Full wwPDB X-ray Structure Validation Report (i)

Aug 28, 2023 – 09:33 PM EDT

PDB ID	:	3PQ2
Title	:	Structure of I274C variant of E. coli KatE[] - Images 1-6
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:

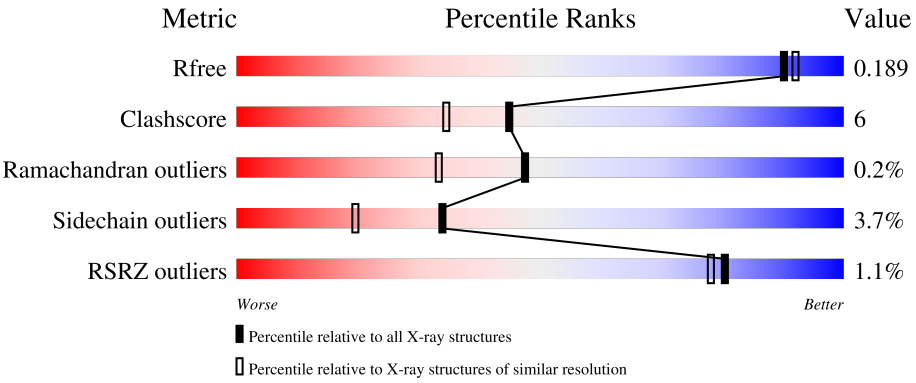
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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% 85% 10%
1	C	753	% 85% 10%
1	D	753	% 86% 10%

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 26834 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.

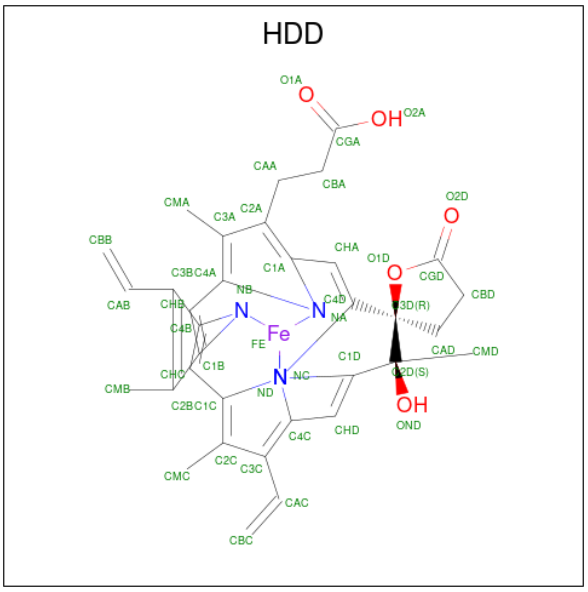
- Molecule 1 is a protein called Catalase HPII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	5	0
			5755	3652	1009	1083	11			
1	B	726	Total	C	N	O	S	0	5	0
			5757	3654	1009	1083	11			
1	C	726	Total	C	N	O	S	0	3	0
			5753	3652	1010	1080	11			
1	D	726	Total	C	N	O	S	0	8	0
			5768	3662	1010	1085	11			

There are 12 discrepancies between the modelled and reference sequences:

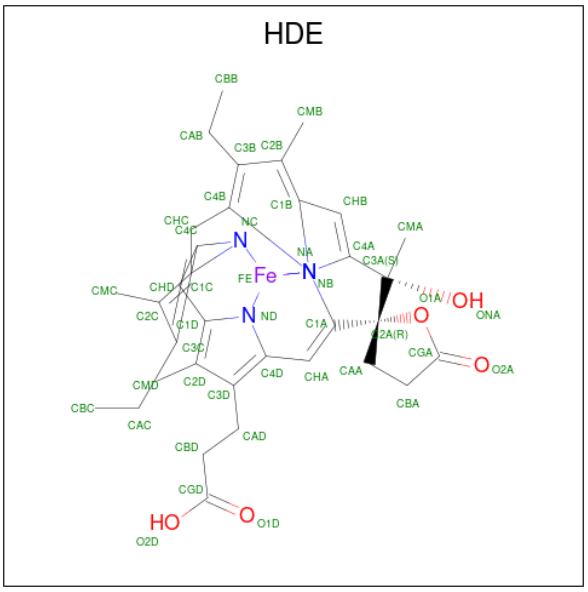
Chain	Residue	Modelled	Actual	Comment	Reference
A	274	CYS	ILE	engineered mutation	UNP P21179
A	438	ALA	CYS	engineered mutation	UNP P21179
A	669	ALA	CYS	engineered mutation	UNP P21179
B	274	CYS	ILE	engineered mutation	UNP P21179
B	438	ALA	CYS	engineered mutation	UNP P21179
B	669	ALA	CYS	engineered mutation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



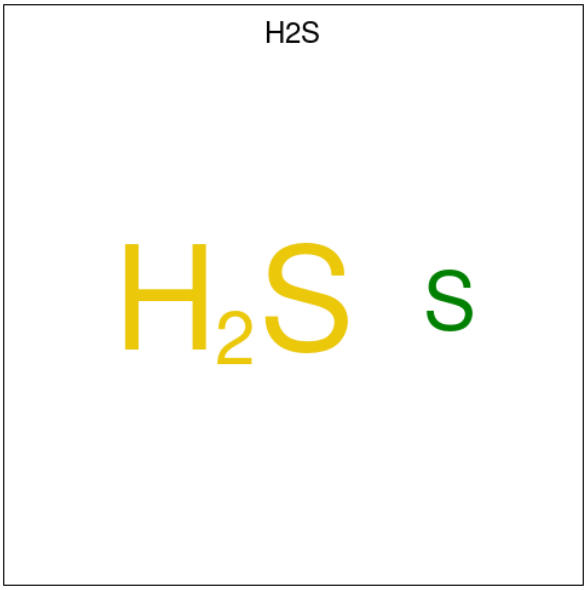
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
2	B	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
2	C	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
2	D	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		

- 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_2S).



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	887	Total	O	0	0
			887	887		
5	B	801	Total	O	0	0
			801	801		

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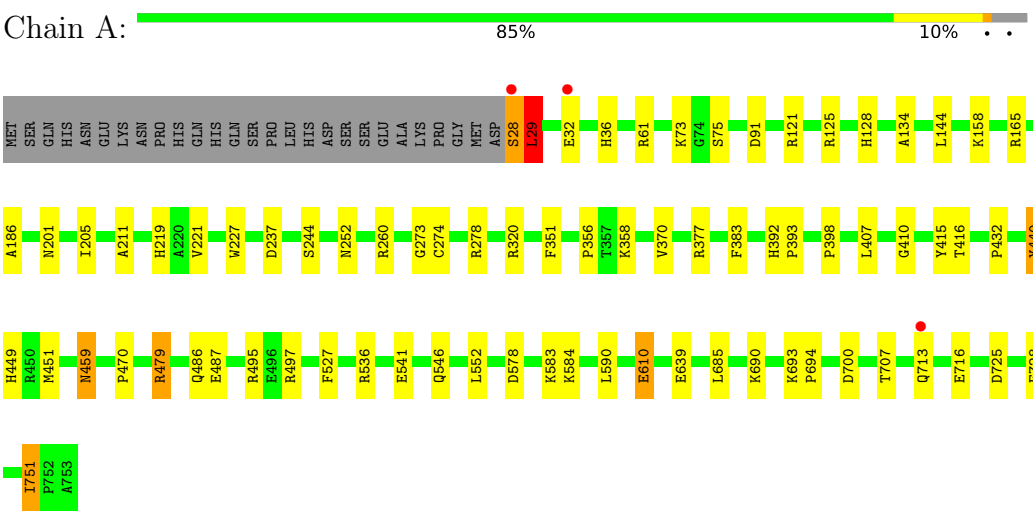
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	845	Total O 845 845	0	0
5	D	912	Total O 912 912	0	0

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.

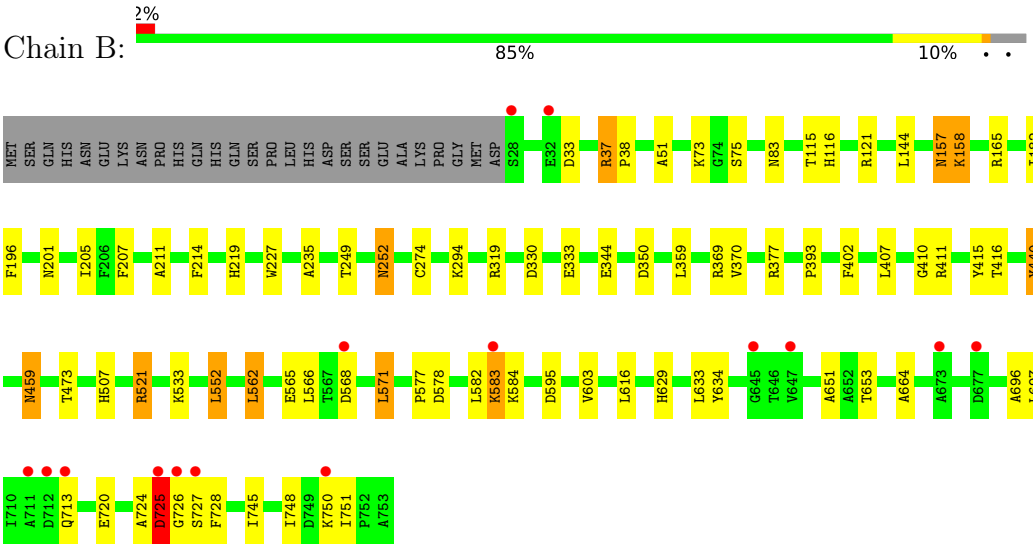
- Molecule 1: Catalase HPII

Chain A:



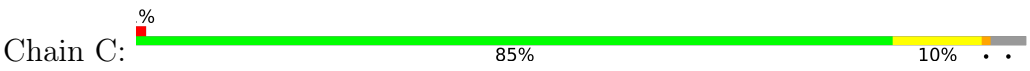
- Molecule 1: Catalase HPII

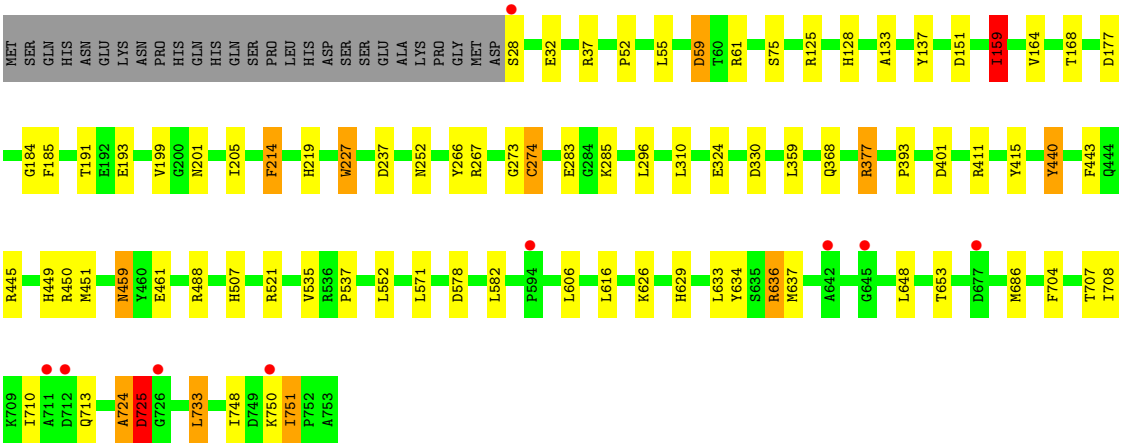
Chain B:



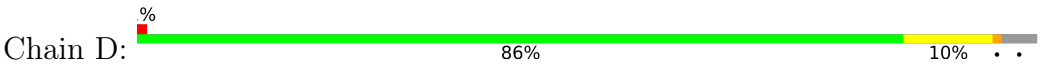
- Molecule 1: Catalase HPII

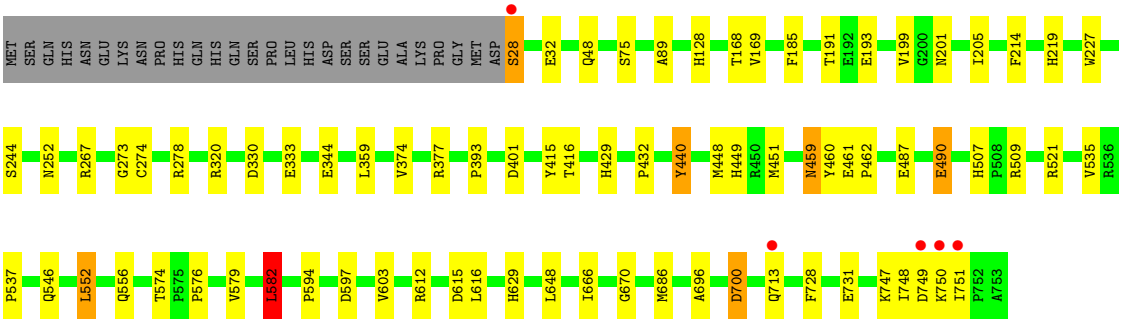
Chain C:





• Molecule 1: Catalase HPII





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)	31.27 – 1.79 31.27 – 1.79	Depositor EDS
% Data completeness (in resolution range)	92.2 (31.27-1.79) 92.2 (31.27-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.39 (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	12150 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	11.1	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	26834	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 3.25% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HDD, H2S, HDE

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	1.18	6/5932 (0.1%)	0.96	12/8064 (0.1%)
1	B	1.14	6/5931 (0.1%)	0.95	5/8062 (0.1%)
1	C	1.13	6/5919 (0.1%)	0.96	13/8047 (0.2%)
1	D	1.22	6/5955 (0.1%)	0.97	9/8095 (0.1%)
All	All	1.17	24/23737 (0.1%)	0.96	39/32268 (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	2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	440	TYR	CE1-CZ	7.34	1.48	1.38
1	A	440	TYR	CE1-CZ	6.96	1.47	1.38
1	D	333	GLU	CD-OE2	-6.74	1.18	1.25
1	D	460	TYR	CD1-CE1	5.72	1.48	1.39
1	B	196	PHE	CE1-CZ	5.67	1.48	1.37
1	A	186	ALA	CA-CB	5.67	1.64	1.52
1	D	199	VAL	CB-CG1	5.51	1.64	1.52
1	C	266	TYR	CD2-CE2	5.48	1.47	1.39
1	C	443	PHE	CE2-CZ	5.45	1.47	1.37
1	C	59	ASP	CB-CG	5.43	1.63	1.51
1	A	134	ALA	CA-CB	5.37	1.63	1.52
1	D	193	GLU	CB-CG	5.30	1.62	1.52
1	B	333	GLU	CD-OE1	-5.29	1.19	1.25
1	A	527	PHE	CE2-CZ	5.29	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	28	SER	CB-OG	5.26	1.49	1.42
1	A	383	PHE	CD2-CE2	5.24	1.49	1.39
1	C	125	ARG	CG-CD	5.21	1.65	1.51
1	A	221	VAL	CB-CG2	5.16	1.63	1.52
1	B	37	ARG	CZ-NH2	5.12	1.39	1.33
1	C	193	GLU	CB-CG	5.11	1.61	1.52
1	D	374	VAL	CB-CG2	5.10	1.63	1.52
1	B	440	TYR	CD1-CE1	5.10	1.47	1.39
1	B	402	PHE	CE2-CZ	5.07	1.47	1.37
1	C	214	PHE	CE1-CZ	5.03	1.47	1.37

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	636	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	C	636	ARG	NE-CZ-NH1	8.47	124.54	120.30
1	C	59	ASP	CB-CG-OD1	7.36	124.92	118.30
1	A	536	ARG	NE-CZ-NH2	7.13	123.86	120.30
1	A	121	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	A	536	ARG	NE-CZ-NH1	-6.75	116.92	120.30
1	C	310	LEU	CB-CG-CD1	6.56	122.16	111.00
1	C	445	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	A	740	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	B	521	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	A	479	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	C	159	ILE	CB-CG1-CD1	-6.01	97.08	113.90
1	A	165	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	B	121	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	D	582	LEU	CB-CG-CD1	5.79	120.84	111.00
1	D	521	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	A	495	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	C	733	LEU	CA-CB-CG	5.72	128.46	115.30
1	D	401	ASP	CB-CG-OD2	5.64	123.38	118.30
1	D	320	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	A	685	LEU	CB-CG-CD1	-5.59	101.49	111.00
1	B	33	ASP	CB-CG-OD1	5.50	123.25	118.30
1	D	615	ASP	CB-CG-OD2	5.50	123.25	118.30
1	C	450	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	320	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	A	377	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	D	612	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	C	37	ARG	NE-CZ-NH2	-5.26	117.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	686	MET	CG-SD-CE	5.24	108.59	100.20
1	B	377	ARG	NE-CZ-NH1	-5.21	117.69	120.30
1	B	350	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	A	29	LEU	CA-CB-CG	5.19	127.23	115.30
1	C	445	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	C	177	ASP	CB-CG-OD1	-5.14	113.67	118.30
1	C	401	ASP	CB-CG-OD2	5.14	122.93	118.30
1	C	377	ARG	NE-CZ-NH1	-5.09	117.76	120.30
1	A	497	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	D	377	ARG	NE-CZ-NH1	-5.03	117.78	120.30
1	D	612	ARG	NE-CZ-NH1	-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	62	0
1	B	5757	0	5587	78	0
1	C	5753	0	5586	56	0
1	D	5768	0	5601	56	0
2	A	44	0	31	9	0
2	B	44	0	31	18	0
2	C	44	0	31	15	0
2	D	44	0	31	10	0
3	A	44	0	36	8	0
3	B	44	0	36	13	0
3	C	44	0	36	13	0
3	D	44	0	36	14	0
4	A	1	0	0	6	0
4	B	1	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	7	0
4	D	1	0	0	7	0
5	A	887	0	0	16	1
5	B	801	0	0	13	0
5	C	845	0	0	21	0
5	D	912	0	0	26	1
All	All	26834	0	22624	299	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (299) 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)
2:B:760[A]:HDD:HBB2	4:B:754:H2S:S	1.29	1.69
1:C:274:CYS:HB3	4:C:754:H2S:S	1.28	1.69
1:D:274:CYS:HB3	4:D:754:H2S:S	1.36	1.66
1:A:274:CYS:HB3	4:A:754:H2S:S	1.33	1.62
1:B:274:CYS:HB3	4:B:754:H2S:S	1.40	1.57
2:D:760[A]:HDD:HBB2	4:D:754:H2S:S	1.48	1.50
2:C:760[A]:HDD:HBB2	4:C:754:H2S:S	1.61	1.38
2:B:760[A]:HDD:CBB	4:B:754:H2S:S	2.18	1.32
3:B:761[B]:HDE:HMC	3:B:761[B]:HDE:CBC	1.57	1.28
1:C:449[B]:HIS:CE1	5:C:3610:HOH:O	1.68	1.27
1:D:449[B]:HIS:CE1	5:D:3616:HOH:O	1.63	1.27
1:C:274:CYS:CB	4:C:754:H2S:S	2.21	1.27
2:D:760[A]:HDD:CBB	4:D:754:H2S:S	2.23	1.25
1:A:274:CYS:CB	4:A:754:H2S:S	2.23	1.24
1:C:578:ASP:HB3	5:C:2919:HOH:O	1.32	1.23
2:C:760[A]:HDD:CBB	4:C:754:H2S:S	2.28	1.21
1:D:451:MET:SD	5:D:3617:HOH:O	1.95	1.20
1:B:274:CYS:CB	4:B:754:H2S:S	2.30	1.20
1:D:274:CYS:CB	4:D:754:H2S:S	2.29	1.20
1:A:716:GLU:HG2	5:A:3090:HOH:O	1.42	1.19
3:D:761[B]:HDE:HBCB	3:D:761[B]:HDE:HMC	1.16	1.14
3:B:761[B]:HDE:CMC	3:B:761[B]:HDE:HBCA	1.70	1.11
3:C:761[B]:HDE:HMC	3:C:761[B]:HDE:HBCB	1.13	1.08
1:A:201:ASN:CG	2:A:760[A]:HDD:HMB2	1.70	1.08
3:A:761[B]:HDE:HBCB	3:A:761[B]:HDE:HMC	1.34	1.06
1:C:267:ARG:HG3	5:C:2916:HOH:O	1.54	1.05
1:B:451:MET:SD	5:B:3614:HOH:O	2.14	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:ASN:CG	2:B:760[A]:HDD:HMB2	1.77	1.04
1:D:201:ASN:CG	2:D:760[A]:HDD:HMB2	1.78	1.04
3:D:761[B]:HDE:HMC	3:D:761[B]:HDE:CBC	1.91	1.01
2:A:760[A]:HDD:HBB2	4:A:754:H2S:S	2.01	1.01
3:C:761[B]:HDE:HMC	3:C:761[B]:HDE:CBC	1.91	0.99
1:B:416:THR:HG21	5:D:2464:HOH:O	1.61	0.98
1:C:440:TYR:HD1	5:C:3454:HOH:O	1.45	0.98
1:A:416[A]:THR:HG21	5:C:3313:HOH:O	1.64	0.97
1:C:451:MET:SD	5:C:3612:HOH:O	2.25	0.95
1:D:416[A]:THR:HG21	5:D:3334:HOH:O	1.68	0.94
1:A:610:GLU:HG2	5:A:3555:HOH:O	1.67	0.94
1:A:28:SER:O	1:A:28:SER:OG	1.76	0.93
1:C:713:GLN:HB3	5:C:3004:HOH:O	1.67	0.93
1:A:29:LEU:HD22	5:C:2405:HOH:O	1.69	0.92
1:D:416[A]:THR:HG23	5:D:3576:HOH:O	1.67	0.92
1:A:274:CYS:SG	2:A:760[A]:HDD:CMB	2.58	0.90
3:D:761[B]:HDE:HMB	3:D:761[B]:HDE:CBB	2.01	0.90
1:C:201:ASN:CG	2:C:760[A]:HDD:HMB2	1.93	0.89
1:D:416[A]:THR:CG2	5:D:3576:HOH:O	2.21	0.89
1:A:451:MET:SD	5:A:3609:HOH:O	2.31	0.89
3:B:761[B]:HDE:HMC	3:B:761[B]:HDE:HBCA	0.89	0.88
3:A:761[B]:HDE:HMC	3:A:761[B]:HDE:CBC	2.03	0.87
3:C:761[B]:HDE:HMB	3:C:761[B]:HDE:CBB	2.05	0.86
2:A:760[A]:HDD:CBB	4:A:754:H2S:S	2.63	0.86
1:A:751:ILE:HD12	1:A:751:ILE:O	1.75	0.86
1:A:274:CYS:SG	2:A:760[A]:HDD:HMB3	2.17	0.85
3:D:761[B]:HDE:HMB	3:D:761[B]:HDE:HBBB	1.58	0.84
1:A:274:CYS:SG	2:A:760[A]:HDD:HMB1	2.17	0.84
3:B:761[B]:HDE:CBC	3:B:761[B]:HDE:CMC	2.33	0.84
1:D:274:CYS:SG	2:D:760[A]:HDD:CMB	2.68	0.82
1:C:274:CYS:SG	2:C:760[A]:HDD:CMB	2.66	0.81
3:B:761[B]:HDE:HMB	3:B:761[B]:HDE:HBBB	1.62	0.81
1:A:201:ASN:ND2	2:A:760[A]:HDD:HMB2	1.94	0.81
1:A:541:GLU:OE2	5:A:2550:HOH:O	1.97	0.80
1:B:521:ARG:NH2	1:B:745:ILE:HD13	1.95	0.80
1:C:274:CYS:SG	2:C:760[A]:HDD:HMB1	2.22	0.79
1:A:690:LYS:HG3	1:A:751:ILE:HD11	1.65	0.78
3:C:761[B]:HDE:HMB	3:C:761[B]:HDE:HBBA	1.65	0.78
3:A:761[B]:HDE:HMB	3:A:761[B]:HDE:HBBB	1.64	0.78
3:C:761[B]:HDE:HBCB	3:C:761[B]:HDE:CMC	1.94	0.77
1:D:748:ILE:O	1:D:751:ILE:HG22	1.86	0.75

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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	2.74	0.75
1:A:610:GLU:CG	5:A:3555:HOH:O	2.29	0.74
1:D:274:CYS:SG	2:D:760[A]:HDD:HMB3	2.27	0.74
1:C:274:CYS:SG	2:C:760[A]:HDD:HMB3	2.27	0.73
1:C:449[B]:HIS:NE2	5:C:3610:HOH:O	1.89	0.73
1:D:274:CYS:SG	2:D:760[A]:HDD:HMB1	2.26	0.73
3:D:761[B]:HDE:HBCB	3:D:761[B]:HDE:CMC	1.95	0.73
1:D:28:SER:HA	5:D:2467:HOH:O	1.87	0.73
1:B:700:ASP:HB2	5:B:3595:HOH:O	1.89	0.72
3:D:761[B]:HDE:HMC	4:D:754:H2S:S	2.29	0.72
1:D:416[B]:THR:HG22	5:D:1415:HOH:O	1.89	0.72
3:C:761[B]:HDE:CBC	3:C:761[B]:HDE:CMC	2.60	0.72
1:B:748:ILE:O	1:B:751:ILE:HG22	1.89	0.71
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.73	0.71
3:B:761[B]:HDE:HMB	3:B:761[B]:HDE:CBB	2.20	0.71
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.73	0.71
1:B:73:LYS:HE3	5:D:3517:HOH:O	1.90	0.70
1:B:583:LYS:NZ	1:B:583:LYS:H	1.89	0.70
1:D:490:GLU:OE1	5:D:2308:HOH:O	2.09	0.70
1:B:274:CYS:SG	2:B:760[A]:HDD:HMB1	2.33	0.69
1:B:274:CYS:SG	2:B:760[A]:HDD:HMB3	2.32	0.69
1:B:521:ARG:HH22	1:B:745:ILE:HD13	1.57	0.69
3:B:761[B]:HDE:HMC	3:B:761[B]:HDE:HBCB	1.68	0.69
1:B:274:CYS:SG	2:B:760[A]:HDD:HBB1	2.33	0.68
1:B:115:THR:HG21	5:D:3420:HOH:O	1.94	0.68
1:A:610:GLU:OE1	5:A:2394:HOH:O	2.12	0.68
3:D:761[B]:HDE:HMB	3:D:761[B]:HDE:HBBA	1.73	0.67
1:D:440:TYR:CZ	5:D:3517:HOH:O	2.48	0.67
3:C:761[B]:HDE:HMB	3:C:761[B]:HDE:HBBB	1.76	0.67
1:C:59:ASP:OD2	5:C:2529:HOH:O	2.13	0.67
1:B:201:ASN:OD1	2:B:760[A]:HDD:HMB2	1.95	0.66
1:C:324:GLU:OE1	5:C:2088:HOH:O	2.14	0.66
1:B:449[B]:HIS:HD2	5:B:3613:HOH:O	1.78	0.65
1:C:449[A]:HIS:HD2	5:C:3611:HOH:O	1.79	0.65
1:D:731:GLU:OE2	5:D:3028:HOH:O	2.15	0.65
1:A:244:SER:HA	1:A:546[B]:GLN:NE2	2.11	0.65
1:D:629:HIS:HD2	5:D:1554:HOH:O	1.78	0.65
1:B:274:CYS:HB3	2:B:760[A]:HDD:CBB	2.27	0.65
1:A:416[B]:THR:HG22	5:A:900:HOH:O	1.95	0.64
3:D:761[B]:HDE:CBC	3:D:761[B]:HDE:CMC	2.59	0.64
1:D:449[A]:HIS:HE1	5:D:1789:HOH:O	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533[A]:LYS:HE2	5:B:3100:HOH:O	1.96	0.64
3:B:761[B]:HDE:CMC	3:B:761[B]:HDE:HBCB	2.26	0.64
1:A:700:ASP:HB2	5:A:3594:HOH:O	1.97	0.63
3:D:761[B]:HDE:HBCB	4:D:754:H2S:S	2.39	0.63
3:C:761[B]:HDE:HMC	4:C:754:H2S:S	2.38	0.63
1:B:201:ASN:ND2	2:B:760[A]:HDD:HMB2	2.15	0.62
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.83	0.62
1:C:578:ASP:HB2	1:C:582:LEU:O	2.00	0.62
1:C:201:ASN:ND2	2:C:760[A]:HDD:HMB2	2.14	0.62
1:C:274:CYS:HB3	2:C:760[A]:HDD:CBB	2.30	0.62
3:A:761[B]:HDE:HMB	3:A:761[B]:HDE:CBB	2.30	0.61
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.83	0.61
1:B:449[B]:HIS:HE1	5:D:1789:HOH:O	1.84	0.61
1:D:267:ARG:HG3	5:D:1920:HOH:O	2.01	0.60
2:B:760[A]:HDD:HMB1	2:B:760[A]:HDD:HBB1	1.83	0.59
1:A:36:HIS:HE1	5:A:1872:HOH:O	1.86	0.59
1:A:274:CYS:CA	4:A:754:H2S:S	2.90	0.59
1:A:29:LEU:HB2	5:C:2405:HOH:O	2.03	0.59
1:A:751:ILE:O	1:A:751:ILE:CD1	2.48	0.58
1:A:201:ASN:ND2	2:A:760[A]:HDD:CMB	2.67	0.58
1:C:368:GLN:NE2	5:C:1787:HOH:O	2.23	0.58
1:D:201:ASN:ND2	2:D:760[A]:HDD:HMB2	2.18	0.58
1:A:125:ARG:HB3	3:A:761[B]:HDE:HBA	1.84	0.57
1:C:274:CYS:CB	2:C:760[A]:HDD:CBB	2.82	0.57
1:B:629:HIS:HD2	5:B:1053:HOH:O	1.87	0.57
1:B:37:ARG:HD3	5:B:2886:HOH:O	2.03	0.57
1:C:440:TYR:CD1	5:C:3454:HOH:O	2.32	0.57
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.08	0.57
1:D:597:ASP:OD2	5:D:2709:HOH:O	2.17	0.57
3:B:761[B]:HDE:HMC	4:B:754:H2S:S	2.44	0.57
1:C:199:VAL:HG12	3:C:761[B]:HDE:HHDA	1.85	0.56
1:D:449[A]:HIS:HD2	5:D:3615:HOH:O	1.88	0.56
1:C:629:HIS:HD2	5:C:1129:HOH:O	1.87	0.56
1:D:670:GLY:O	1:D:700:ASP:OD2	2.23	0.56
3:A:761[B]:HDE:CBC	3:A:761[B]:HDE:CMC	2.77	0.56
2:B:760[A]:HDD:CBC	2:B:760[A]:HDD:HMC1	2.35	0.56
1:A:610:GLU:CD	5:A:3555:HOH:O	2.43	0.56
1:D:244:SER:HA	1:D:546[B]:GLN:NE2	2.21	0.56
1:B:214:PHE:CD2	2:B:760[A]:HDD:HMC2	2.40	0.55
1:A:639:GLU:HG3	5:A:2414:HOH:O	2.06	0.55
1:A:583:LYS:O	1:A:584:LYS:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:760[A]:HDD:CBB	2:B:760[A]:HDD:HMB1	2.38	0.54
1:C:359:LEU:H	1:C:507:HIS:HD2	1.55	0.54
1:C:634:TYR:O	1:C:653:THR:HA	2.08	0.54
1:A:725:ASP:H	1:A:728:PHE:HB3	1.71	0.54
1:C:28:SER:HA	5:C:2891:HOH:O	2.08	0.54
1:A:36:HIS:CD2	1:A:36:HIS:H	2.26	0.54
1:B:724:ALA:O	1:B:725:ASP:O	2.25	0.54
3:D:761[B]:HDE:CBB	3:D:761[B]:HDE:CMB	2.74	0.54
1:B:73:LYS:CE	5:D:3517:HOH:O	2.51	0.53
1:B:411:ARG:HG2	3:B:761[B]:HDE:C3B	2.38	0.53
1:B:116:HIS:HB2	5:B:3039:HOH:O	2.08	0.53
1:B:583:LYS:H	1:B:583:LYS:HZ2	1.53	0.53
1:B:393:PRO:HD2	1:B:415:TYR:CG	2.43	0.53
1:A:29:LEU:HD23	5:C:3144:HOH:O	2.09	0.53
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.24	0.53
2:C:760[A]:HDD:HMC1	2:C:760[A]:HDD:HBC1	1.89	0.53
1:B:274:CYS:CB	2:B:760[A]:HDD:CBB	2.88	0.52
1:B:521:ARG:NH2	1:B:745:ILE:HG21	2.24	0.52
3:D:761[B]:HDE:HBBB	3:D:761[B]:HDE:CMB	2.34	0.52
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.93	0.52
1:B:73:LYS:CD	5:D:3517:HOH:O	2.57	0.52
2:B:760[A]:HDD:HMC1	2:B:760[A]:HDD:HBC1	1.92	0.52
1:A:610:GLU:OE2	5:A:3555:HOH:O	2.19	0.52
1:B:274:CYS:CB	2:B:760[A]:HDD:HBB1	2.39	0.52
2:C:760[A]:HDD:HMC1	2:C:760[A]:HDD:CBC	2.39	0.51
3:A:761[B]:HDE:HBCB	3:A:761[B]:HDE:CMC	2.20	0.51
1:D:278:ARG:HH12	1:D:487:GLU:CD	2.14	0.51
1:D:696:ALA:HB1	1:D:728:PHE:CZ	2.46	0.50
1:C:274:CYS:CA	4:C:754:H2S:S	2.96	0.50
1:B:583:LYS:O	1:B:584:LYS:HB3	2.12	0.50
2:A:760[A]:HDD:CAB	4:A:754:H2S:S	2.99	0.50
2:B:760[A]:HDD:CMB	2:B:760[A]:HDD:HBB1	2.42	0.50
1:B:359:LEU:H	1:B:507:HIS:HD2	1.58	0.50
1:B:157:ASN:C	1:B:157:ASN:HD22	2.16	0.49
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.28	0.49
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.28	0.49
1:B:583:LYS:H	1:B:583:LYS:HZ3	1.60	0.49
1:D:393:PRO:HD2	1:D:415:TYR:CG	2.48	0.49
1:A:273:GLY:C	1:A:274:CYS:SG	2.91	0.48
1:B:634:TYR:O	1:B:653:THR:HA	2.12	0.48
1:B:407:LEU:HG	3:B:761[B]:HDE:HABA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:ARG:HG3	5:B:776:HOH:O	2.13	0.48
1:B:521:ARG:HH22	1:B:745:ILE:CD1	2.24	0.48
1:D:274:CYS:CB	2:D:760[A]:HDD:CBB	2.91	0.48
3:B:761[B]:HDE:CBC	4:B:754:H2S:S	3.02	0.48
1:C:151:ASP:OD1	5:C:3101:HOH:O	2.20	0.48
1:C:725:ASP:O	5:C:2403:HOH:O	2.19	0.48
1:B:577:PRO:HG2	5:B:2668:HOH:O	2.13	0.48
1:B:211:ALA:CB	1:B:410:GLY:HA3	2.44	0.47
1:C:393:PRO:HD2	1:C:415:TYR:CG	2.50	0.47
1:D:603:VAL:HG11	1:D:666:ILE:HD12	1.97	0.47
1:B:144:LEU:HD11	1:B:370:VAL:HG13	1.96	0.46
1:D:556:GLN:NE2	5:D:2773:HOH:O	2.48	0.46
1:B:319:ARG:HD3	1:C:227:TRP:O	2.15	0.46
1:C:214:PHE:CD1	2:C:760[A]:HDD:CAC	2.99	0.46
1:C:273:GLY:C	1:C:274:CYS:SG	2.94	0.46
1:B:725:ASP:OD2	1:B:727:SER:N	2.48	0.46
1:C:52:PRO:HG2	1:C:55:LEU:HD12	1.97	0.46
1:A:351:PHE:HB2	1:A:358:LYS:HG3	1.97	0.46
1:D:128:HIS:CE1	1:D:169:VAL:HG22	2.51	0.46
3:C:761[B]:HDE:HBCB	4:C:754:H2S:S	2.54	0.46
1:B:83:ASN:HB3	1:D:429:HIS:CG	2.51	0.46
1:B:725:ASP:OD2	1:B:726:GLY:N	2.48	0.46
1:D:273:GLY:C	1:D:274:CYS:SG	2.95	0.46
1:B:696:ALA:HB1	1:B:728:PHE:CZ	2.51	0.45
1:D:214:PHE:CD1	2:D:760[A]:HDD:HAC	2.51	0.45
1:D:359:LEU:HD21	5:D:2971:HOH:O	2.16	0.45
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.47	0.45
1:C:440:TYR:HB3	5:C:3454:HOH:O	2.17	0.45
1:A:393:PRO:HD2	1:A:415:TYR:CD2	2.51	0.45
1:D:552:LEU:HD22	1:D:552:LEU:HA	1.85	0.45
1:A:448:MET:HG3	1:A:449[B]:HIS:CD2	2.51	0.45
1:B:157:ASN:HD22	1:B:158:LYS:N	2.15	0.45
3:C:761[B]:HDE:HBBA	3:C:761[B]:HDE:CMB	2.41	0.45
1:D:359:LEU:H	1:D:507:HIS:HD2	1.64	0.45
1:D:594:PRO:HA	5:D:2866:HOH:O	2.16	0.45
2:C:760[A]:HDD:HBC1	2:C:760[A]:HDD:CMC	2.47	0.44
1:C:274:CYS:CB	2:C:760[A]:HDD:HBB1	2.46	0.44
1:A:260:ARG:HD3	1:A:590:LEU:HD21	1.99	0.44
3:C:761[B]:HDE:HMAA	3:C:761[B]:HDE:HAAA	1.81	0.44
1:C:535:VAL:O	1:C:537:PRO:HD3	2.18	0.44
1:B:578:ASP:HB3	1:B:582:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ILE:HG22	1:B:183:ARG:N	2.33	0.44
1:B:38:PRO:HG2	1:B:51:ALA:HB2	2.00	0.44
1:D:128:HIS:HA	1:D:168:THR:O	2.18	0.44
3:D:761[B]:HDE:HBBA	3:D:761[B]:HDE:CMB	2.41	0.43
1:B:294:LYS:HB2	5:B:1089:HOH:O	2.17	0.43
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.33	0.43
1:B:451:MET:HE1	1:D:451:MET:HE2	1.99	0.43
1:C:748:ILE:O	1:C:751:ILE:HG22	2.18	0.43
1:B:651:ALA:O	5:B:1845:HOH:O	2.21	0.43
1:C:411:ARG:HG2	3:C:761[B]:HDE:C3B	2.49	0.43
1:C:686:MET:HB3	1:C:751:ILE:HD11	1.99	0.43
1:C:184:GLY:HA3	2:C:760[A]:HDD:HMA2	2.01	0.43
1:D:416[A]:THR:HG21	5:D:3576:HOH:O	2.01	0.43
1:A:128:HIS:HA	1:A:168:THR:O	2.18	0.43
1:A:61:ARG:HG2	1:A:61:ARG:HH11	1.83	0.43
1:C:359:LEU:C	1:C:359:LEU:HD12	2.39	0.43
1:D:449[A]:HIS:CE1	5:D:1789:HOH:O	2.64	0.43
1:A:578:ASP:OD1	1:A:583:LYS:NZ	2.50	0.42
1:A:128:HIS:CE1	1:A:169:VAL:HG22	2.54	0.42
1:A:393:PRO:HD2	1:A:415:TYR:CG	2.54	0.42
1:A:479:ARG:NH2	5:A:2607:HOH:O	2.43	0.42
1:B:603:VAL:HG22	1:B:664:ALA:HB3	2.01	0.42
1:B:697:LEU:O	1:B:720:GLU:HA	2.20	0.42
1:D:509:ARG:HD2	1:D:576:PRO:HD2	2.02	0.42
1:A:356:PRO:HG3	1:A:407:LEU:HB2	2.02	0.42
1:B:165:ARG:HD3	3:B:761[B]:HDE:O2D	2.20	0.42
1:C:704:PHE:O	1:C:707:THR:HG22	2.19	0.42
1:D:535:VAL:O	1:D:537:PRO:HD3	2.19	0.42
1:C:128:HIS:HA	1:C:168:THR:O	2.19	0.42
3:D:761[B]:HDE:CBC	4:D:754:H2S:S	3.06	0.42
1:B:235:ALA:HB1	1:B:533[A]:LYS:HD3	2.00	0.42
1:C:133:ALA:HA	1:C:164:VAL:O	2.20	0.42
1:A:392:HIS:HB2	1:A:415:TYR:HB3	1.94	0.41
1:D:448:MET:O	1:D:449[A]:HIS:HB2	2.20	0.41
1:C:296:LEU:HD23	1:C:296:LEU:HA	1.82	0.41
1:D:214:PHE:CD1	2:D:760[A]:HDD:CAC	3.03	0.41
1:A:443:PHE:CZ	1:A:470:PRO:HD2	2.55	0.41
1:B:274:CYS:CA	4:B:754:H2S:S	3.05	0.41
3:D:761[B]:HDE:HMAA	3:D:761[B]:HDE:HAAA	1.87	0.41
1:B:562:LEU:HA	1:C:637:MET:HB2	2.01	0.41
1:B:521:ARG:HH21	1:B:745:ILE:HG21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ASN:CG	3:A:761[B]:HDE:HAC	2.40	0.41
1:B:252:ASN:HD22	1:B:252:ASN:HA	1.78	0.41
1:C:359:LEU:H	1:C:507:HIS:CD2	2.35	0.41
1:B:344:GLU:CD	1:B:344:GLU:H	2.24	0.41
1:B:451:MET:HE2	1:D:451:MET:HE1	2.02	0.41
1:A:486:GLN:OE1	5:A:2605:HOH:O	2.22	0.41
1:A:700:ASP:HB2	5:A:2575:HOH:O	2.20	0.41
1:B:207:PHE:O	1:B:249:THR:HA	2.21	0.41
1:B:393:PRO:HD2	1:B:415:TYR:CD2	2.56	0.41
5:B:3376:HOH:O	1:D:28:SER:HB3	2.20	0.41
1:D:459:ASN:HD22	1:D:459:ASN:H	1.69	0.41
1:A:91:ASP:OD1	1:C:461:GLU:OE1	2.38	0.41
1:A:144:LEU:HD11	1:A:370:VAL:HG13	2.02	0.41
1:B:473:THR:O	1:D:89:ALA:HA	2.20	0.41
1:C:724:ALA:O	1:C:725:ASP:CB	2.69	0.40
1:D:461:GLU:HA	1:D:462:PRO:C	2.42	0.40
1:B:37:ARG:HA	1:B:38:PRO:HD3	1.90	0.40
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.52	0.40
1:D:579:VAL:O	1:D:582:LEU:HB2	2.22	0.40
1:B:726:GLY:O	5:B:2261:HOH:O	2.22	0.40
1:A:61:ARG:HD2	5:A:3208:HOH:O	2.21	0.40
1:A:693:LYS:HA	1:A:694:PRO:HD3	1.95	0.40
1:B:709:LYS:HA	1:B:709:LYS:HD3	1.99	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:3241:HOH:O	5:D:2457:HOH:O[2_646]	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%)	709 (97%)	19 (3%)	1 (0%)	51	36
1	B	729/753 (97%)	709 (97%)	18 (2%)	2 (0%)	41	27
1	C	727/753 (96%)	705 (97%)	20 (3%)	2 (0%)	41	27
1	D	732/753 (97%)	712 (97%)	19 (3%)	1 (0%)	51	36
All	All	2917/3012 (97%)	2835 (97%)	76 (3%)	6 (0%)	47	33

All (6) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	614/634 (97%)	595 (97%)	19 (3%)	40	25
1	B	614/634 (97%)	593 (97%)	21 (3%)	37	22
1	C	612/634 (96%)	582 (95%)	30 (5%)	25	11
1	D	617/634 (97%)	595 (96%)	22 (4%)	35	20
All	All	2457/2536 (97%)	2365 (96%)	92 (4%)	34	19

All (92) 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	73	LYS
1	A	185	PHE

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Mol	Chain	Res	Type
1	A	205	ILE
1	A	227	TRP
1	A	237	ASP
1	A	252	ASN
1	A	398	PRO
1	A	432	PRO
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	610	GLU
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	252	ASN
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	595	ASP
1	B	616	LEU
1	B	633	LEU
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

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Mol	Chain	Res	Type
1	C	237	ASP
1	C	252	ASN
1	C	274	CYS
1	C	283	GLU
1	C	285	LYS
1	C	377	ARG
1	C	440	TYR
1	C	459	ASN
1	C	488[A]	ARG
1	C	488[B]	ARG
1	C	521	ARG
1	C	552	LEU
1	C	571	LEU
1	C	606	LEU
1	C	616	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	48	GLN
1	D	185	PHE
1	D	191	THR
1	D	205	ILE
1	D	227	TRP
1	D	252	ASN
1	D	344	GLU
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

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Mol	Chain	Res	Type
1	D	747	LYS
1	D	749	ASP
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	486	GLN
1	A	515	GLN
1	A	556	GLN
1	B	157	ASN
1	B	252	ASN
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
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	$\#\|Z\| > 2$
3	HDE	D	761[B]	1,5	44,52,52	2.63	14 (31%)	41,89,89	2.68	19 (46%)
3	HDE	B	761[B]	1,5	44,52,52	2.63	14 (31%)	41,89,89	2.52	17 (41%)
2	HDD	B	760[A]	1,5	41,52,52	2.04	13 (31%)	31,89,89	2.32	7 (22%)
2	HDD	D	760[A]	1,5	41,52,52	2.47	14 (34%)	31,89,89	2.27	10 (32%)
2	HDD	A	760[A]	1,5	41,52,52	2.17	11 (26%)	31,89,89	2.16	9 (29%)
3	HDE	C	761[B]	1,5	44,52,52	2.42	13 (29%)	41,89,89	2.57	18 (43%)
2	HDD	C	760[A]	1,5	41,52,52	2.19	13 (31%)	31,89,89	2.44	15 (48%)
3	HDE	A	761[B]	1,5	44,52,52	2.56	15 (34%)	41,89,89	2.58	19 (46%)

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

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

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

All (107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	761[B]	HDE	CHC-C4B	-8.46	1.42	1.51
3	B	761[B]	HDE	CHC-C4B	-7.99	1.43	1.51
2	D	760[A]	HDD	FE-ND	7.57	2.25	1.95
2	C	760[A]	HDD	FE-ND	7.32	2.24	1.95
3	C	761[B]	HDE	C4C-C3C	7.25	1.48	1.38
3	B	761[B]	HDE	C4C-C3C	7.21	1.48	1.38
3	A	761[B]	HDE	C4C-C3C	7.08	1.47	1.38
3	D	761[B]	HDE	C4C-C3C	6.50	1.47	1.38
3	A	761[B]	HDE	CHC-C1C	-6.18	1.44	1.51
2	A	760[A]	HDD	O1D-C3D	-5.99	1.37	1.46
3	C	761[B]	HDE	CHC-C4B	-5.86	1.45	1.51
3	B	761[B]	HDE	CHD-C4C	-5.37	1.45	1.51
3	C	761[B]	HDE	O1A-CGA	5.30	1.44	1.35
3	A	761[B]	HDE	O1A-CGA	5.30	1.44	1.35
3	D	761[B]	HDE	CHD-C4C	-5.25	1.45	1.51
3	D	761[B]	HDE	CHD-C1D	-5.11	1.45	1.51
2	B	760[A]	HDD	C3C-C2C	-5.08	1.33	1.40
3	A	761[B]	HDE	CHD-C1D	-5.06	1.45	1.51
3	D	761[B]	HDE	CHC-C1C	-5.02	1.46	1.51
3	A	761[B]	HDE	CHC-C4B	-4.94	1.46	1.51
2	D	760[A]	HDD	C3B-C2B	-4.89	1.33	1.40
2	D	760[A]	HDD	O1D-C3D	-4.87	1.38	1.46
2	A	760[A]	HDD	C3B-C2B	-4.85	1.33	1.40
3	B	761[B]	HDE	CHD-C1D	-4.71	1.46	1.51
3	B	761[B]	HDE	O1A-CGA	4.59	1.43	1.35
2	A	760[A]	HDD	C3C-C2C	-4.52	1.34	1.40
2	D	760[A]	HDD	C3C-C2C	-4.49	1.34	1.40
3	C	761[B]	HDE	CHC-C1C	-4.47	1.46	1.51
2	C	760[A]	HDD	C3C-C2C	-4.20	1.34	1.40
2	A	760[A]	HDD	FE-ND	4.19	2.12	1.95
3	C	761[B]	HDE	CHD-C1D	-4.19	1.46	1.51
2	B	760[A]	HDD	FE-ND	4.08	2.11	1.95
3	A	761[B]	HDE	CHD-C4C	-4.04	1.47	1.51
3	D	761[B]	HDE	O1A-CGA	4.04	1.42	1.35
2	B	760[A]	HDD	O1D-C3D	-3.96	1.40	1.46
3	B	761[B]	HDE	C1A-NA	3.95	1.44	1.37
2	C	760[A]	HDD	C3B-C2B	-3.94	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	761[B]	HDE	CHC-C1C	-3.91	1.47	1.51
2	D	760[A]	HDD	CHD-C1D	3.91	1.42	1.36
3	C	761[B]	HDE	CHD-C4C	-3.89	1.47	1.51
2	B	760[A]	HDD	C3B-C2B	-3.86	1.35	1.40
3	D	761[B]	HDE	C4A-NA	3.82	1.44	1.37
3	A	761[B]	HDE	C4A-NA	3.79	1.44	1.37
3	B	761[B]	HDE	C3B-C2B	3.74	1.48	1.37
3	C	761[B]	HDE	C3B-C2B	3.68	1.48	1.37
3	A	761[B]	HDE	C3B-C2B	3.67	1.48	1.37
3	D	761[B]	HDE	C3B-C2B	3.62	1.48	1.37
2	A	760[A]	HDD	C3C-CAC	3.61	1.55	1.47
2	D	760[A]	HDD	C3B-CAB	3.59	1.55	1.47
3	A	761[B]	HDE	C3C-C2C	3.57	1.48	1.37
2	C	760[A]	HDD	CMD-C2D	3.54	1.58	1.53
2	C	760[A]	HDD	O1D-C3D	-3.48	1.41	1.46
2	D	760[A]	HDD	C3C-CAC	3.47	1.55	1.47
2	C	760[A]	HDD	CHA-C4D	3.46	1.41	1.36
3	A	761[B]	HDE	C3D-C2D	3.40	1.47	1.37
3	D	761[B]	HDE	C1A-NA	3.39	1.43	1.37
2	D	760[A]	HDD	CHA-C4D	3.36	1.41	1.36
3	C	761[B]	HDE	C3D-C2D	3.34	1.47	1.37
3	D	761[B]	HDE	C3C-C2C	3.32	1.47	1.37
3	C	761[B]	HDE	C3C-C2C	3.28	1.47	1.37
2	D	760[A]	HDD	CMD-C2D	3.28	1.57	1.53
3	C	761[B]	HDE	C1A-NA	3.27	1.43	1.37
2	C	760[A]	HDD	CHD-C1D	3.21	1.41	1.36
2	C	760[A]	HDD	C3B-CAB	3.17	1.54	1.47
3	D	761[B]	HDE	C3D-C2D	3.10	1.46	1.37
3	A	761[B]	HDE	C1C-C2C	3.06	1.42	1.38
3	B	761[B]	HDE	C3C-C2C	3.03	1.46	1.37
2	B	760[A]	HDD	C3B-CAB	2.97	1.53	1.47
3	A	761[B]	HDE	C1A-NA	2.96	1.42	1.37
2	A	760[A]	HDD	C3B-CAB	2.95	1.53	1.47
2	A	760[A]	HDD	CMC-C2C	2.92	1.57	1.51
3	B	761[B]	HDE	C4A-NA	2.90	1.42	1.37
3	B	761[B]	HDE	C4D-CHA	2.89	1.49	1.41
2	B	760[A]	HDD	CMD-C2D	2.89	1.57	1.53
2	B	760[A]	HDD	C3C-CAC	2.75	1.53	1.47
2	B	760[A]	HDD	C4D-ND	2.72	1.42	1.37
3	C	761[B]	HDE	C4A-NA	2.71	1.42	1.37
2	D	760[A]	HDD	OND-C2D	2.66	1.47	1.42
2	A	760[A]	HDD	CHD-C1D	2.66	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	761[B]	HDE	C3D-C2D	2.60	1.45	1.37
2	C	760[A]	HDD	C1A-NA	2.59	1.41	1.36
3	A	761[B]	HDE	C1B-NB	2.56	1.41	1.36
2	D	760[A]	HDD	CAA-C2A	2.48	1.55	1.52
3	B	761[B]	HDE	CHB-C4A	-2.45	1.32	1.36
3	D	761[B]	HDE	C4D-CHA	2.43	1.47	1.41
3	C	761[B]	HDE	C4D-CHA	2.41	1.47	1.41
3	A	761[B]	HDE	C1B-CHB	2.40	1.47	1.41
3	C	761[B]	HDE	C1B-CHB	2.28	1.47	1.41
3	A	761[B]	HDE	C4D-CHA	2.20	1.47	1.41
3	B	761[B]	HDE	O1A-C2A	-2.20	1.43	1.46
2	B	760[A]	HDD	CMA-C3A	2.19	1.56	1.51
2	B	760[A]	HDD	CAA-C2A	2.17	1.55	1.52
2	C	760[A]	HDD	C3C-CAC	2.15	1.52	1.47
2	C	760[A]	HDD	CMC-C2C	2.15	1.56	1.51
3	D	761[B]	HDE	C1B-NB	2.14	1.40	1.36
2	A	760[A]	HDD	CAA-C2A	2.13	1.55	1.52
2	B	760[A]	HDD	CHA-C4D	2.13	1.39	1.36
2	D	760[A]	HDD	O2D-CGD	2.12	1.28	1.22
2	B	760[A]	HDD	C1A-NA	2.10	1.40	1.36
2	A	760[A]	HDD	OND-C2D	2.09	1.46	1.42
2	B	760[A]	HDD	CHD-C1D	2.09	1.39	1.36
2	C	760[A]	HDD	C1C-NC	2.07	1.40	1.36
2	D	760[A]	HDD	O1D-CGD	-2.07	1.32	1.35
2	A	760[A]	HDD	O2D-CGD	2.04	1.28	1.22
3	D	761[B]	HDE	C1B-CHB	2.03	1.46	1.41
2	C	760[A]	HDD	CAA-C2A	2.02	1.55	1.52
2	D	760[A]	HDD	C1A-NA	2.01	1.40	1.36

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	760[A]	HDD	O1D-CGD-CBD	-7.92	102.20	110.19
2	B	760[A]	HDD	O1D-CGD-O2D	7.21	127.23	120.80
2	C	760[A]	HDD	O1D-CGD-O2D	6.68	126.76	120.80
2	D	760[A]	HDD	O1D-CGD-O2D	5.99	126.15	120.80
3	A	761[B]	HDE	CHD-C1D-C2D	-5.98	119.53	129.53
2	D	760[A]	HDD	O1D-CGD-CBD	-5.79	104.35	110.19
3	A	761[B]	HDE	CHC-C4B-C3B	-5.71	122.79	129.68
3	A	761[B]	HDE	CHD-C4C-C3C	-5.60	122.92	129.68
2	B	760[A]	HDD	O1D-CGD-CBD	-5.29	104.85	110.19
3	B	761[B]	HDE	CHC-C4B-C3B	-5.29	123.29	129.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	761[B]	HDE	CHD-C1D-C2D	-5.25	120.75	129.53
3	B	761[B]	HDE	CHD-C1D-C2D	-5.19	120.86	129.53
3	D	761[B]	HDE	CBC-CAC-C3C	-5.16	99.12	112.27
3	C	761[B]	HDE	C1B-CHB-C4A	-5.07	120.07	130.12
3	C	761[B]	HDE	CMA-C3A-C4A	-4.99	103.76	112.63
3	D	761[B]	HDE	CHC-C4B-C3B	-4.85	123.82	129.68
3	D	761[B]	HDE	CAD-CBD-CGD	-4.78	100.36	113.76
3	B	761[B]	HDE	CBC-CAC-C3C	-4.65	100.42	112.27
3	D	761[B]	HDE	C1B-CHB-C4A	-4.58	121.04	130.12
3	D	761[B]	HDE	C4C-CHD-C1D	4.49	123.82	112.87
3	C	761[B]	HDE	CBC-CAC-C3C	-4.47	100.88	112.27
2	C	760[A]	HDD	OND-C2D-CMD	-4.46	101.39	109.59
3	B	761[B]	HDE	C4C-CHD-C1D	4.45	123.73	112.87
3	D	761[B]	HDE	CHD-C1D-C2D	-4.41	122.16	129.53
3	C	761[B]	HDE	CHC-C1C-C2C	-4.36	122.24	129.53
3	D	761[B]	HDE	CHC-C1C-C2C	-4.30	122.33	129.53
3	A	761[B]	HDE	CAD-CBD-CGD	-4.28	101.76	113.76
3	B	761[B]	HDE	CHC-C1C-C2C	-4.17	122.55	129.53
3	B	761[B]	HDE	C1C-C2C-C3C	-4.14	101.40	105.81
3	B	761[B]	HDE	C1B-CHB-C4A	-4.08	122.03	130.12
3	C	761[B]	HDE	CHC-C4B-C3B	-4.06	124.78	129.68
2	D	760[A]	HDD	C2B-C3B-C4B	3.99	109.69	106.90
3	A	761[B]	HDE	CHC-C1C-C2C	-3.91	122.98	129.53
3	D	761[B]	HDE	C4D-CHA-C1A	-3.80	122.60	130.12
3	C	761[B]	HDE	C4C-CHD-C1D	3.78	122.09	112.87
3	B	761[B]	HDE	C1B-C2B-C3B	-3.77	104.38	107.00
3	B	761[B]	HDE	C4D-CHA-C1A	-3.75	122.69	130.12
2	C	760[A]	HDD	O1D-CGD-CBD	-3.75	106.41	110.19
2	A	760[A]	HDD	CAD-CBD-CGD	-3.68	98.87	104.56
3	D	761[B]	HDE	C1C-C2C-C3C	-3.66	101.91	105.81
3	C	761[B]	HDE	C4D-CHA-C1A	-3.66	122.87	130.12
3	C	761[B]	HDE	C1C-C2C-C3C	-3.55	102.03	105.81
3	A	761[B]	HDE	C1B-CHB-C4A	-3.50	123.19	130.12
3	A	761[B]	HDE	C1C-C2C-C3C	-3.44	102.15	105.81
2	B	760[A]	HDD	CMB-C2B-C3B	3.43	131.10	124.68
3	A	761[B]	HDE	C4C-CHD-C1D	3.43	121.23	112.87
2	B	760[A]	HDD	C1A-CHA-C4D	-3.42	123.34	130.12
3	D	761[B]	HDE	CHD-C4C-C3C	-3.39	125.58	129.68
3	C	761[B]	HDE	CHD-C4C-C3C	-3.39	125.59	129.68
2	B	760[A]	HDD	C2B-C3B-C4B	3.38	109.26	106.90
2	B	760[A]	HDD	CAA-CBA-CGA	-3.37	104.31	113.76
2	C	760[A]	HDD	CMA-C3A-C4A	-3.29	123.40	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	761[B]	HDE	C3A-C4A-CHB	-3.27	118.87	124.28
3	D	761[B]	HDE	CMC-C2C-C3C	3.23	131.03	124.94
2	D	760[A]	HDD	CAA-CBA-CGA	-3.23	104.72	113.76
3	D	761[B]	HDE	CBB-CAB-C3B	-3.19	104.13	112.27
3	D	761[B]	HDE	C1B-C2B-C3B	-3.19	104.78	107.00
3	B	761[B]	HDE	CAD-CBD-CGD	-3.18	104.83	113.76
3	A	761[B]	HDE	C4B-CHC-C1C	3.17	120.61	112.87
2	C	760[A]	HDD	C2B-C3B-C4B	3.16	109.11	106.90
3	B	761[B]	HDE	C3A-C4A-CHB	-3.10	119.16	124.28
3	D	761[B]	HDE	CMA-C3A-C4A	-3.09	107.13	112.63
3	A	761[B]	HDE	CAB-C3B-C4B	-3.04	123.53	127.19
3	B	761[B]	HDE	CHD-C4C-C3C	-3.04	126.00	129.68
2	D	760[A]	HDD	OND-C2D-CMD	-3.04	104.00	109.59
2	C	760[A]	HDD	CMC-C2C-C1C	-3.03	123.81	128.46
2	A	760[A]	HDD	CAA-CBA-CGA	-2.99	105.39	113.76
2	B	760[A]	HDD	OND-C2D-CMD	-2.98	104.11	109.59
3	A	761[B]	HDE	C1B-C2B-C3B	-2.95	104.94	107.00
3	C	761[B]	HDE	CMC-C2C-C3C	2.92	130.45	124.94
2	D	760[A]	HDD	C4A-C3A-C2A	2.90	109.02	107.00
2	D	760[A]	HDD	C2D-C1D-CHD	2.88	129.03	124.28
2	A	760[A]	HDD	CMC-C2C-C1C	-2.88	124.04	128.46
3	C	761[B]	HDE	O1A-CGA-O2A	2.83	123.33	120.80
3	A	761[B]	HDE	CMB-C2B-C3B	2.72	130.07	124.94
3	A	761[B]	HDE	C4D-CHA-C1A	-2.71	124.74	130.12
2	C	760[A]	HDD	C3C-C4C-NC	-2.70	105.72	109.21
3	C	761[B]	HDE	CMD-C2D-C3D	2.69	130.02	124.94
3	B	761[B]	HDE	CMB-C2B-C3B	2.68	130.00	124.94
3	D	761[B]	HDE	C4B-CHC-C1C	2.68	119.40	112.87
3	C	761[B]	HDE	C3A-C4A-CHB	-2.67	119.87	124.28
2	C	760[A]	HDD	OND-C2D-C1D	-2.67	106.50	111.92
3	D	761[B]	HDE	O1A-CGA-O2A	2.67	123.18	120.80
3	D	761[B]	HDE	CMB-C2B-C3B	2.67	129.97	124.94
3	A	761[B]	HDE	O1A-CGA-O2A	2.66	123.17	120.80
3	C	761[B]	HDE	C4B-CHC-C1C	2.61	119.24	112.87
2	C	760[A]	HDD	CAA-CBA-CGA	-2.60	106.48	113.76
2	D	760[A]	HDD	C3C-C4C-NC	-2.58	105.87	109.21
3	B	761[B]	HDE	C4B-CHC-C1C	2.58	119.16	112.87
2	C	760[A]	HDD	C3B-C4B-NB	-2.56	106.11	110.94
3	C	761[B]	HDE	CMB-C2B-C1B	-2.56	124.53	128.46
3	B	761[B]	HDE	C4C-C3C-C2C	2.56	109.74	105.93
2	C	760[A]	HDD	CMD-C2D-C1D	2.54	117.14	112.63
2	C	760[A]	HDD	C4C-CHD-C1D	-2.48	125.21	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	761[B]	HDE	C1D-C2D-C3D	-2.48	103.17	105.81
3	C	761[B]	HDE	CAD-CBD-CGD	-2.44	106.92	113.76
2	C	760[A]	HDD	C4A-C3A-C2A	2.38	108.65	107.00
2	A	760[A]	HDD	C4A-C3A-C2A	2.36	108.64	107.00
3	A	761[B]	HDE	ONA-C3A-CMA	-2.36	105.24	109.59
3	B	761[B]	HDE	O1A-CGA-O2A	2.36	122.90	120.80
3	C	761[B]	HDE	CMB-C2B-C3B	2.35	129.36	124.94
3	A	761[B]	HDE	CMB-C2B-C1B	-2.27	124.97	128.46
3	A	761[B]	HDE	CMD-C2D-C3D	2.25	129.19	124.94
2	D	760[A]	HDD	CMA-C3A-C4A	-2.20	125.08	128.46
2	A	760[A]	HDD	C2B-C3B-C4B	2.17	108.42	106.90
2	A	760[A]	HDD	CMD-C2D-C1D	-2.15	108.81	112.63
2	D	760[A]	HDD	CMC-C2C-C1C	-2.14	125.17	128.46
3	B	761[B]	HDE	C1D-C2D-C3D	-2.13	103.54	105.81
3	D	761[B]	HDE	CMB-C2B-C1B	-2.12	125.21	128.46
2	A	760[A]	HDD	C3B-C4B-NB	-2.10	106.98	110.94
2	C	760[A]	HDD	C2D-C1D-CHD	2.08	127.72	124.28
2	A	760[A]	HDD	C4C-CHD-C1D	-2.02	126.11	130.12
2	C	760[A]	HDD	CMC-C2C-C3C	2.02	128.45	124.68
3	A	761[B]	HDE	CBC-CAC-C3C	-2.01	107.15	112.27

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
3	D	761[B]	HDE	CAD-CBD-CGD-O2D

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

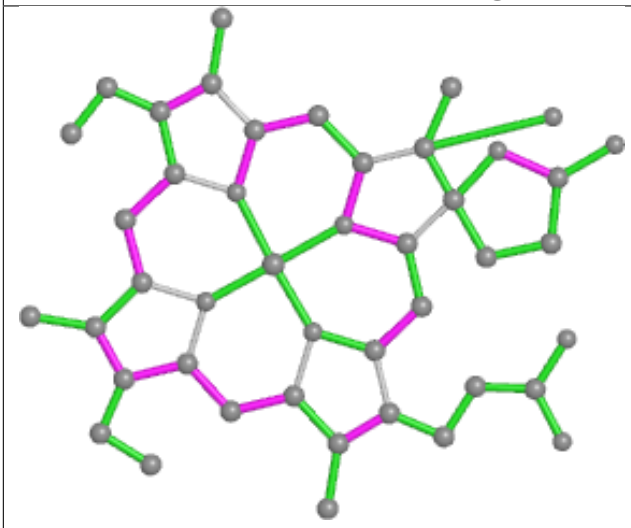
There are no ring outliers.

8 monomers are involved in 100 short contacts:

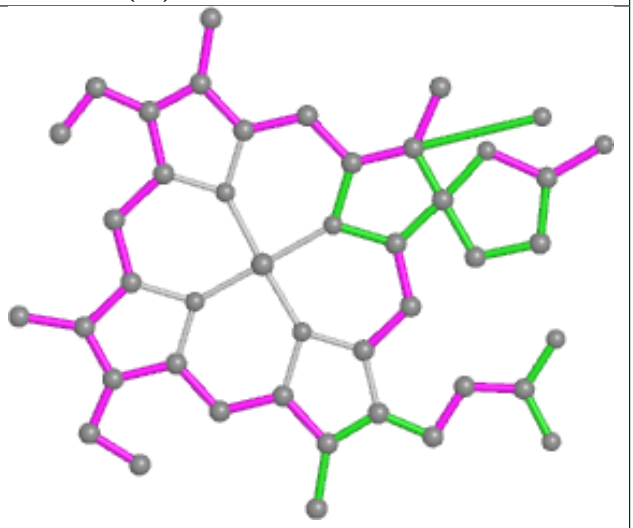
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	761[B]	HDE	14	0
3	B	761[B]	HDE	13	0
2	B	760[A]	HDD	18	0
2	D	760[A]	HDD	10	0
2	A	760[A]	HDD	9	0
3	C	761[B]	HDE	13	0
2	C	760[A]	HDD	15	0
3	A	761[B]	HDE	8	0

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.

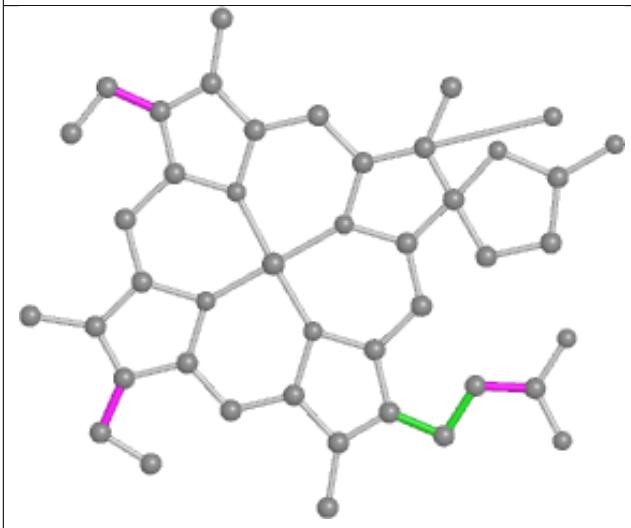
Ligand HDE D 761 (B)



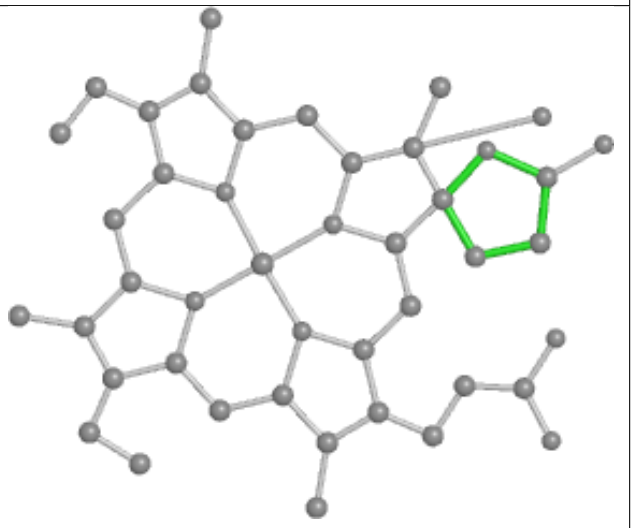
Bond lengths



Bond angles

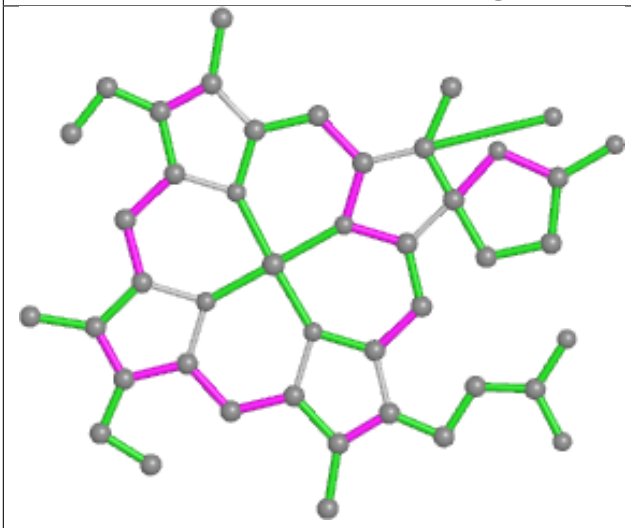


Torsions

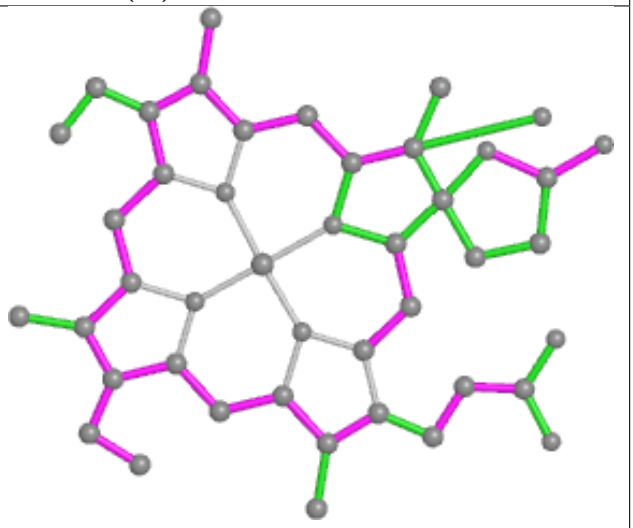


Rings

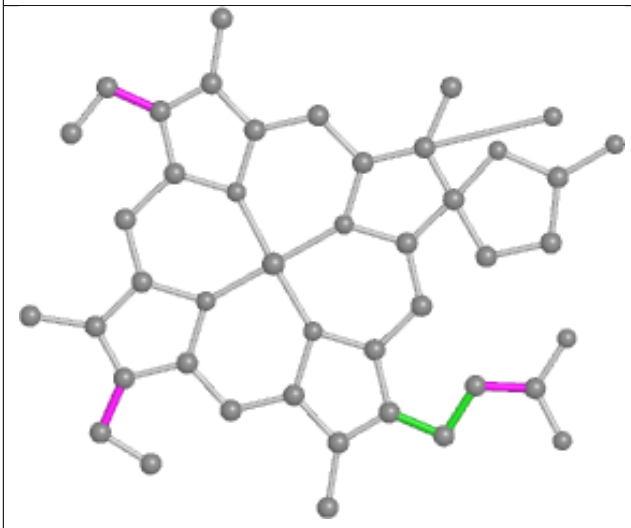
Ligand HDE B 761 (B)



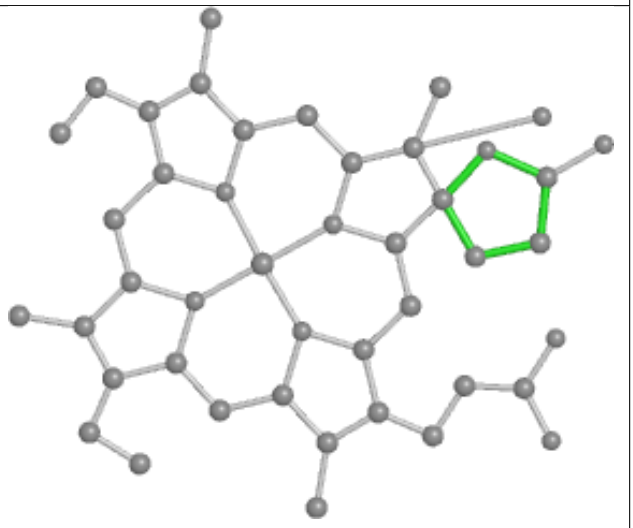
Bond lengths



Bond angles

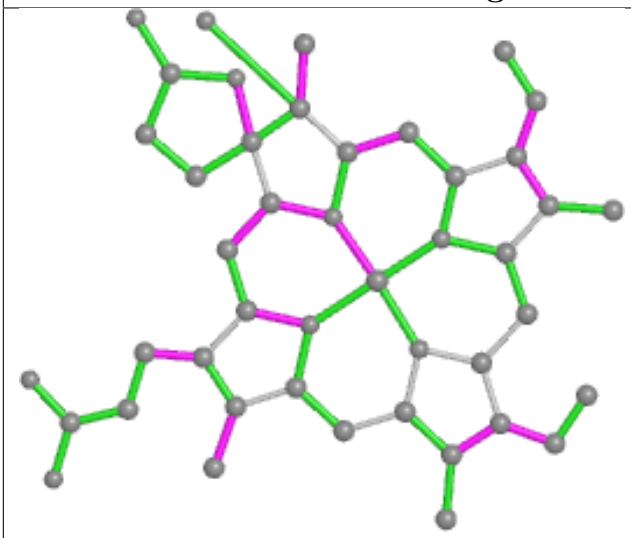


Torsions

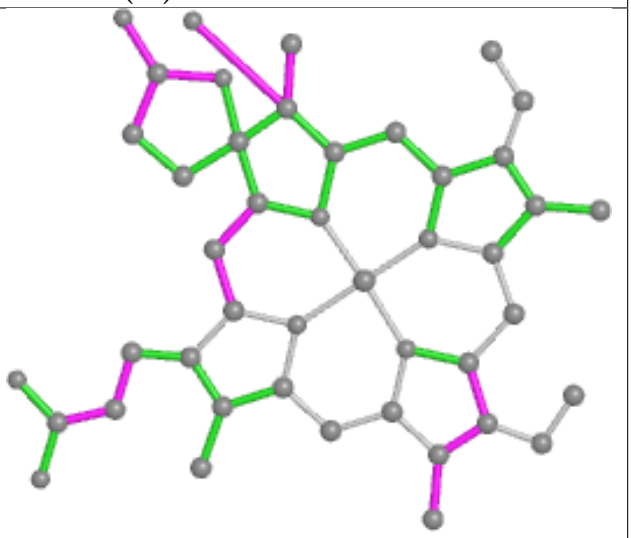


Rings

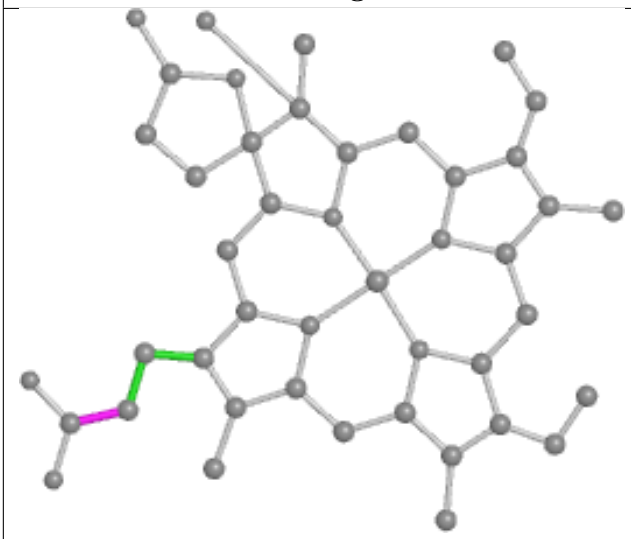
Ligand HDD B 760 (A)



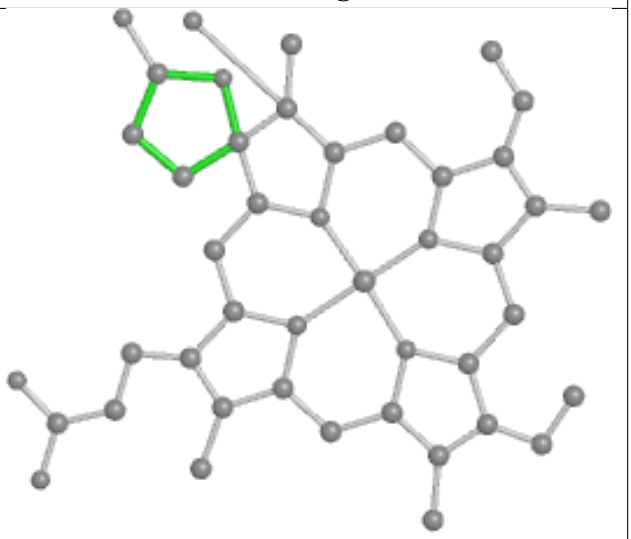
Bond lengths



Bond angles

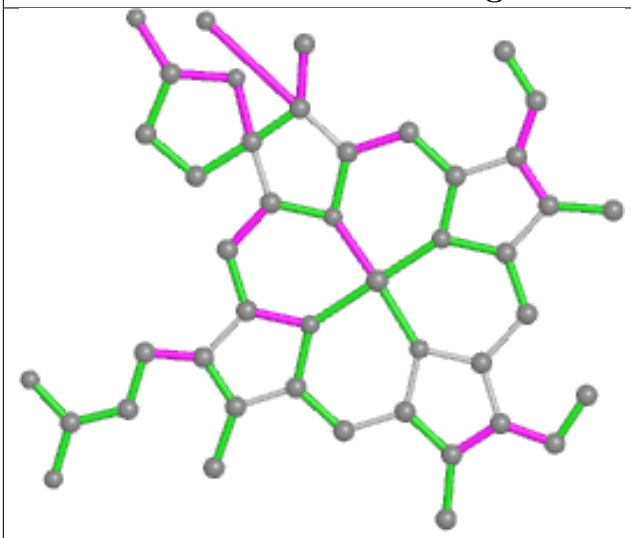


Torsions

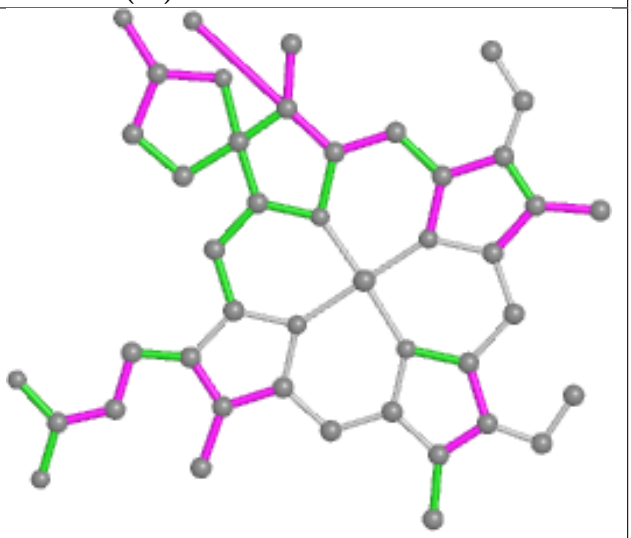


Rings

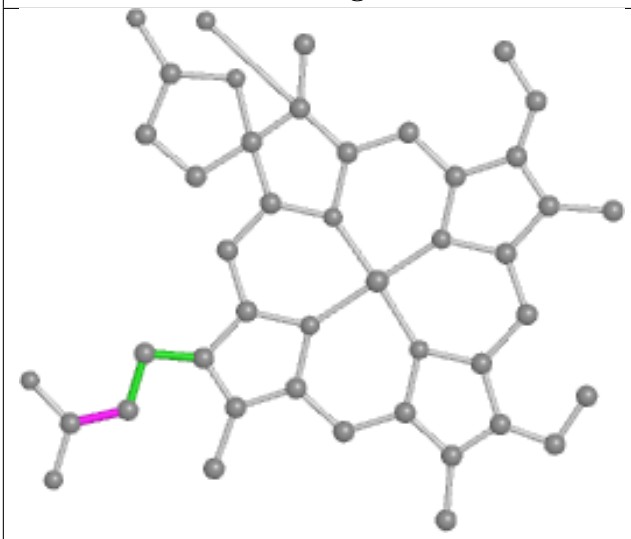
Ligand HDD D 760 (A)



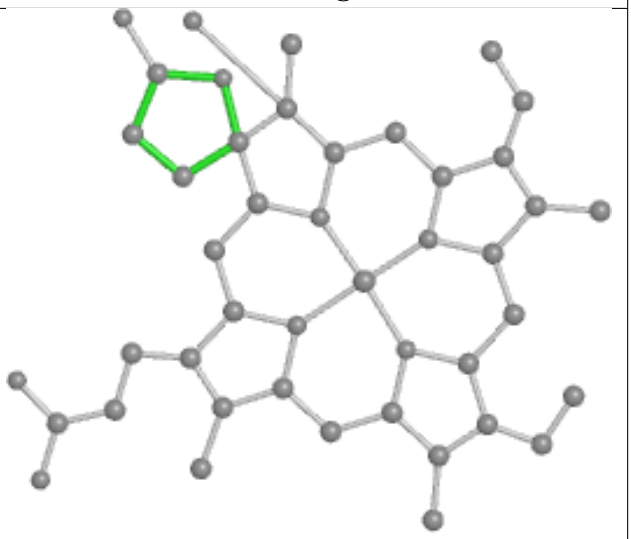
Bond lengths



Bond angles

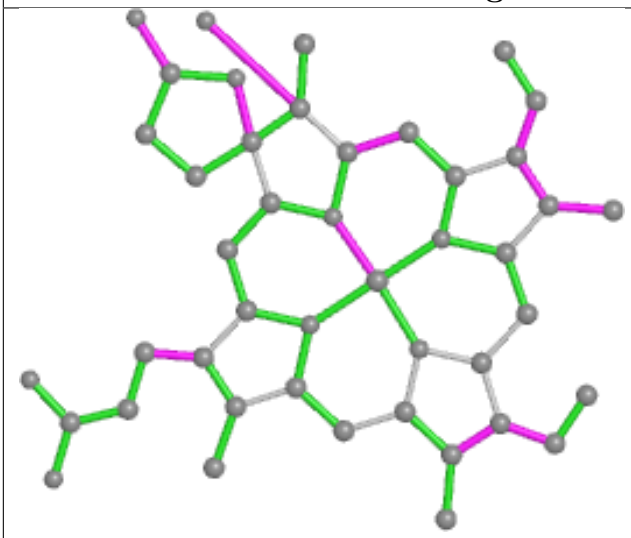


Torsions

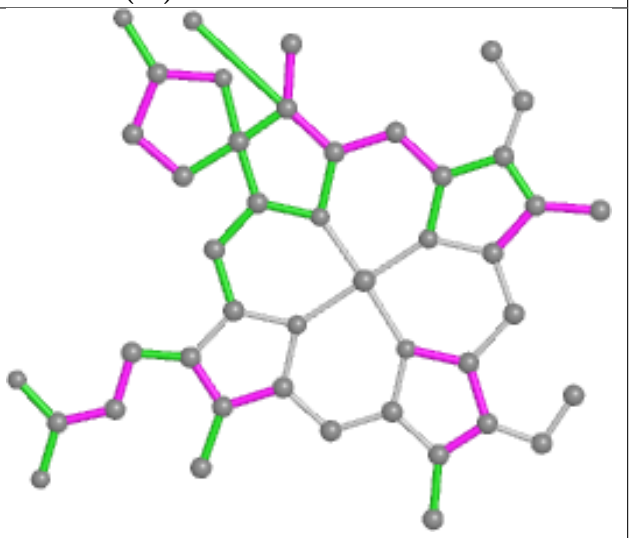


Rings

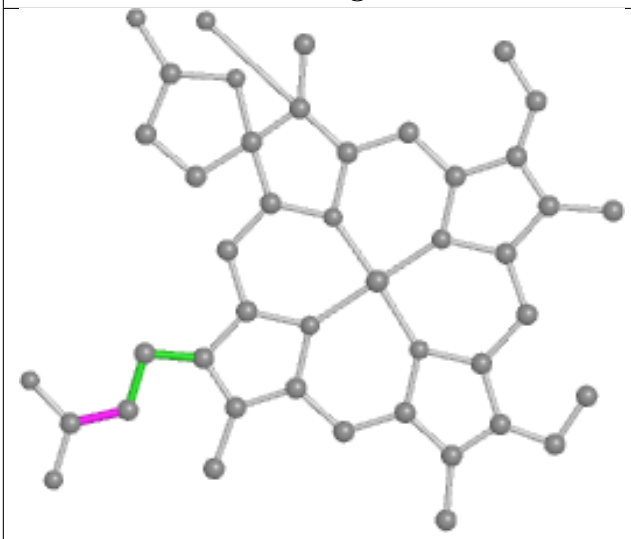
Ligand HDD A 760 (A)



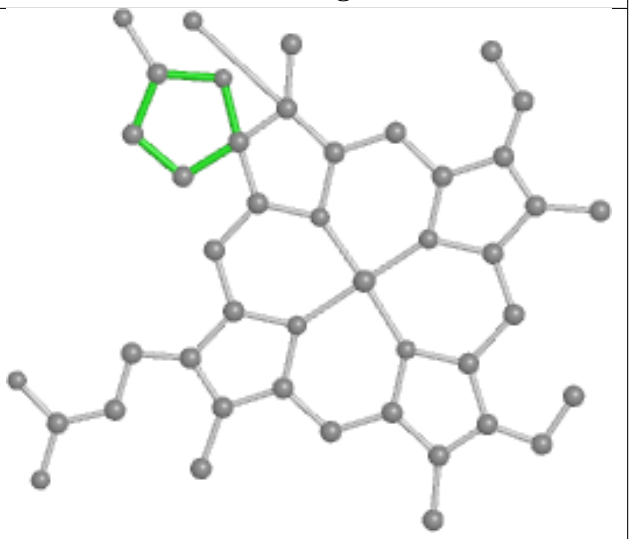
Bond lengths



Bond angles

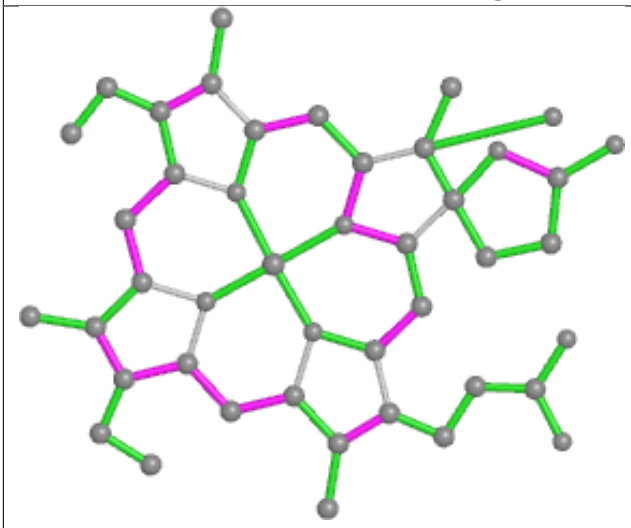


Torsions

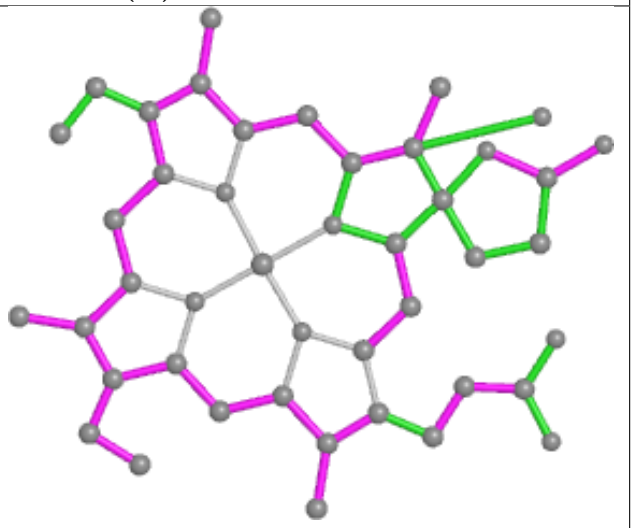


Rings

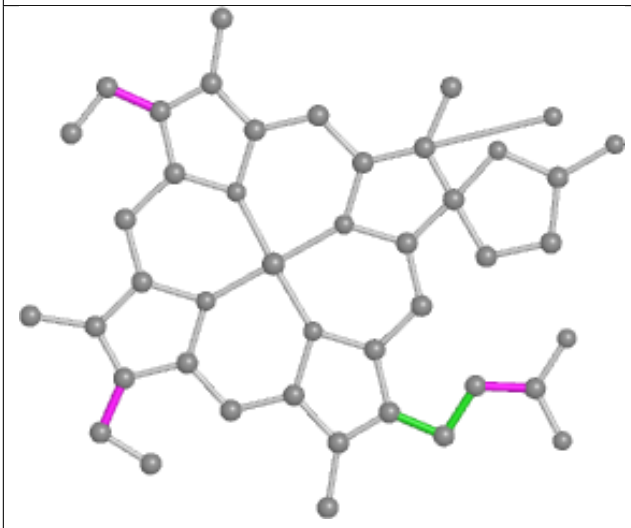
Ligand HDE C 761 (B)



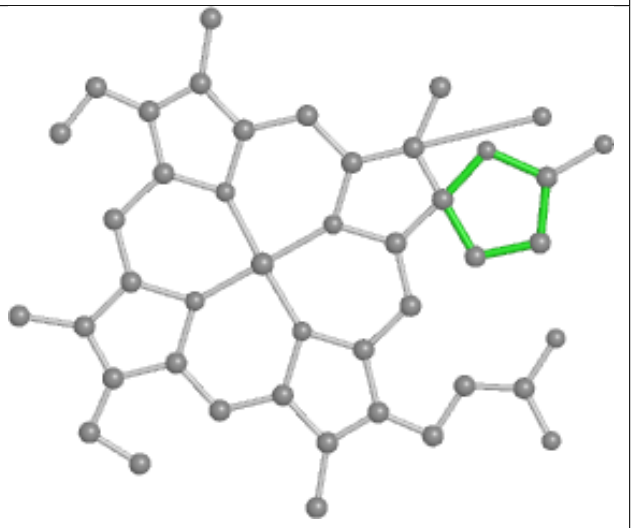
Bond lengths



Bond angles

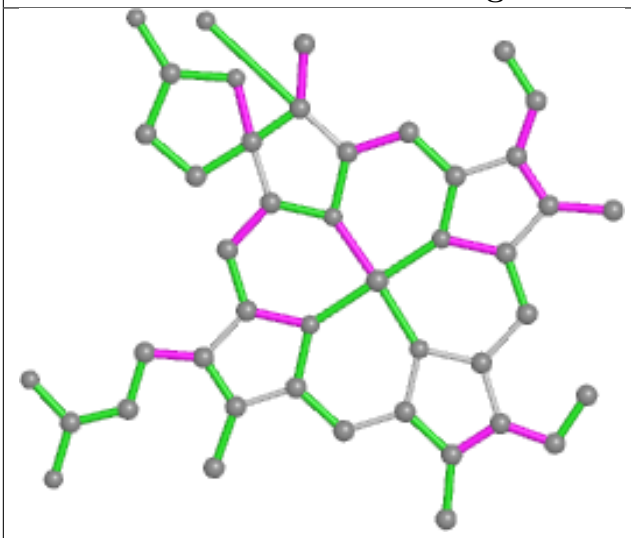


Torsions

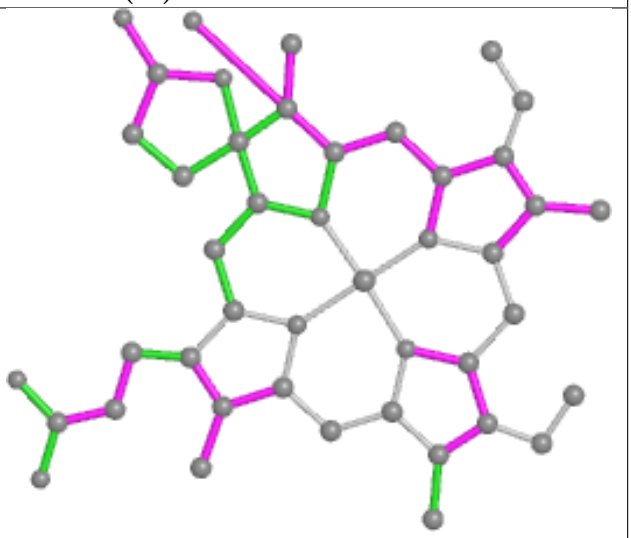


Rings

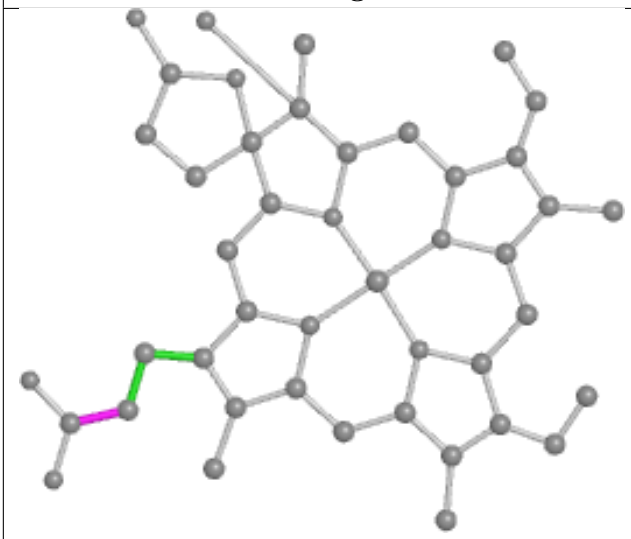
Ligand HDD C 760 (A)



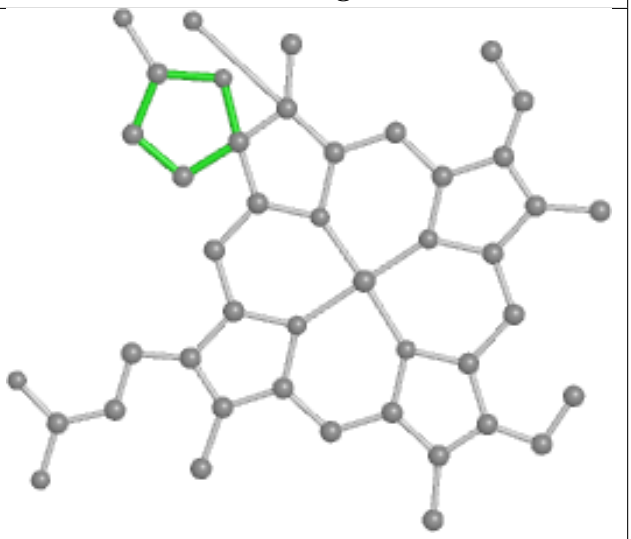
Bond lengths



Bond angles

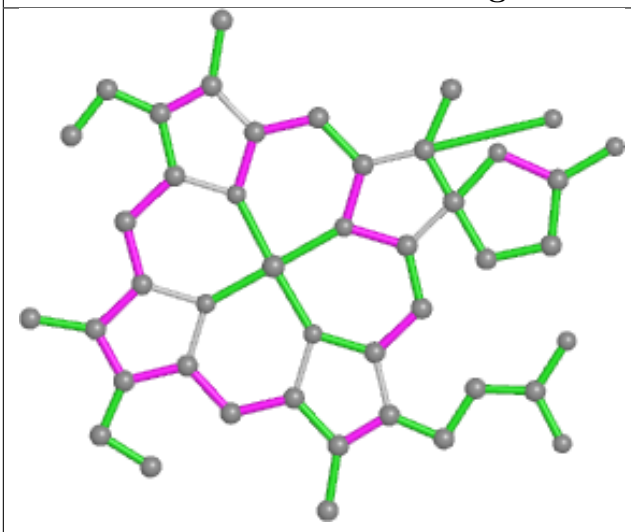


Torsions

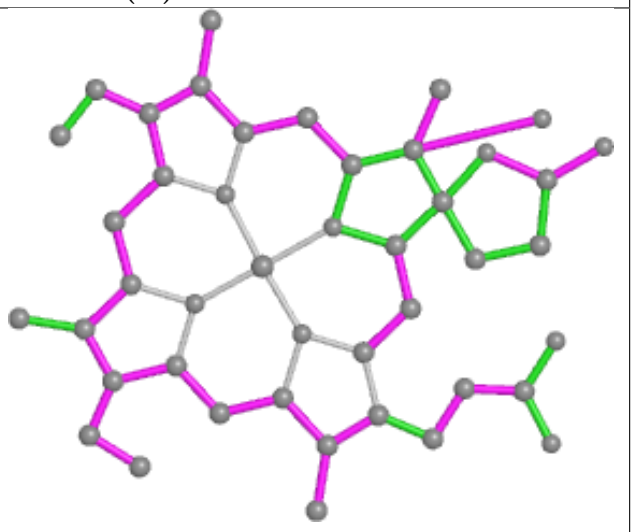


Rings

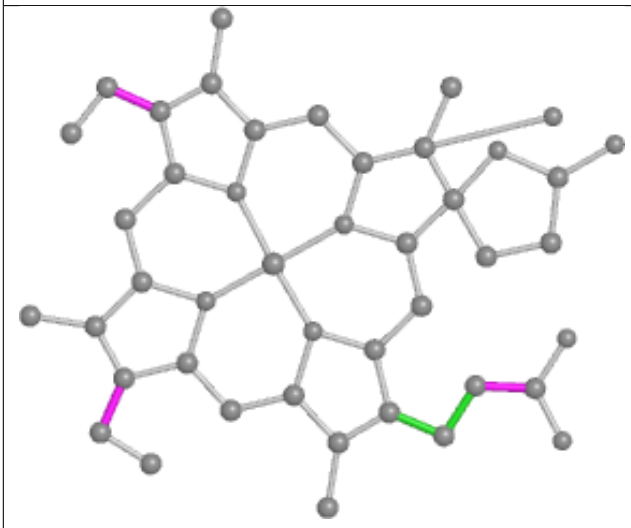
Ligand HDE A 761 (B)



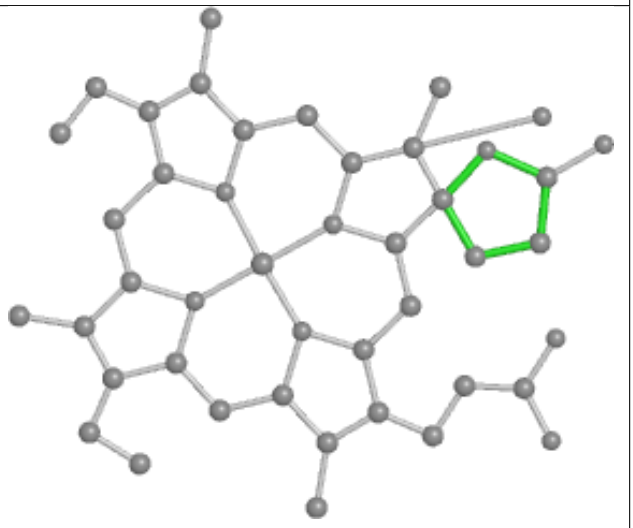
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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, 9, 26, 43	2 (0%)
1	B	726/753 (96%)	-0.46	15 (2%) 63 59	4, 11, 32, 47	2 (0%)
1	C	726/753 (96%)	-0.50	9 (1%) 79 76	4, 11, 31, 46	2 (0%)
1	D	726/753 (96%)	-0.62	5 (0%) 87 86	3, 9, 27, 43	1 (0%)
All	All	2904/3012 (96%)	-0.55	32 (1%) 80 78	3, 10, 30, 47	7 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	726	GLY	5.1
1	B	32	GLU	3.5
1	D	28	SER	3.5
1	B	28	SER	3.5
1	B	713	GLN	3.4
1	B	673	ALA	3.1
1	D	749	ASP	3.1
1	A	713	GLN	3.0
1	A	28	SER	2.9
1	C	726	GLY	2.9
1	C	750	LYS	2.8
1	B	727	SER	2.7
1	A	32	GLU	2.7
1	C	712	ASP	2.7
1	B	583	LYS	2.6
1	C	594	PRO	2.5
1	B	647	VAL	2.4
1	C	28	SER	2.4
1	D	750	LYS	2.4
1	B	568	ASP	2.3
1	D	713	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	645	GLY	2.3
1	C	642	ALA	2.3
1	B	677	ASP	2.3
1	D	751	ILE	2.2
1	B	712	ASP	2.2
1	B	725	ASP	2.2
1	C	645	GLY	2.2
1	C	677	ASP	2.2
1	C	711	ALA	2.1
1	B	750	LYS	2.1
1	B	711	ALA	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)

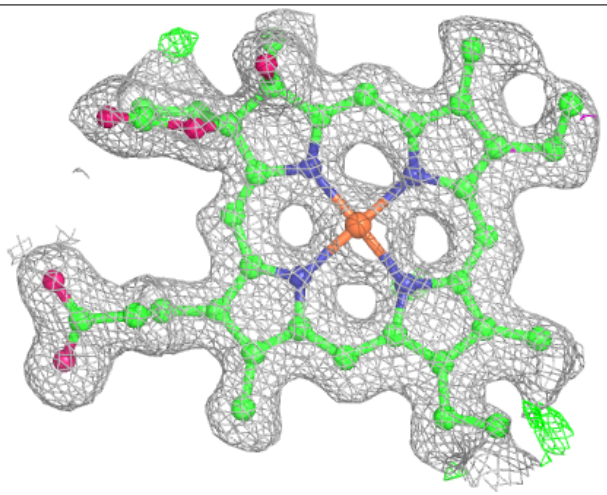
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

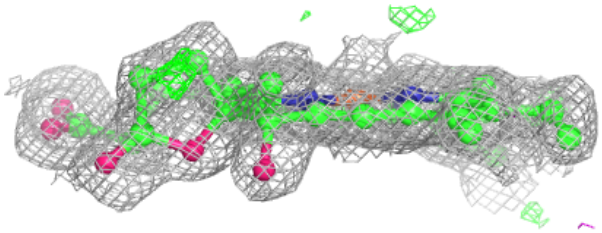
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	H2S	D	754	1/1	0.95	0.29	20,20,20,20	1
4	H2S	A	754	1/1	0.96	0.28	24,24,24,24	1
4	H2S	C	754	1/1	0.98	0.38	26,26,26,26	1
4	H2S	B	754	1/1	0.98	0.26	22,22,22,22	1
3	HDE	A	761[B]	44/44	0.99	0.07	2,7,11,11	44
3	HDE	B	761[B]	44/44	0.99	0.07	3,10,12,14	44
3	HDE	C	761[B]	44/44	0.99	0.07	3,9,12,14	44
3	HDE	D	761[B]	44/44	0.99	0.06	2,8,11,16	44
2	HDD	A	760[A]	44/44	0.99	0.06	2,3,8,10	44
2	HDD	B	760[A]	44/44	0.99	0.07	2,4,6,10	44
2	HDD	C	760[A]	44/44	0.99	0.07	2,4,10,12	44
2	HDD	D	760[A]	44/44	0.99	0.06	2,3,8,12	44

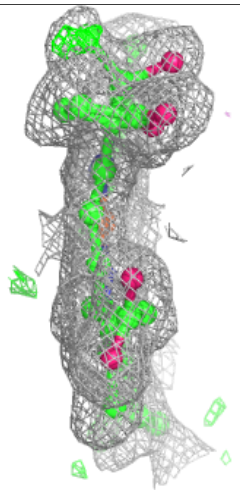
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HDE 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)

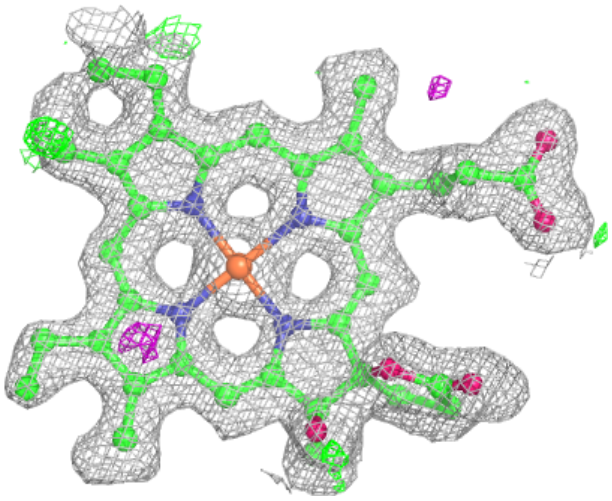


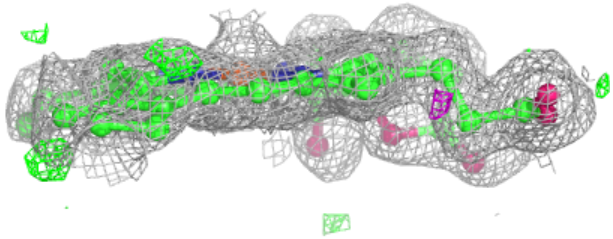


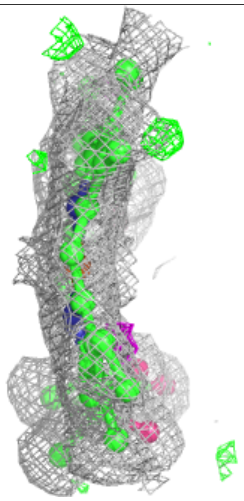


Electron density around HDE B 761 (B):

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

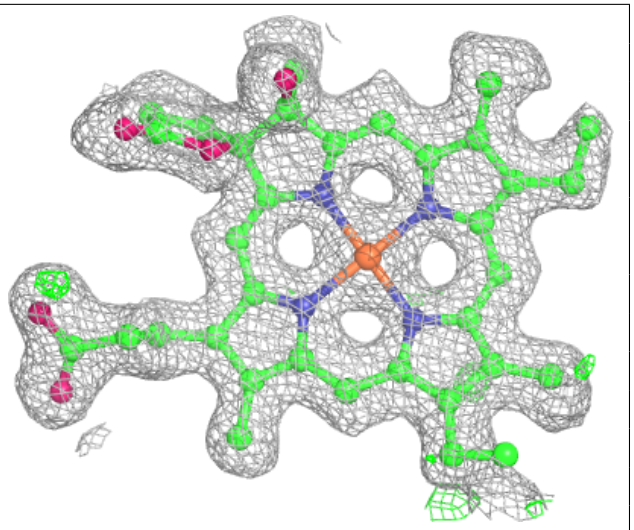


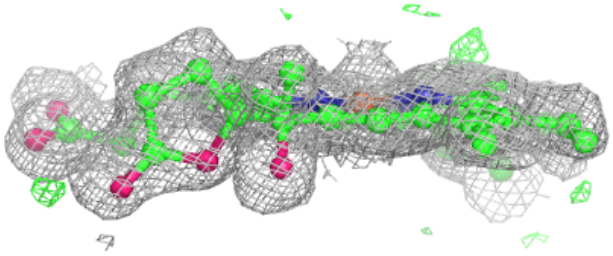


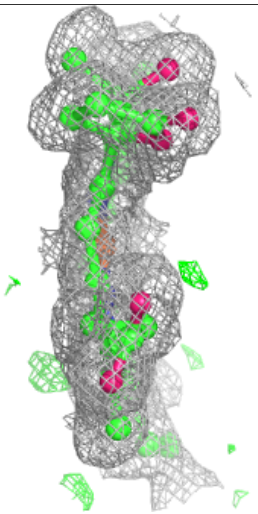


Electron density around HDE C 761 (B):

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







Electron density around HDE D 761 (B):

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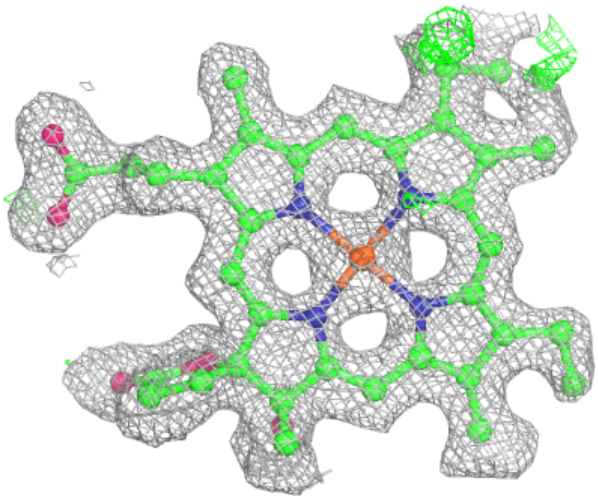
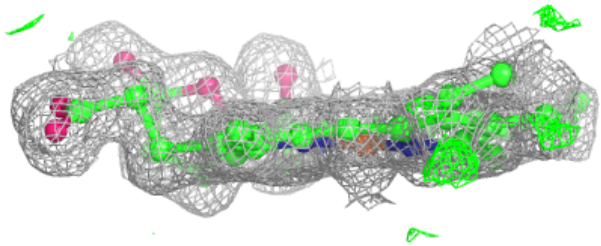
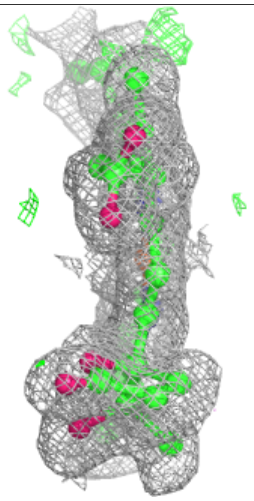
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

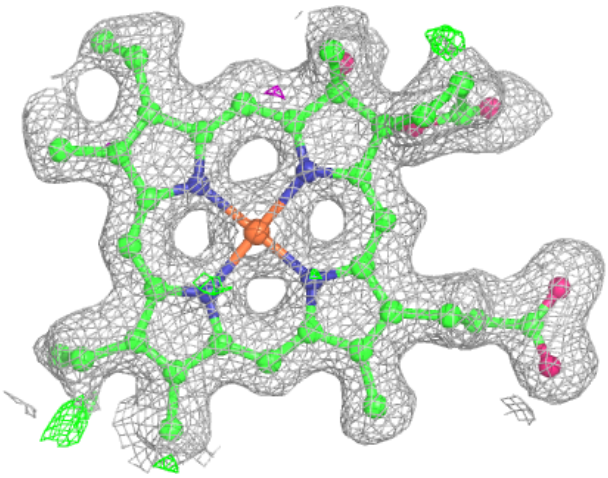


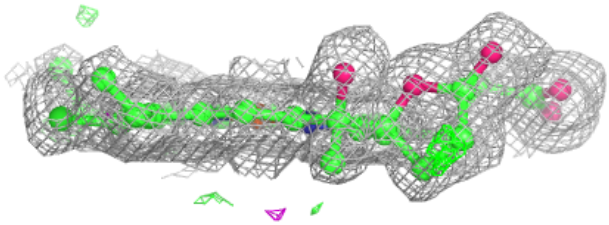


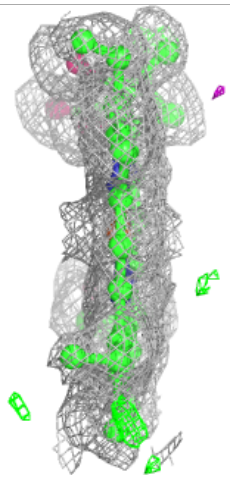


Electron density around HDD A 760 (A):

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

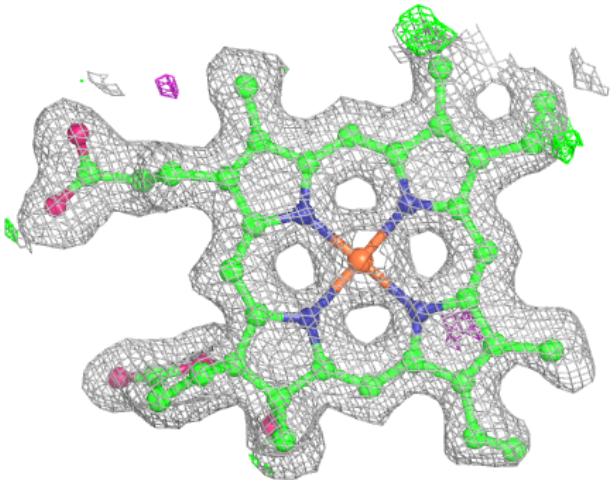


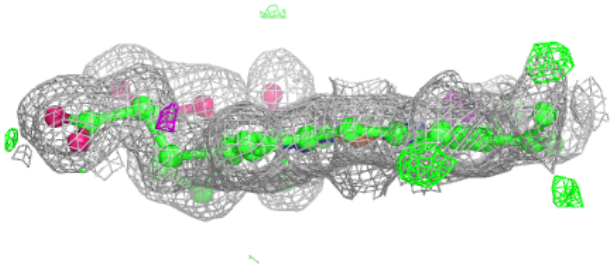


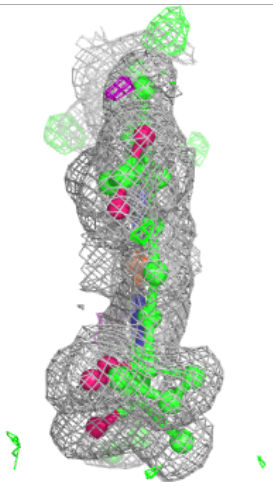


Electron density around HDD B 760 (A):

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

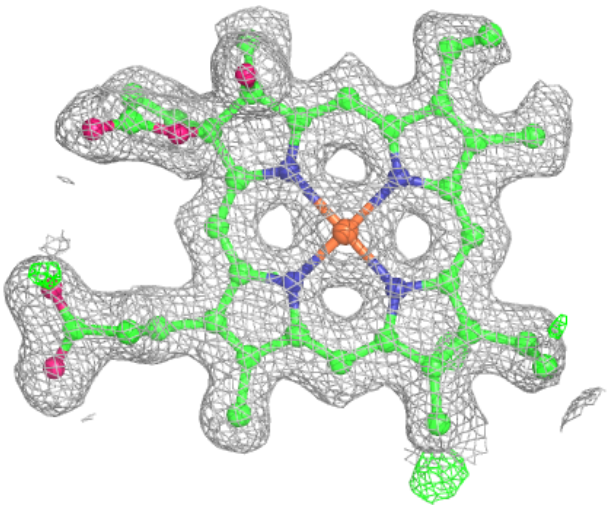


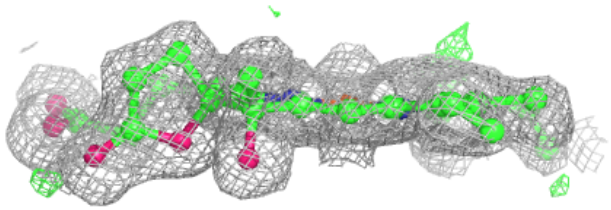


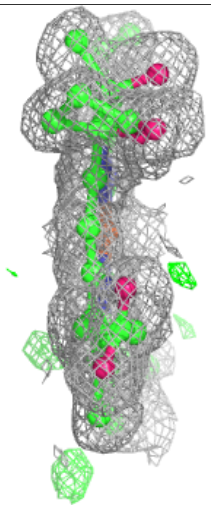


Electron density around HDD C 760 (A):

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

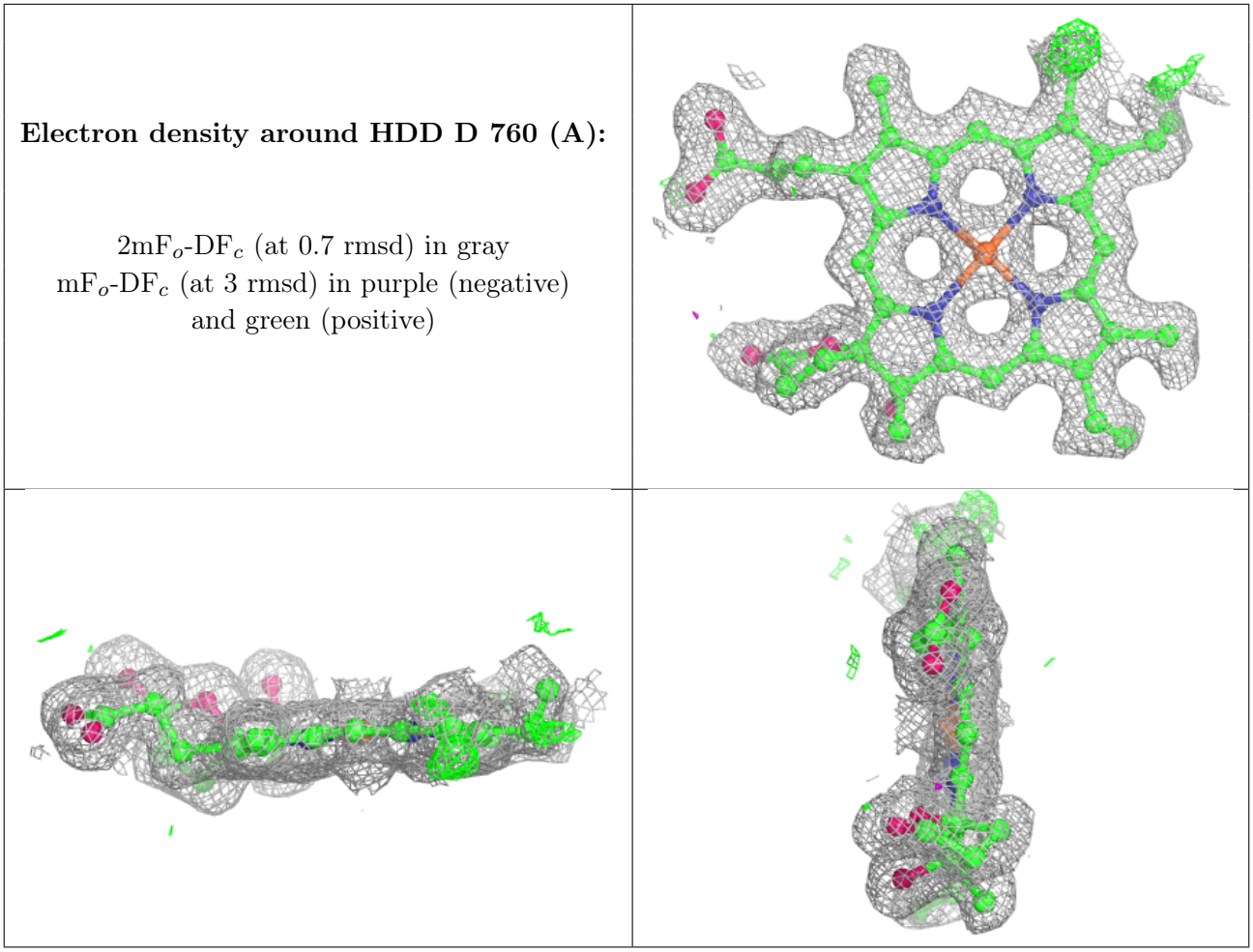






Electron density around HDD D 760 (A):

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



6.5 Other polymers (i)

There are no such residues in this entry.