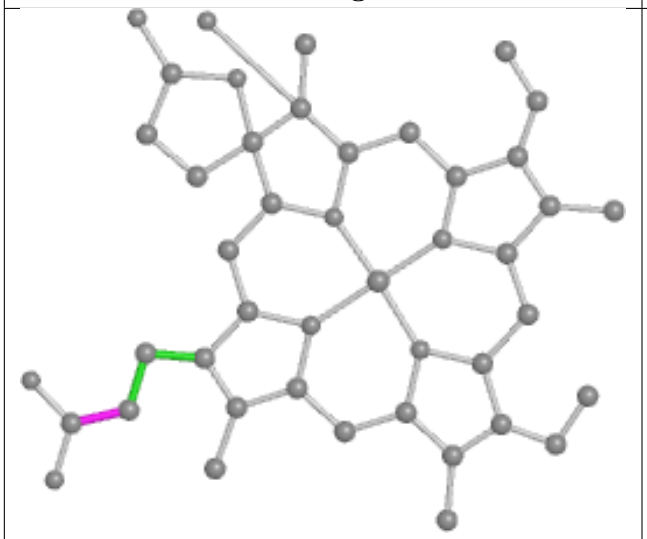
Ligand HDD C 760 (A)



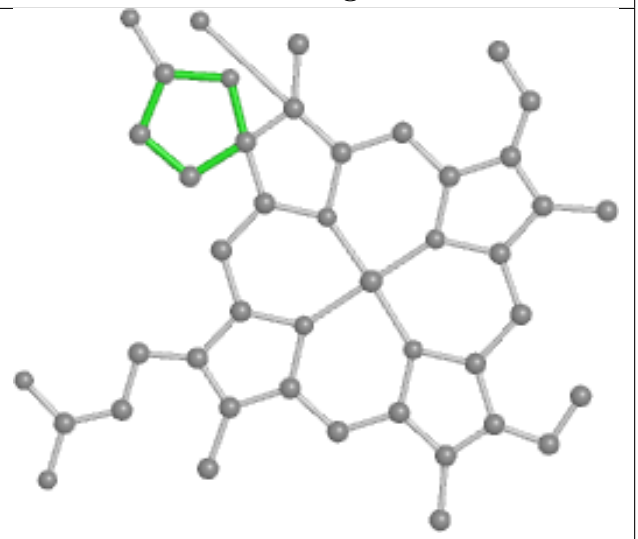
Bond lengths



Bond angles

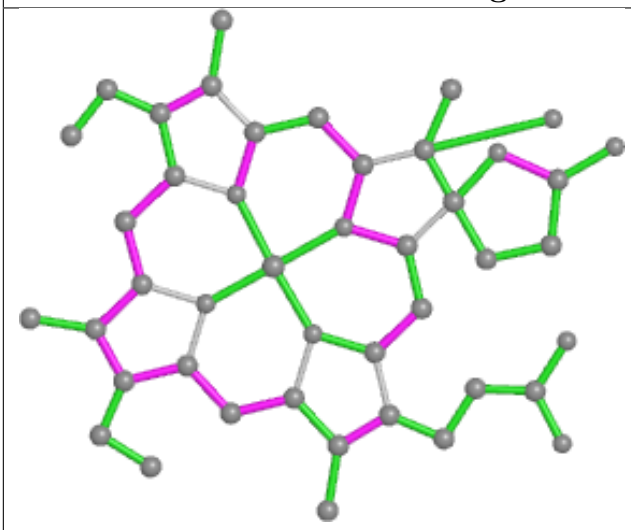


Torsions

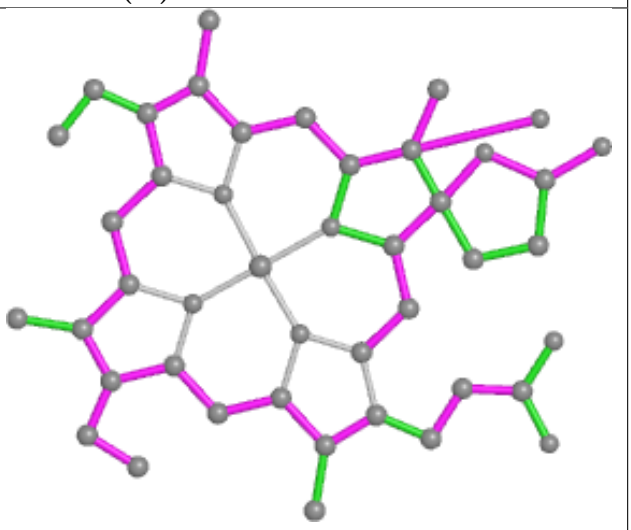


Rings

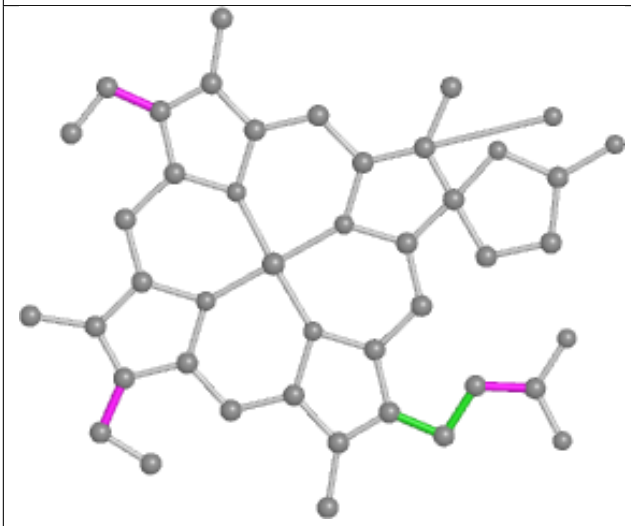
Ligand HDE B 761 (B)



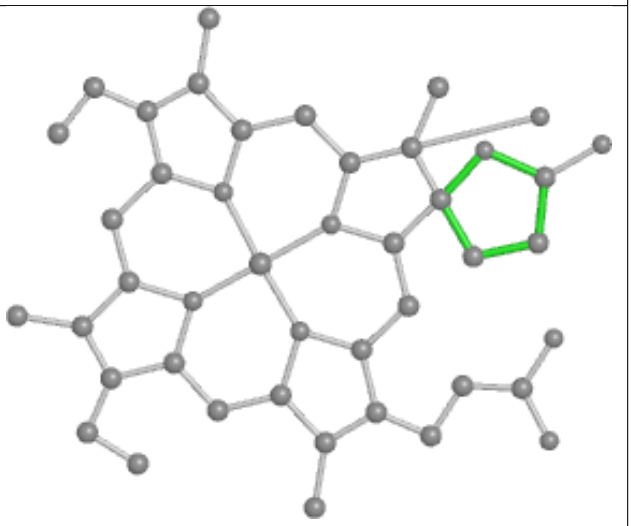
Bond lengths



Bond angles

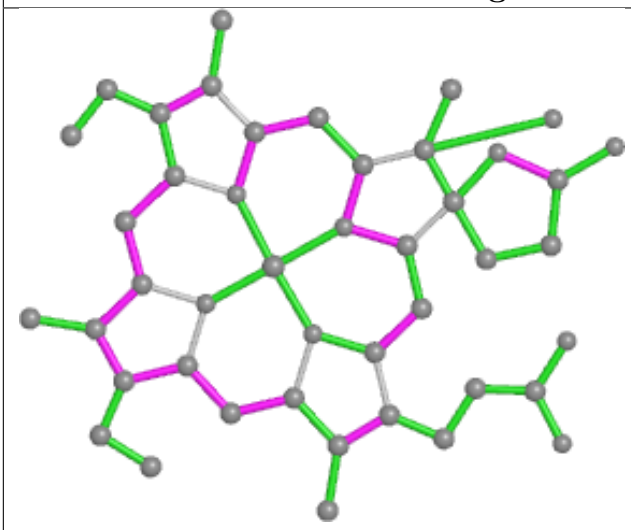


Torsions

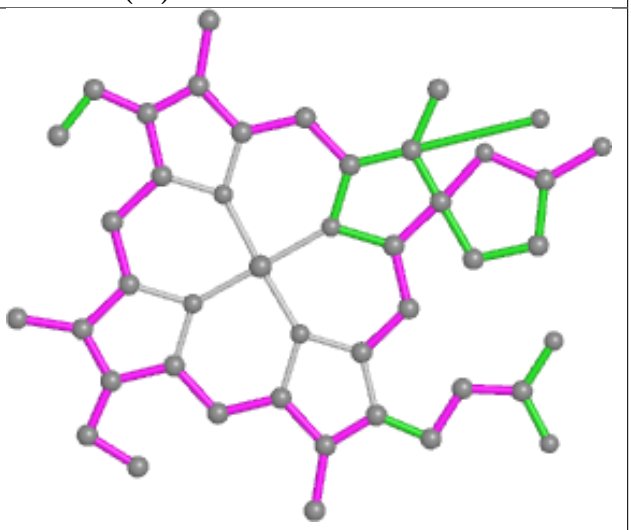


Rings

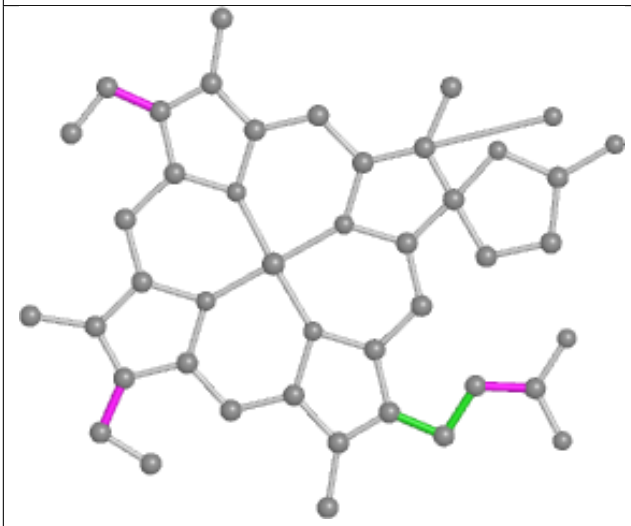
Ligand HDE A 761 (B)



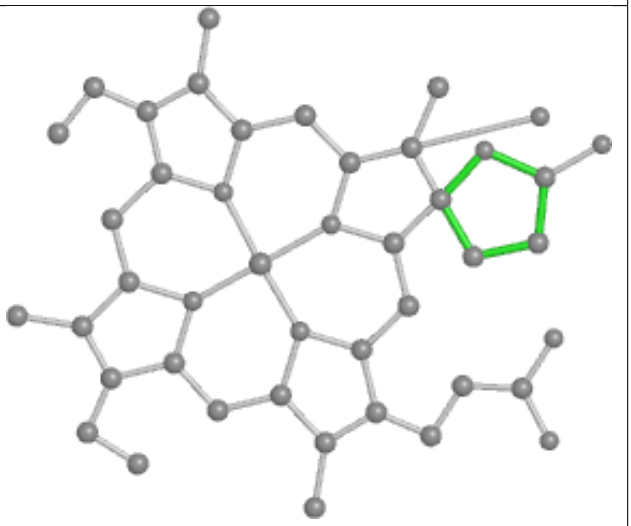
Bond lengths



Bond angles

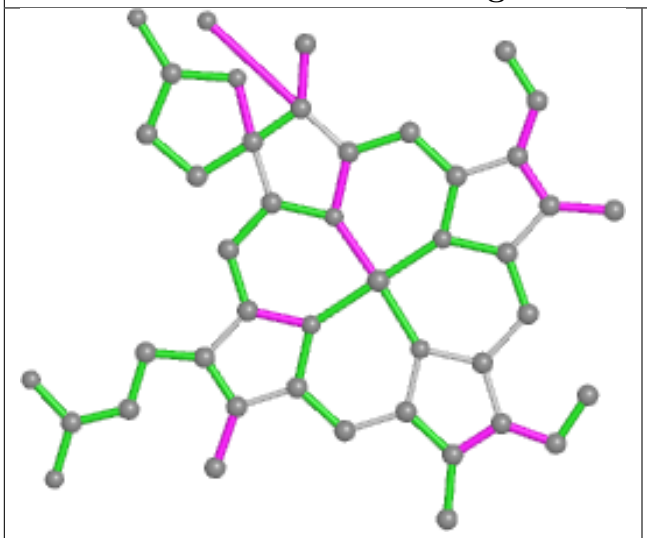


Torsions

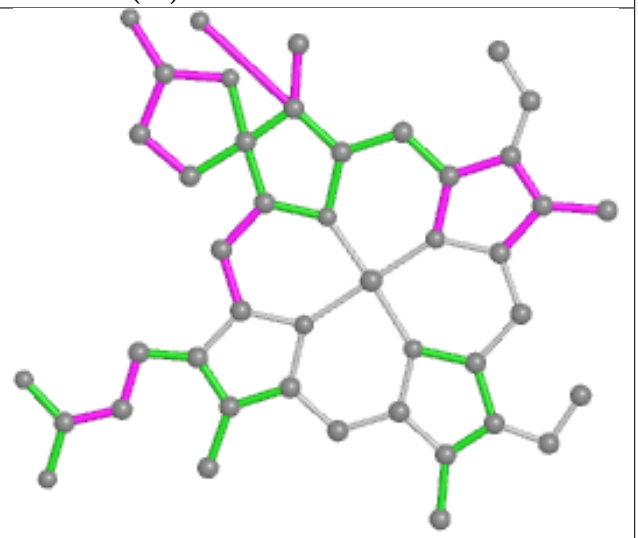


Rings

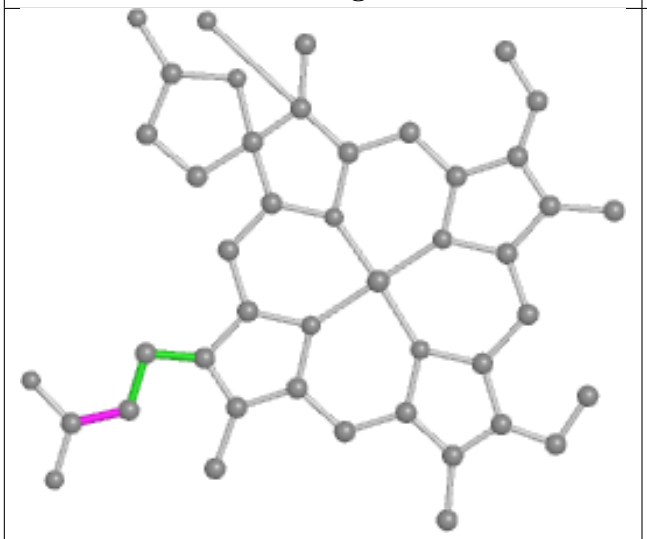
Ligand HDD B 760 (A)



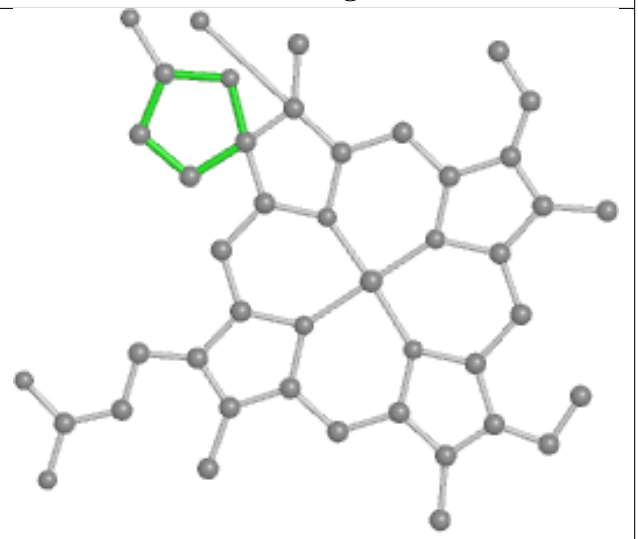
Bond lengths



Bond angles

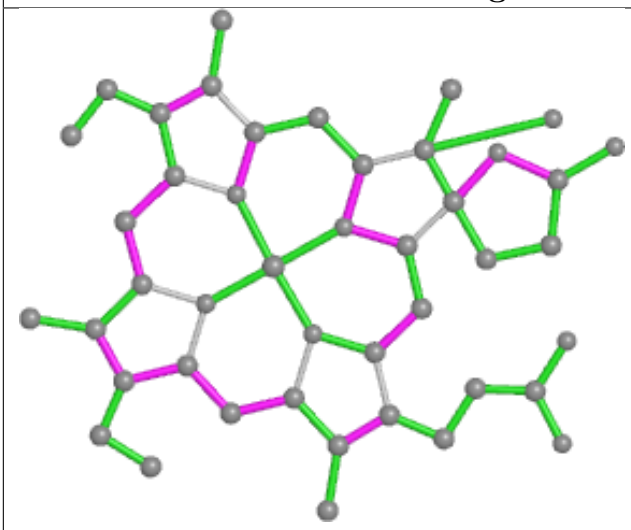


Torsions

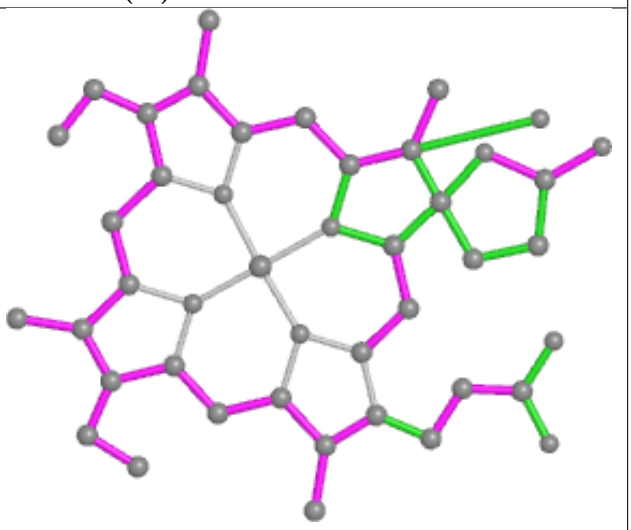


Rings

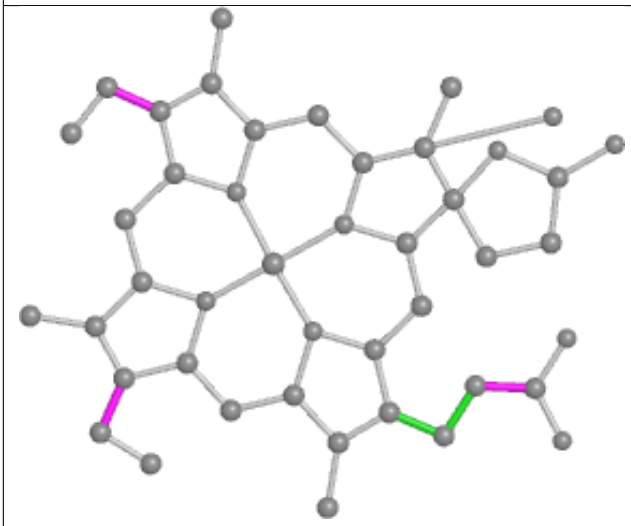
Ligand HDE D 761 (B)



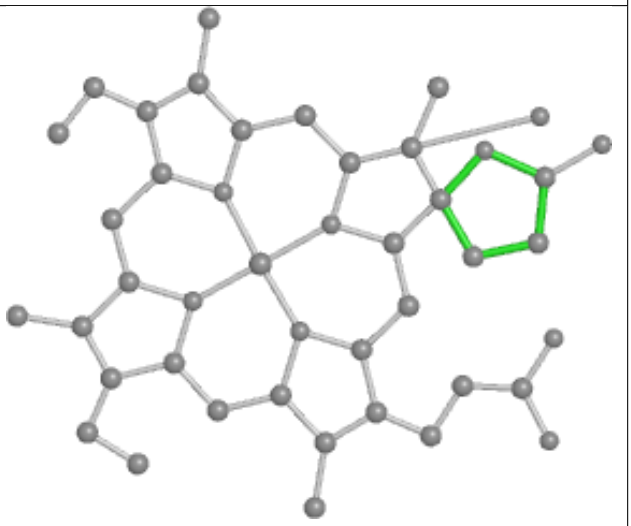
Bond lengths



Bond angles

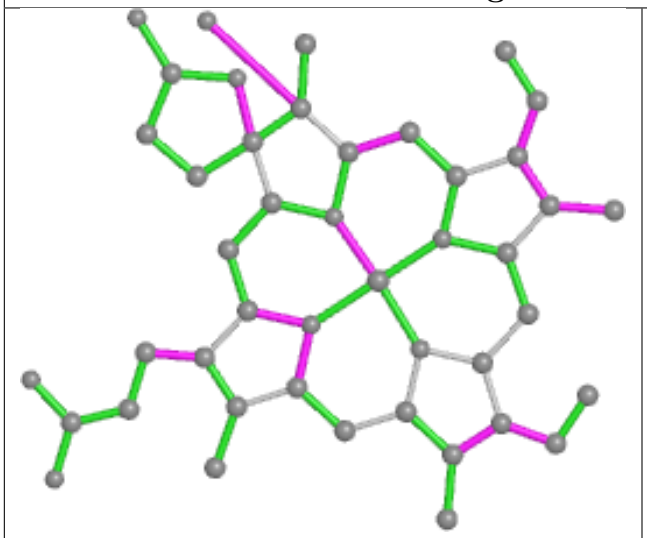


Torsions

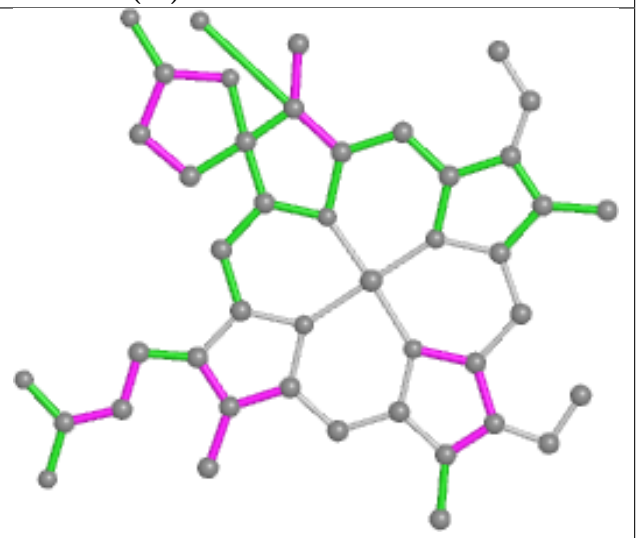


Rings

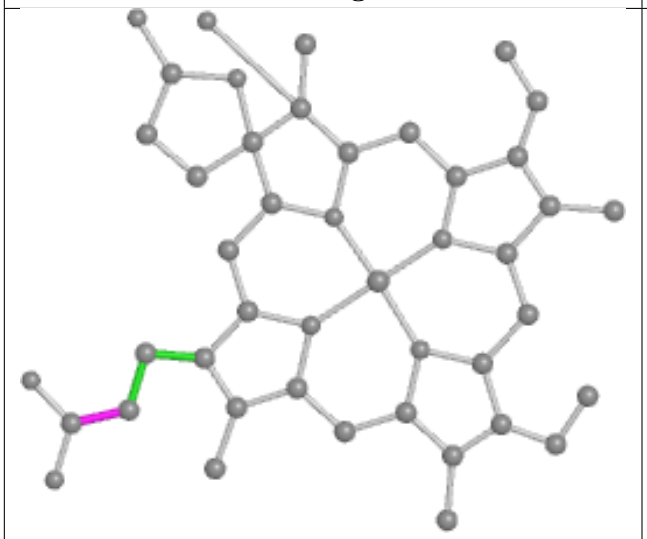
Ligand HDD A 760 (A)



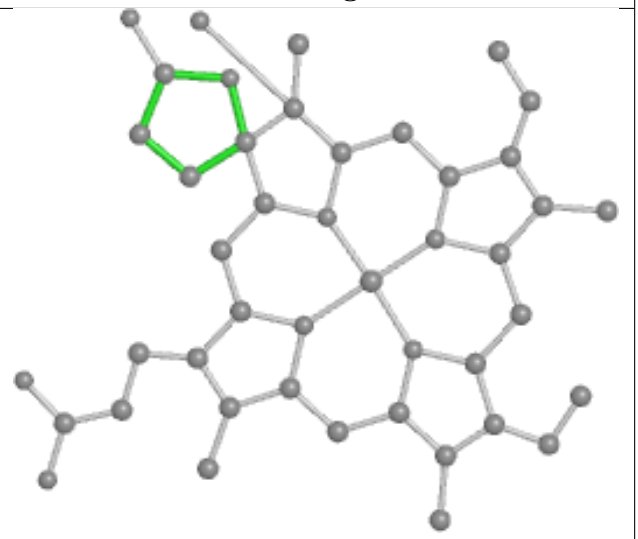
Bond lengths



Bond angles

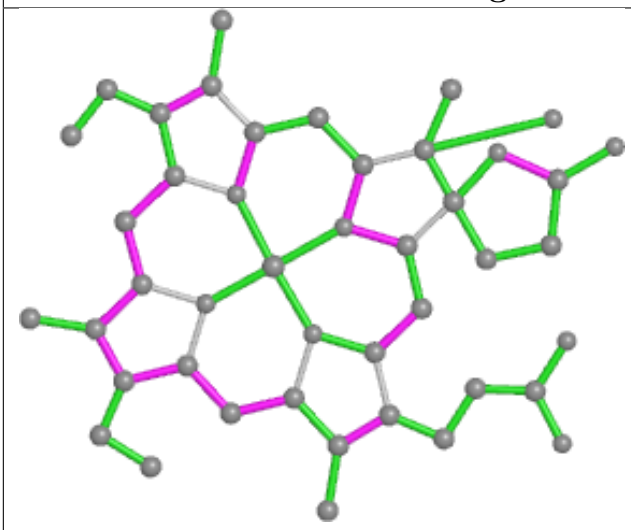


Torsions

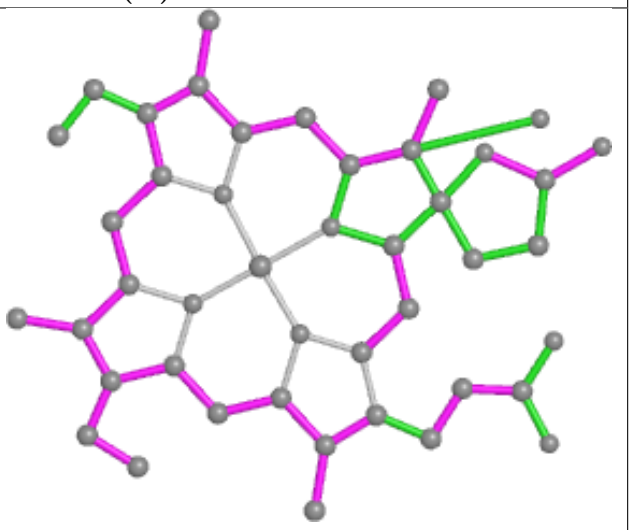


Rings

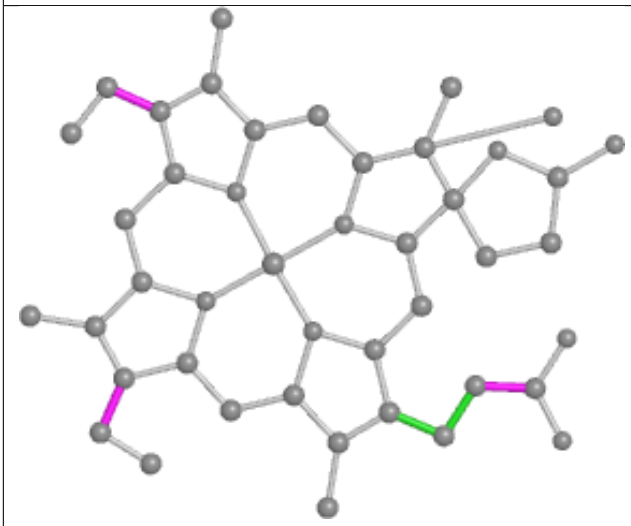
Ligand HDE C 761 (B)



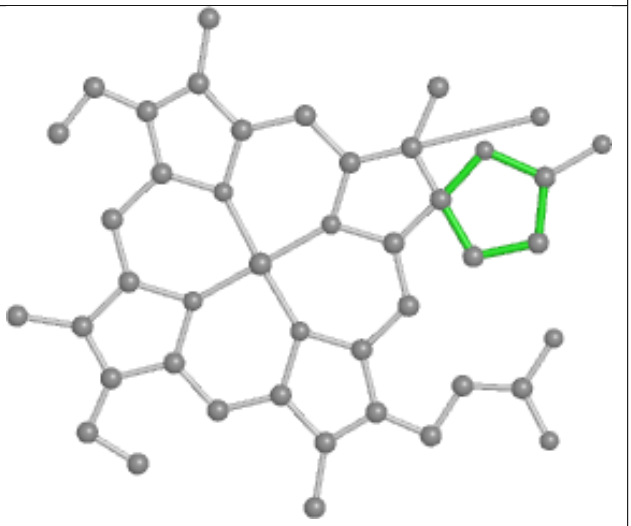
Bond lengths



Bond angles

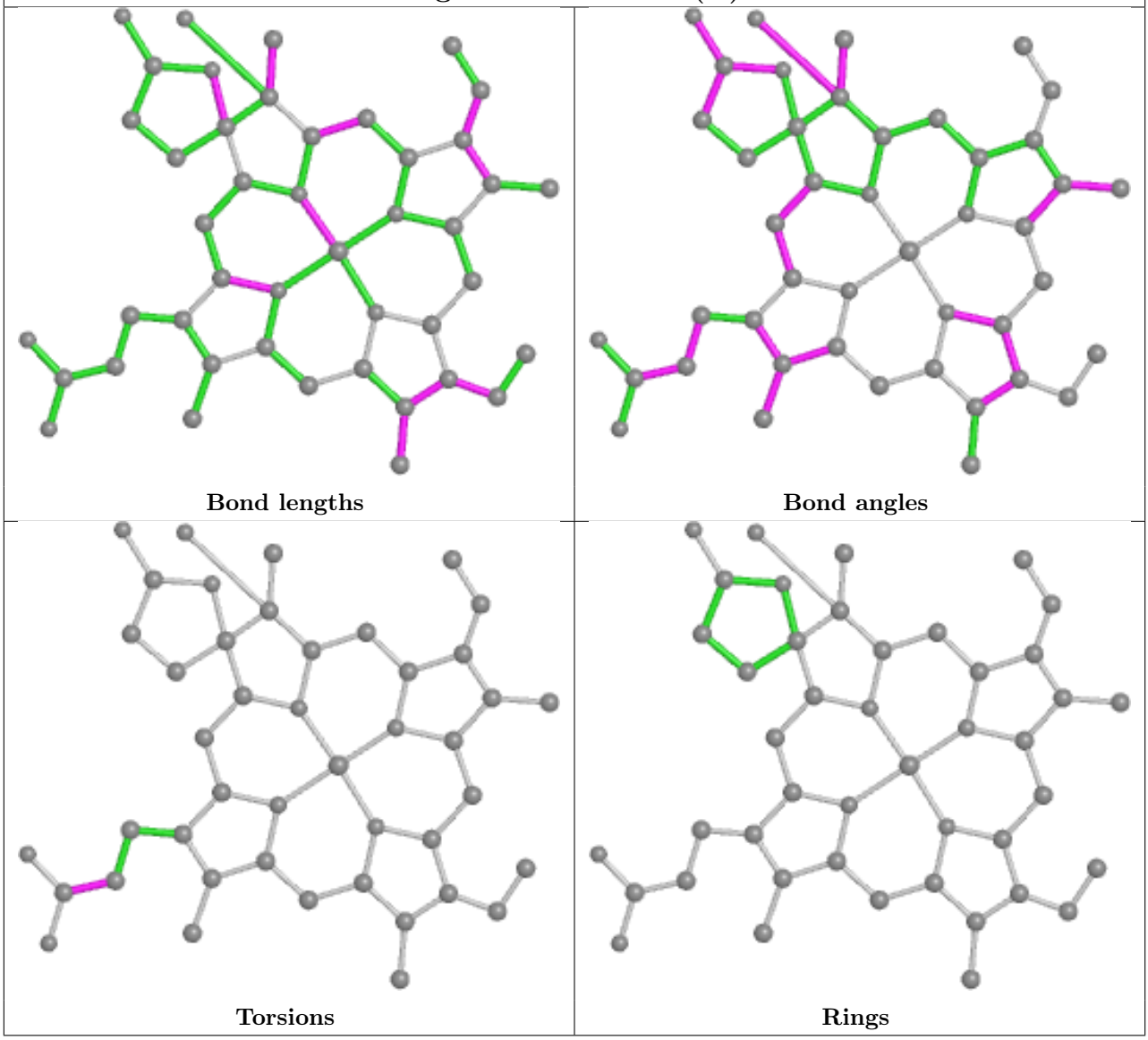


Torsions



Rings

Ligand HDD D 760 (A)



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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	726/753 (96%)	-0.62	3 (0%)	92	90	3, 10, 26, 44	2 (0%)
1	B	726/753 (96%)	-0.45	15 (2%)	63	59	3, 11, 32, 47	2 (0%)
1	C	726/753 (96%)	-0.48	10 (1%)	75	72	3, 11, 31, 46	2 (0%)
1	D	726/753 (96%)	-0.61	6 (0%)	86	84	3, 10, 27, 44	1 (0%)
All	All	2904/3012 (96%)	-0.54	34 (1%)	79	76	3, 10, 30, 47	7 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	726	GLY	3.8
1	C	594	PRO	3.6
1	B	32	GLU	3.5
1	A	28	SER	3.4
1	B	713	GLN	3.4
1	B	28	SER	3.1
1	D	28	SER	3.1
1	A	32	GLU	3.0
1	B	712	ASP	2.9
1	C	726	GLY	2.8
1	B	673	ALA	2.8
1	B	568	ASP	2.7
1	C	672	ILE	2.7
1	A	713	GLN	2.6
1	D	713	GLN	2.6
1	C	712	ASP	2.5
1	B	727	SER	2.5
1	D	750	LYS	2.4
1	B	725	ASP	2.4
1	B	677	ASP	2.3
1	B	552	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	710	ILE	2.3
1	C	750	LYS	2.3
1	B	647	VAL	2.3
1	B	583	LYS	2.2
1	C	673	ALA	2.2
1	B	569	ASP	2.2
1	D	712	ASP	2.1
1	B	641	THR	2.1
1	C	572	ASN	2.1
1	C	32	GLU	2.1
1	C	714	GLY	2.1
1	D	749	ASP	2.1
1	C	552	LEU	2.1

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	H2S	C	754	1/1	0.96	0.26	20,20,20,20	1
4	H2S	D	754	1/1	0.96	0.28	23,23,23,23	1
4	H2S	A	754	1/1	0.97	0.35	28,28,28,28	1
4	H2S	B	754	1/1	0.97	0.20	26,26,26,26	1
3	HDE	C	761[B]	44/44	0.98	0.08	3,11,13,15	44
2	HDD	B	760[A]	44/44	0.98	0.07	2,3,6,7	44
2	HDD	C	760[A]	44/44	0.98	0.08	2,4,9,14	44
2	HDD	D	760[A]	44/44	0.98	0.07	2,3,7,12	44
3	HDE	B	761[B]	44/44	0.98	0.07	2,9,13,14	44
3	HDE	A	761[B]	44/44	0.99	0.08	2,7,10,13	44

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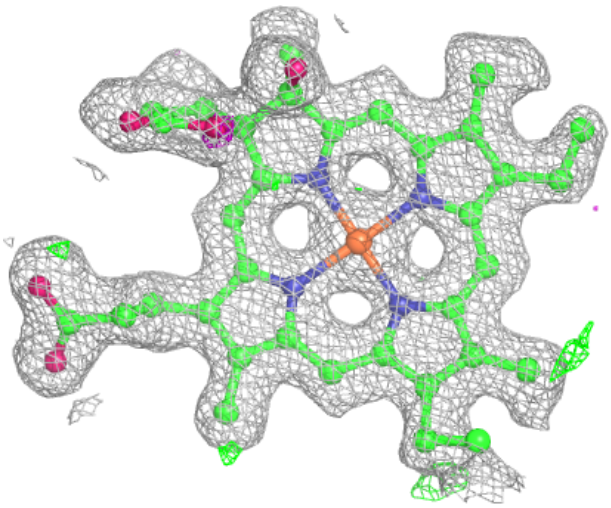
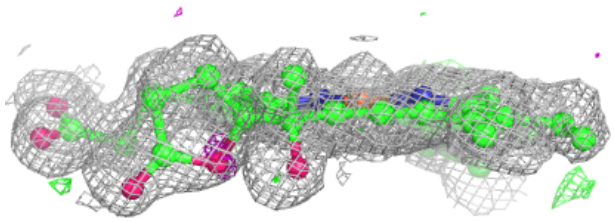
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HDE	D	761[B]	44/44	0.99	0.07	2,8,12,16	44
2	HDD	A	760[A]	44/44	0.99	0.09	2,3,6,9	44

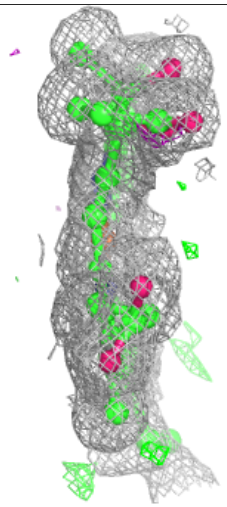
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HDE C 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)

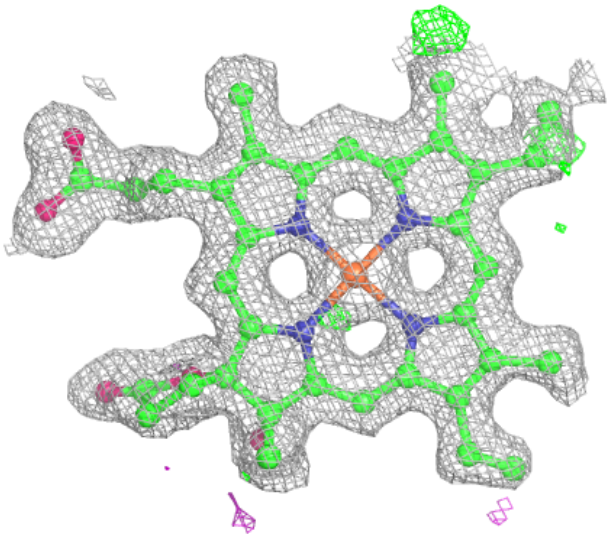


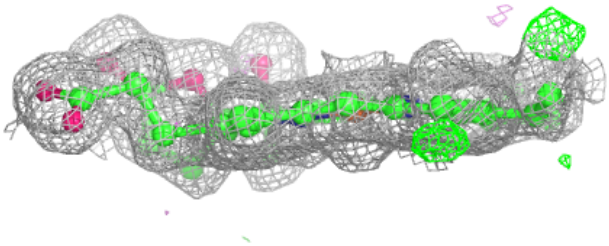


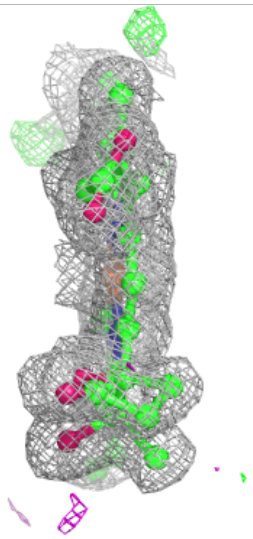


Electron density around HDD B 760 (A):

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

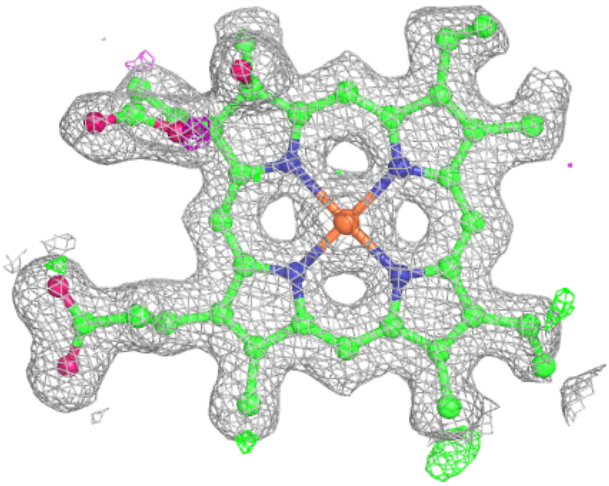


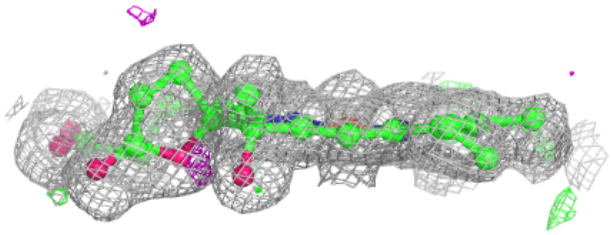


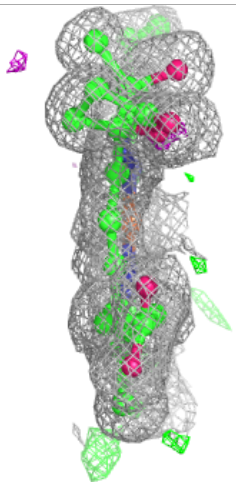


Electron density around HDD C 760 (A):

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

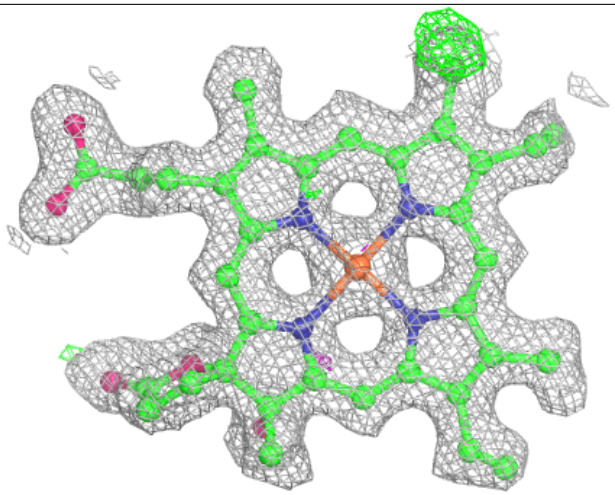


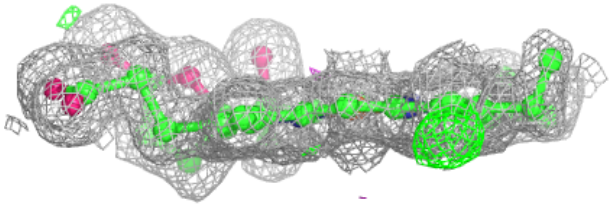


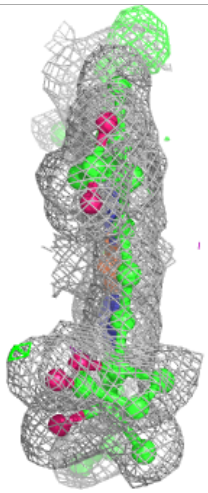


Electron density around HDD D 760 (A):

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

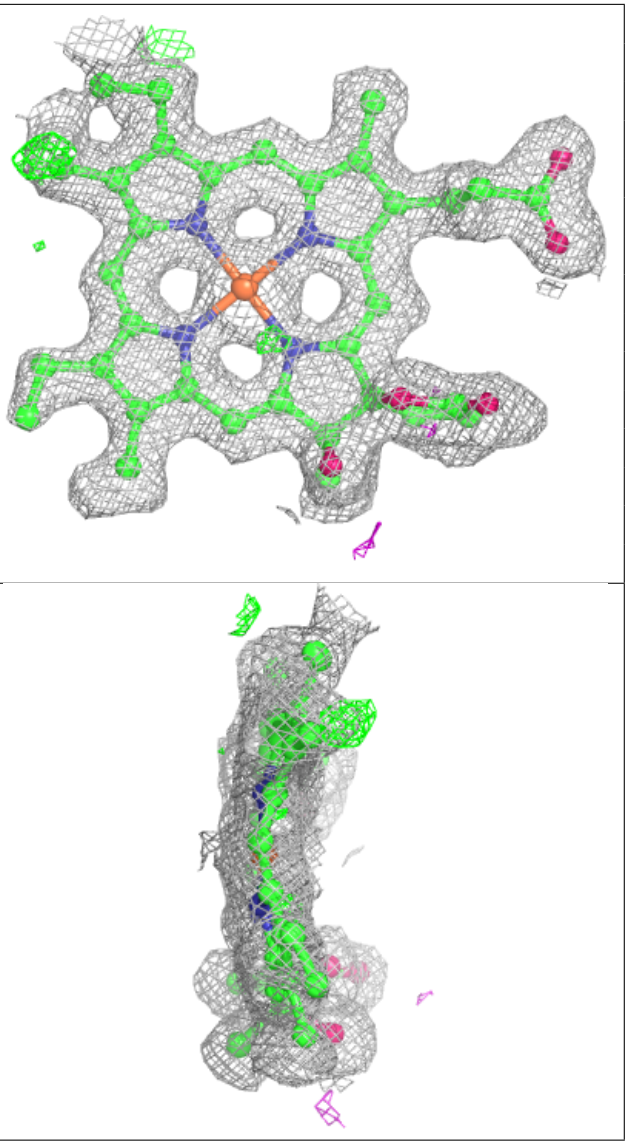






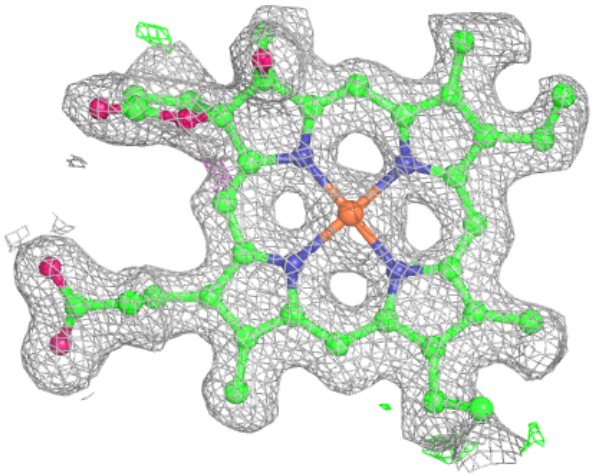
Electron density around HDE B 761 (B):

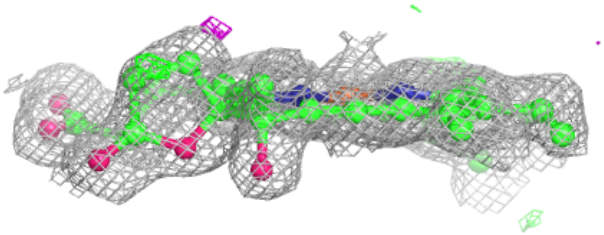
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

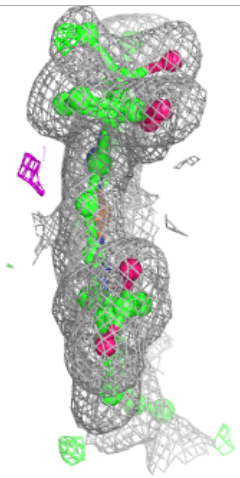


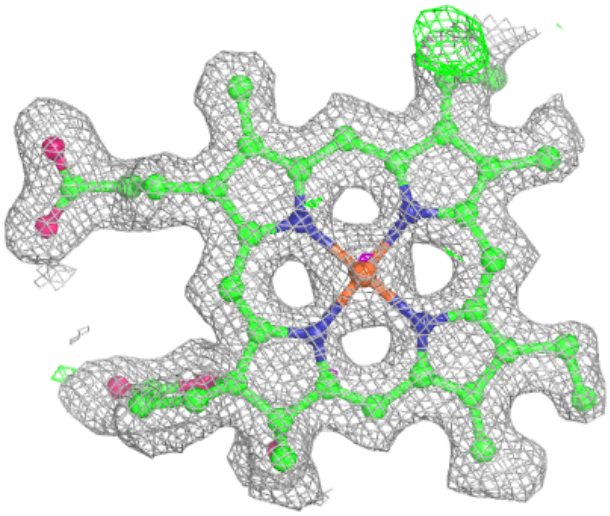
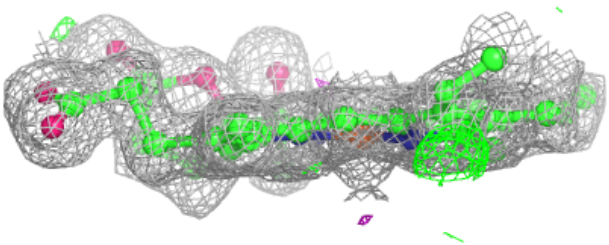
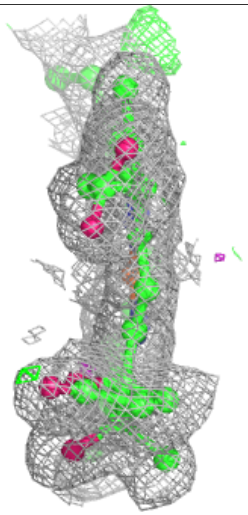
Electron density around HDE A 761 (B):

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



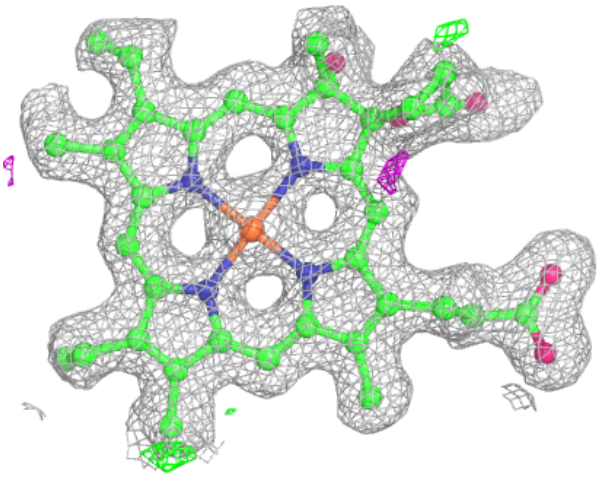


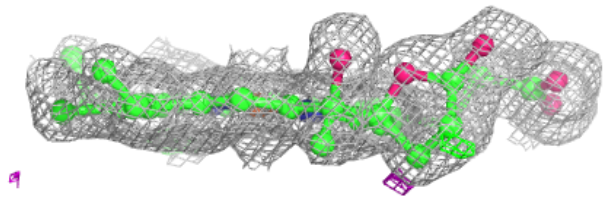


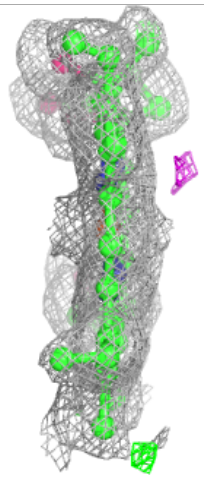
Electron density around HDE D 761 (B): 2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around HDD 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)







6.5 Other polymers (i)

There are no such residues in this entry.