



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 10:42 AM EDT

PDB ID : 3P9Q / pdb_00003p9q
Title : Structure of I274C variant of E. coli KatE
Authors : Loewen, P.C.; Jha, V.; Louis, S.; Chelikani, P.; Carpena, X.; Fita, I.
Deposited on : 2010-10-18
Resolution : 1.48 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

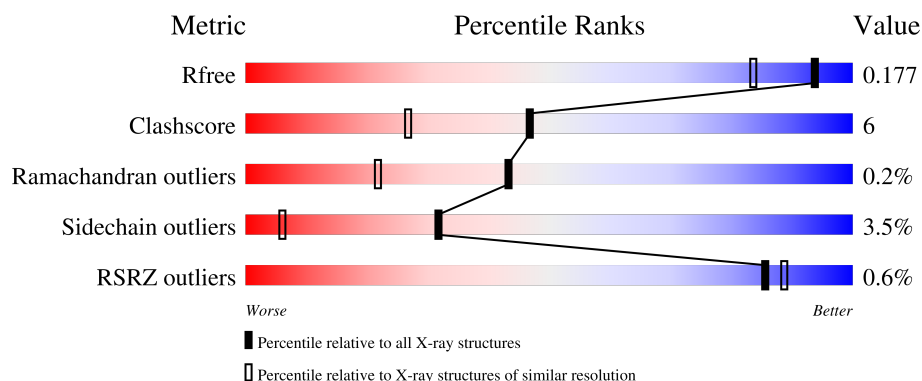
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.48 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}	180053	6779 (1.50-1.46)
Clashscore	190562	7025 (1.50-1.46)
Ramachandran outliers	187476	6917 (1.50-1.46)
Sidechain outliers	187428	6914 (1.50-1.46)
RSRZ outliers	180081	6781 (1.50-1.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	753	% 84% 11% • •
1	B	753	% 83% 12% • •
1	C	753	% 84% 11% • •
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
2	HDD	A	760[A]	X	-	-	-
2	HDD	B	760[A]	X	-	-	-
2	HDD	C	760[A]	X	-	-	-
2	HDD	D	760[A]	X	-	-	-
3	HDE	A	761[B]	X	-	-	-
4	H2S	A	754[A]	-	-	X	-
4	H2S	B	754[A]	-	-	X	-
4	H2S	C	754[A]	-	-	X	-
4	H2S	D	754[A]	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26893 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

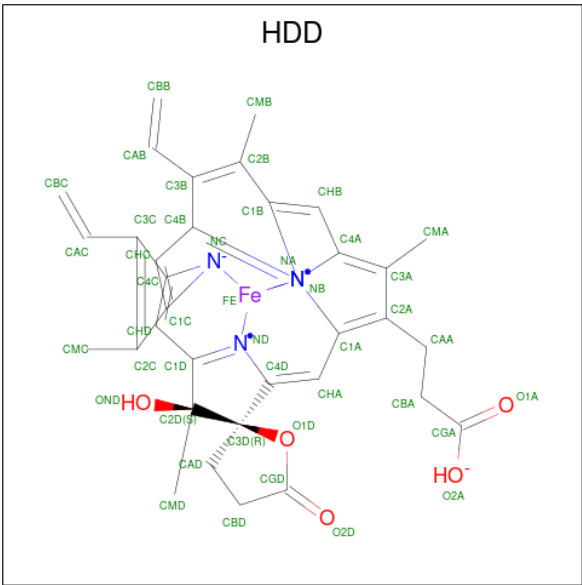
- Molecule 1 is a protein called Catalase HP11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	4	0
			5760	3658	1010	1081	11			
1	D	726	Total	C	N	O	S	0	8	0
			5769	3661	1012	1085	11			

There are 12 discrepancies between the modelled and reference sequences:

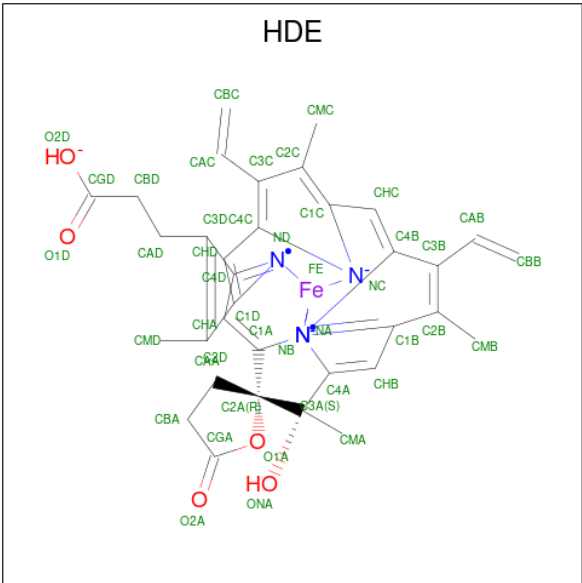
Chain	Residue	Modelled	Actual	Comment	Reference
A	274	CYS	ILE	engineered mutation	UNP P21179
A	438	ALA	CYS	engineered mutation	UNP P21179
A	669	ALA	CYS	engineered mutation	UNP P21179
B	274	CYS	ILE	engineered mutation	UNP P21179
B	438	ALA	CYS	engineered mutation	UNP P21179
B	669	ALA	CYS	engineered mutation	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 (CCD ID: HDD) (formula: C₃₄H₃₂FeN₄O₅).



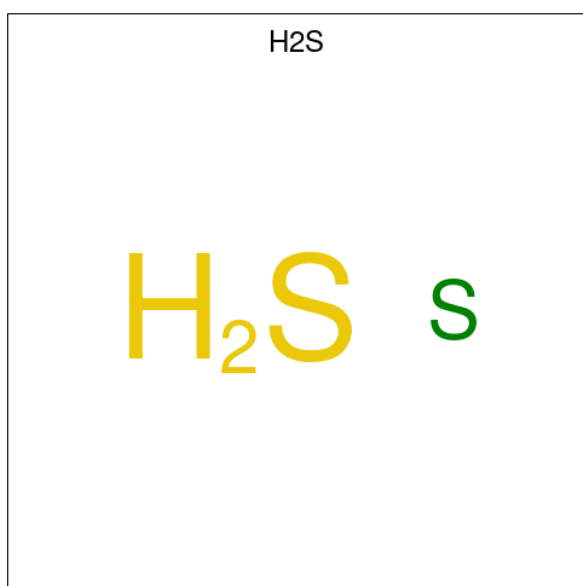
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
2	B	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
2	C	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
2	D	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		

- Molecule 3 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE 17R, 18S (CCD ID: HDE) (formula: $C_{34}H_{32}FeN_4O_5$).



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

- Molecule 4 is HYDROSULFURIC ACID (CCD ID: H2S) (formula: H₂S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	895	Total 895	O 895	0	0
5	B	803	Total 803	O 803	0	0

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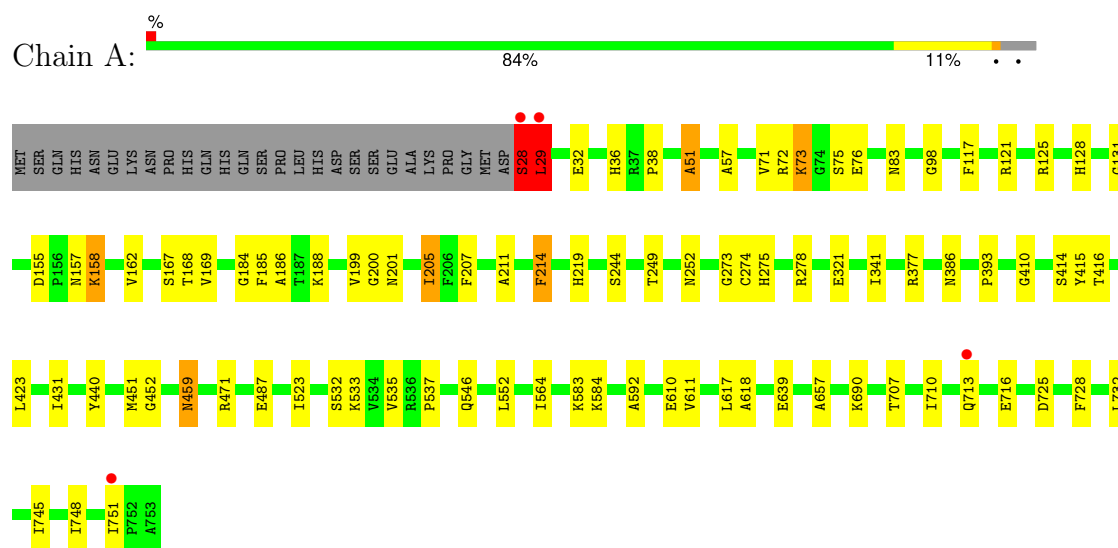
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	865	Total 865	O 865	0	0
5	D	933	Total 933	O 933	0	0

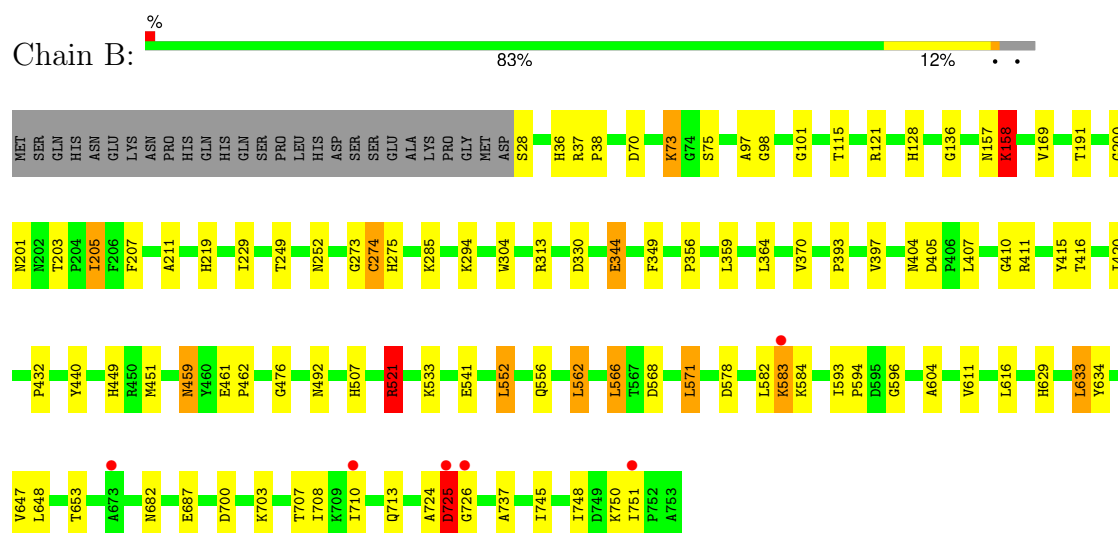
3 Residue-property plots [i](#)

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.

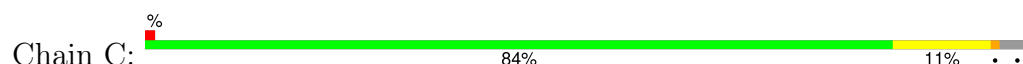
• Molecule 1: Catalase HP1I

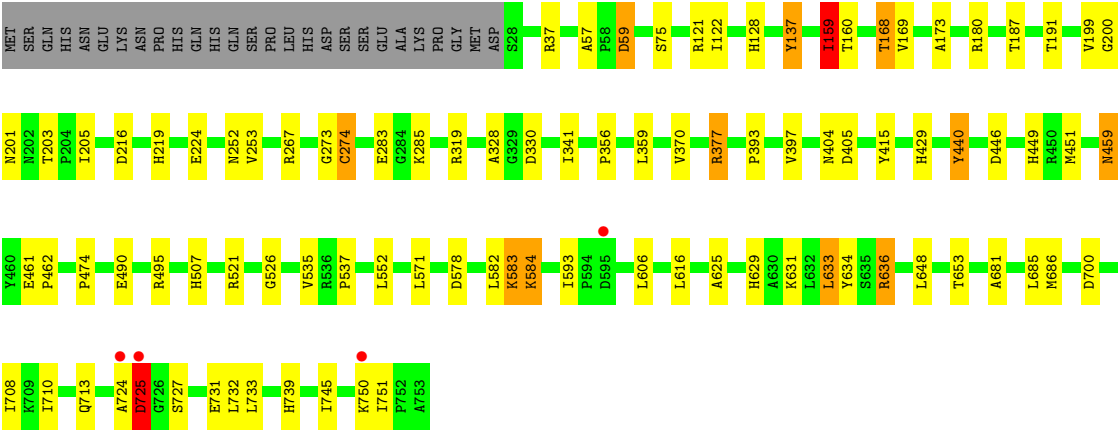


• Molecule 1: Catalase HP1I

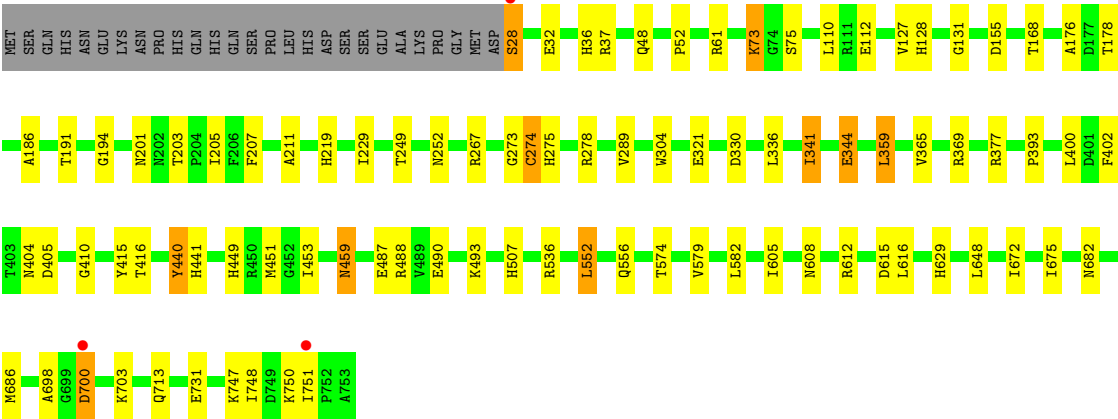
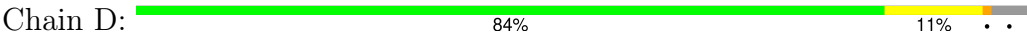


• Molecule 1: Catalase HP1I





● Molecule 1: Catalase HP11



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.66Å 133.02Å 122.59Å 90.00° 109.59° 90.00°	Depositor
Resolution (Å)	28.55 – 1.48 28.55 – 1.48	Depositor EDS
% Data completeness (in resolution range)	91.7 (28.55-1.48) 91.7 (28.55-1.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 1.48Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.143 , 0.177 0.143 , 0.177	Depositor DCC
R_{free} test set	21507 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	10.7	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	26893	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.62	33/5932 (0.6%)	1.34	13/8064 (0.2%)
1	B	1.56	20/5931 (0.3%)	1.31	12/8062 (0.1%)
1	C	1.55	27/5932 (0.5%)	1.29	12/8065 (0.1%)
1	D	1.63	29/5957 (0.5%)	1.32	10/8098 (0.1%)
All	All	1.59	109/23752 (0.5%)	1.32	47/32289 (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	A	0	1
1	B	0	1
1	C	1	3
All	All	1	5

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	LEU	N-CA	-9.22	1.33	1.46
1	D	341	ILE	N-CA	8.53	1.52	1.45
1	B	98	GLY	N-CA	8.53	1.54	1.45
1	D	341	ILE	CA-CB	-8.33	1.48	1.54
1	C	59	ASP	CG-OD1	7.76	1.40	1.25
1	A	341	ILE	N-CA	7.62	1.51	1.45
1	D	365	VAL	CA-CB	7.62	1.64	1.54
1	A	71	VAL	CA-CB	7.55	1.63	1.54
1	C	370	VAL	CA-CB	7.49	1.65	1.55
1	C	159	ILE	CG1-CD1	-7.49	1.22	1.51
1	A	275	HIS	N-CA	7.28	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	131	GLY	N-CA	7.26	1.53	1.45
1	C	59	ASP	CB-CG	7.15	1.70	1.52
1	B	37	ARG	CZ-NH2	7.06	1.42	1.33
1	B	200	GLY	N-CA	7.01	1.51	1.44
1	C	187	THR	N-CA	7.01	1.54	1.46
1	C	397	VAL	N-CA	7.00	1.52	1.46
1	A	72	ARG	C-O	6.85	1.32	1.23
1	D	605	ILE	N-CA	6.71	1.55	1.46
1	A	657	ALA	CA-CB	6.67	1.62	1.53
1	A	745	ILE	CA-CB	6.60	1.57	1.54
1	C	526	GLY	N-CA	6.58	1.53	1.45
1	C	593	ILE	N-CA	6.52	1.51	1.46
1	C	137	TYR	C-O	-6.45	1.16	1.23
1	C	203	THR	N-CA	6.45	1.51	1.45
1	C	474	PRO	CA-C	6.42	1.58	1.52
1	D	28	SER	CA-C	6.42	1.66	1.52
1	D	28	SER	CB-OG	6.34	1.54	1.42
1	D	203	THR	N-CA	6.34	1.51	1.45
1	B	397	VAL	N-CA	6.16	1.52	1.46
1	D	155	ASP	N-CA	6.15	1.54	1.46
1	D	682	ASN	N-CA	-6.15	1.39	1.46
1	C	168	THR	C-O	6.12	1.30	1.23
1	C	168	THR	N-CA	6.10	1.52	1.45
1	C	377	ARG	CZ-NH1	6.08	1.41	1.32
1	A	185	PHE	CA-CB	6.05	1.60	1.52
1	B	611	VAL	CA-CB	5.91	1.61	1.54
1	C	495	ARG	CZ-NH1	5.88	1.41	1.32
1	C	180	ARG	N-CA	5.87	1.53	1.46
1	C	625	ALA	CA-CB	5.87	1.62	1.53
1	A	51	ALA	CA-CB	5.86	1.61	1.53
1	A	214	PHE	C-O	-5.81	1.19	1.24
1	B	420	ILE	C-O	5.81	1.31	1.24
1	C	739	HIS	N-CA	5.80	1.53	1.46
1	A	321	GLU	CD-OE1	5.80	1.36	1.25
1	D	178	THR	CA-CB	5.79	1.60	1.52
1	A	341	ILE	CA-CB	-5.74	1.50	1.54
1	D	336	LEU	N-CA	5.72	1.53	1.46
1	D	536	ARG	N-CA	5.69	1.54	1.46
1	A	167	SER	N-CA	5.67	1.52	1.46
1	A	186	ALA	N-CA	5.65	1.52	1.46
1	A	205	ILE	CA-C	-5.64	1.47	1.52
1	C	319	ARG	CD-NE	5.63	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	446	ASP	N-CA	5.61	1.53	1.46
1	C	328	ALA	C-O	5.61	1.31	1.24
1	D	579	VAL	CA-CB	5.60	1.60	1.53
1	A	184	GLY	N-CA	5.59	1.52	1.44
1	D	377	ARG	CZ-NH2	5.59	1.40	1.33
1	B	521	ARG	CG-CD	5.59	1.69	1.52
1	D	493	LYS	N-CA	5.58	1.53	1.46
1	A	452	GLY	C-O	5.56	1.29	1.24
1	A	386	ASN	C-O	5.55	1.30	1.24
1	B	203	THR	N-CA	5.53	1.50	1.45
1	D	453	ILE	CA-CB	5.51	1.59	1.53
1	B	136	GLY	N-CA	5.50	1.52	1.45
1	B	205	ILE	CA-CB	5.50	1.61	1.54
1	D	186	ALA	CA-C	-5.49	1.46	1.52
1	A	423	LEU	N-CA	5.48	1.52	1.46
1	B	476	GLY	N-CA	5.46	1.52	1.44
1	A	57	ALA	CA-CB	5.45	1.59	1.53
1	C	377	ARG	CZ-NH2	5.43	1.40	1.33
1	A	131	GLY	N-CA	5.43	1.51	1.45
1	B	356	PRO	C-O	-5.43	1.18	1.23
1	A	564	ILE	CA-CB	5.40	1.61	1.54
1	D	359	LEU	N-CA	5.37	1.52	1.45
1	C	200	GLY	N-CA	5.36	1.49	1.44
1	B	492	ASN	CG-ND2	-5.36	1.22	1.33
1	B	725	ASP	C-O	5.35	1.30	1.24
1	A	618	ALA	CA-CB	5.30	1.61	1.53
1	D	321	GLU	CD-OE1	5.30	1.35	1.25
1	A	117	PHE	CA-C	5.29	1.59	1.52
1	C	160	THR	N-CA	5.28	1.53	1.46
1	C	57	ALA	CA-CB	5.27	1.59	1.53
1	A	76	GLU	N-CA	5.25	1.52	1.46
1	D	402	PHE	CA-CB	5.23	1.60	1.53
1	B	275	HIS	N-CA	5.22	1.52	1.45
1	A	710	ILE	CA-CB	5.21	1.60	1.54
1	B	229	ILE	CA-CB	5.21	1.60	1.54
1	D	176	ALA	C-O	5.21	1.30	1.23
1	B	38	PRO	C-O	5.20	1.29	1.23
1	C	122	ILE	CA-CB	5.19	1.59	1.55
1	D	304	TRP	N-CA	5.17	1.52	1.46
1	D	675	ILE	N-CA	5.17	1.51	1.46
1	A	200	GLY	N-CA	5.17	1.49	1.44
1	B	647	VAL	CA-CB	5.15	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	289	VAL	N-CA	5.15	1.52	1.46
1	D	400	LEU	N-CA	5.13	1.52	1.45
1	D	194	GLY	N-CA	5.12	1.49	1.45
1	A	592	ALA	C-O	5.11	1.30	1.24
1	A	98	GLY	N-CA	5.08	1.51	1.45
1	A	611	VAL	CA-CB	5.08	1.59	1.54
1	B	687	GLU	CA-C	5.07	1.59	1.52
1	C	173	ALA	N-CA	5.07	1.52	1.46
1	D	608	ASN	N-CA	5.05	1.52	1.45
1	D	698	ALA	N-CA	5.05	1.52	1.46
1	A	523	ILE	C-O	5.05	1.29	1.24
1	B	541	GLU	C-O	5.03	1.30	1.24
1	A	523	ILE	CA-CB	-5.02	1.48	1.54
1	A	592	ALA	N-CA	5.01	1.52	1.46

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	SER	CA-C-N	-10.18	103.34	123.09
1	A	28	SER	C-N-CA	-10.18	103.34	123.09
1	B	648	LEU	CA-C-N	7.58	127.86	119.90
1	B	648	LEU	C-N-CA	7.58	127.86	119.90
1	B	158	LYS	CA-CB-CG	-7.37	99.37	114.10
1	C	725	ASP	N-CA-C	7.31	126.37	110.80
1	C	37	ARG	NE-CZ-NH2	-7.21	112.71	119.20
1	C	636	ARG	NE-CZ-NH1	6.75	128.25	121.50
1	C	636	ARG	NE-CZ-NH2	-6.66	113.21	119.20
1	D	229	ILE	N-CA-C	-6.59	103.78	109.19
1	D	344	GLU	CA-CB-CG	6.47	127.03	114.10
1	A	431	ILE	N-CA-C	-6.28	102.80	108.95
1	A	157	ASN	CA-C-N	-6.09	114.67	122.77
1	A	157	ASN	C-N-CA	-6.09	114.67	122.77
1	D	686	MET	CG-SD-CE	6.06	114.22	100.90
1	A	158[A]	LYS	CB-CA-C	6.05	119.99	110.19
1	A	158[B]	LYS	CB-CA-C	6.05	119.99	110.19
1	A	377	ARG	CG-CD-NE	-5.77	99.31	112.00
1	D	615	ASP	N-CA-C	-5.76	104.91	111.07
1	B	593	ILE	CA-C-N	5.70	126.96	119.84
1	B	593	ILE	C-N-CA	5.70	126.96	119.84
1	B	344	GLU	CA-CB-CG	5.61	125.32	114.10
1	C	37	ARG	CB-CG-CD	-5.58	98.47	111.30
1	A	583	LYS	N-CA-C	-5.57	106.65	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	216	ASP	N-CA-C	5.56	117.02	111.07
1	B	349	PHE	CA-C-N	-5.55	113.01	122.56
1	B	349	PHE	C-N-CA	-5.55	113.01	122.56
1	A	471	ARG	NE-CZ-NH1	-5.55	115.95	121.50
1	B	73	LYS	CA-CB-CG	-5.51	103.07	114.10
1	C	253	VAL	CA-C-O	-5.41	115.33	120.95
1	C	356	PRO	N-CA-C	-5.40	109.06	114.68
1	A	72	ARG	CG-CD-NE	-5.37	100.18	112.00
1	A	158[A]	LYS	CA-C-O	5.32	126.06	120.36
1	A	158[B]	LYS	CA-C-O	5.32	126.06	120.36
1	D	612	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	C	745	ILE	O-C-N	5.25	123.78	120.42
1	D	110	LEU	CA-C-O	-5.24	115.32	120.82
1	B	562	LEU	CD1-CG-CD2	5.19	122.22	110.80
1	B	304	TRP	N-CA-C	5.18	116.61	111.07
1	C	253	VAL	O-C-N	5.16	126.88	121.87
1	B	313	ARG	N-CA-C	5.16	116.99	111.36
1	D	304	TRP	N-CA-C	5.12	116.55	111.07
1	D	377	ARG	CG-CD-NE	-5.05	100.89	112.00
1	C	341	ILE	CA-C-N	-5.05	114.52	119.92
1	C	341	ILE	C-N-CA	-5.05	114.52	119.92
1	D	112	GLU	N-CA-C	-5.05	105.86	111.36
1	D	61	ARG	NE-CZ-NH1	-5.01	116.49	121.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	159	ILE	CB

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	ARG	Sidechain
1	B	121	ARG	Sidechain
1	C	121	ARG	Sidechain
1	C	724	ALA	Peptide
1	C	725	ASP	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5755	0	5582	56	0
1	B	5757	0	5587	60	0
1	C	5760	0	5591	57	0
1	D	5769	0	5597	52	0
2	A	44	0	31	6	0
2	B	44	0	31	13	0
2	C	44	0	31	12	0
2	D	44	0	31	7	0
3	A	44	0	36	9	0
3	B	44	0	36	14	0
3	C	44	0	36	6	0
3	D	44	0	36	9	0
4	A	1	0	0	3	0
4	B	1	0	0	2	0
4	C	1	0	0	3	0
4	D	1	0	0	2	0
5	A	895	0	0	10	1
5	B	803	0	0	18	0
5	C	865	0	0	19	0
5	D	933	0	0	24	1
All	All	26893	0	22625	263	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 (263) 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:C:760[A]:HDD:HBB2	4:C:754[A]:H2S:S	1.30	1.70
2:B:760[A]:HDD:HBB2	4:B:754[A]:H2S:S	1.22	1.68
2:B:760[A]:HDD:CBB	4:B:754[A]:H2S:S	2.08	1.38
2:C:760[A]:HDD:CBB	4:C:754[A]:H2S:S	2.17	1.33
5:B:2705:HOH:O	1:D:73:LYS:HD3	1.26	1.30
1:C:578:ASP:HB3	5:C:2919:HOH:O	1.12	1.27
1:A:451:MET:HE2	1:C:451:MET:HE2	1.20	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LEU:HD22	5:C:2405:HOH:O	1.43	1.17
1:A:201:ASN:ND2	2:A:760[A]:HDD:HMB2	1.62	1.14
1:B:451:MET:SD	5:B:3614:HOH:O	2.05	1.13
1:A:73:LYS:CD	5:C:3442:HOH:O	1.94	1.13
3:D:761[B]:HDE:HBCB	3:D:761[B]:HDE:HMC	1.31	1.12
3:B:761[B]:HDE:HMC	3:B:761[B]:HDE:CBC	1.80	1.11
1:B:451:MET:HE2	1:D:451:MET:HE2	1.23	1.11
3:B:761[B]:HDE:HMC	3:B:761[B]:HDE:HBCB	1.11	1.09
1:C:451:MET:SD	5:C:3612:HOH:O	2.10	1.09
1:C:267:ARG:HG3	5:C:2916:HOH:O	1.51	1.08
2:A:760[A]:HDD:HBB2	4:A:754[A]:H2S:S	1.94	1.08
1:D:416[A]:THR:CG2	5:D:3576:HOH:O	2.03	1.05
1:B:416:THR:HG21	5:D:2464:HOH:O	1.55	1.04
3:B:761[B]:HDE:CBC	3:B:761[B]:HDE:CMC	2.31	1.04
1:B:521:ARG:HH21	1:B:745:ILE:HG21	1.20	1.03
1:D:416[A]:THR:HG23	5:D:3576:HOH:O	1.59	1.02
3:B:761[B]:HDE:HBCB	3:B:761[B]:HDE:CMC	1.85	1.00
1:A:201:ASN:CG	2:A:760[A]:HDD:HMB2	1.85	1.00
1:B:201:ASN:CG	2:B:760[A]:HDD:HMB1	1.88	0.99
3:D:761[B]:HDE:HBCB	3:D:761[B]:HDE:CMC	1.89	0.97
1:A:451:MET:SD	5:A:3609:HOH:O	2.20	0.96
1:A:416[A]:THR:HG21	5:A:3313:HOH:O	1.65	0.96
2:A:760[A]:HDD:CBB	4:A:754[A]:H2S:S	2.54	0.95
3:A:761[B]:HDE:HBCB	3:A:761[B]:HDE:HMC	1.50	0.93
1:B:73:LYS:HE3	5:D:3517:HOH:O	1.71	0.91
1:B:521:ARG:NH2	1:B:745:ILE:HG21	1.85	0.90
1:A:73:LYS:HD3	5:C:3442:HOH:O	1.64	0.89
3:C:761[B]:HDE:HMC	3:C:761[B]:HDE:HBCB	1.55	0.89
1:C:440[B]:TYR:CZ	5:C:1792:HOH:O	2.24	0.88
1:D:201:ASN:CG	2:D:760[A]:HDD:HMB1	1.98	0.88
1:A:716:GLU:HG2	5:A:3090:HOH:O	1.73	0.88
3:B:761[B]:HDE:CMC	3:B:761[B]:HDE:HBCA	2.02	0.87
1:A:28:SER:O	1:A:28:SER:OG	1.86	0.87
1:A:639:GLU:HG3	5:A:2414:HOH:O	1.74	0.87
1:C:201:ASN:CG	2:C:760[A]:HDD:HMB1	2.00	0.86
1:C:137:TYR:HB2	1:C:159:ILE:HD11	1.59	0.84
1:C:713:GLN:HB3	5:C:3004:HOH:O	1.78	0.84
3:C:761[B]:HDE:HMB	3:C:761[B]:HDE:HBBB	1.60	0.82
1:A:201:ASN:CG	2:A:760[A]:HDD:CMB	2.53	0.81
3:C:761[B]:HDE:HBCB	3:C:761[B]:HDE:CMC	2.06	0.81
1:B:748:ILE:O	1:B:751:ILE:HG22	1.78	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:SER:HA	5:D:2467:HOH:O	1.81	0.79
3:A:761[B]:HDE:HBCB	3:A:761[B]:HDE:CMC	2.12	0.77
1:D:416[A]:THR:HG21	5:D:3334:HOH:O	1.84	0.77
1:A:751:ILE:HD12	1:A:751:ILE:O	1.83	0.77
1:B:201:ASN:CG	2:B:760[A]:HDD:CMB	2.58	0.76
3:D:761[B]:HDE:CMC	3:D:761[B]:HDE:CBC	2.62	0.76
3:D:761[B]:HDE:HMB	3:D:761[B]:HDE:HBBB	1.69	0.75
1:C:685:LEU:N	1:C:685:LEU:HD22	2.02	0.73
1:D:700:ASP:OD1	5:D:3236:HOH:O	2.07	0.73
1:D:731:GLU:OE2	5:D:3028:HOH:O	2.07	0.72
1:D:416[B]:THR:HG22	5:D:1415:HOH:O	1.91	0.71
1:D:440:TYR:CZ	5:D:3517:HOH:O	2.42	0.71
2:C:760[A]:HDD:HBB1	2:C:760[A]:HDD:CMB	2.21	0.70
1:D:416[A]:THR:HG21	5:D:3576:HOH:O	1.76	0.69
1:C:578:ASP:OD1	5:C:3157:HOH:O	2.08	0.69
2:B:760[A]:HDD:CMB	2:B:760[A]:HDD:HBB1	2.23	0.69
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.78	0.67
1:D:703:LYS:NZ	5:D:2744:HOH:O	2.26	0.67
2:C:760[A]:HDD:HBC1	2:C:760[A]:HDD:CMC	2.27	0.64
1:C:725:ASP:O	5:C:2403:HOH:O	2.14	0.64
1:D:629:HIS:HD2	5:D:1554:HOH:O	1.80	0.64
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.27	0.64
1:B:700:ASP:HB2	5:B:3595:HOH:O	1.97	0.63
1:B:533[A]:LYS:HE2	5:B:3100:HOH:O	1.98	0.63
1:B:70:ASP:OD1	5:B:2761:HOH:O	2.15	0.63
1:C:578:ASP:HB2	1:C:582:LEU:O	1.98	0.63
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.83	0.62
3:B:761[B]:HDE:HMBB	3:B:761[B]:HDE:CBB	2.31	0.61
1:C:583:LYS:O	1:C:584:LYS:HB3	2.00	0.61
1:D:201:ASN:CG	2:D:760[A]:HDD:CMB	2.71	0.61
1:A:532:SER:OG	5:A:2410:HOH:O	2.15	0.61
1:B:449[B]:HIS:HE1	5:D:1789:HOH:O	1.84	0.60
1:D:267:ARG:HG3	5:D:1920:HOH:O	2.01	0.60
1:D:341:ILE:HD12	5:D:3022:HOH:O	2.02	0.59
3:B:761[B]:HDE:HBCA	3:B:761[B]:HDE:HMCA	1.85	0.59
1:D:440:TYR:CE2	5:D:3517:HOH:O	2.55	0.59
1:A:273:GLY:C	1:A:274:CYS:SG	2.85	0.58
1:A:201:ASN:ND2	2:A:760[A]:HDD:CMB	2.53	0.58
1:C:273:GLY:C	1:C:274:CYS:SG	2.86	0.58
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.86	0.58
1:C:629:HIS:HD2	5:C:1129:HOH:O	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416[B]:THR:HG22	5:A:901:HOH:O	2.03	0.58
3:A:761[B]:HDE:CMC	3:A:761[B]:HDE:CBC	2.81	0.57
1:B:521:ARG:NH2	1:B:745:ILE:CG2	2.64	0.57
1:A:36:HIS:CD2	1:A:36:HIS:H	2.23	0.57
3:C:761[B]:HDE:HMB	3:C:761[B]:HDE:CBB	2.32	0.57
1:B:115:THR:CG2	5:B:3420:HOH:O	2.54	0.56
3:D:761[B]:HDE:HBBB	3:D:761[B]:HDE:CMB	2.32	0.56
1:B:726:GLY:HA2	5:B:3590:HOH:O	2.06	0.56
3:C:761[B]:HDE:CMC	3:C:761[B]:HDE:CBC	2.82	0.56
1:C:201:ASN:CG	2:C:760[A]:HDD:CMB	2.76	0.56
1:B:359:LEU:H	1:B:507:HIS:HD2	1.54	0.56
1:C:59:ASP:OD2	5:C:2529:HOH:O	2.17	0.56
1:C:681:ALA:O	1:C:685:LEU:HD23	2.05	0.55
1:D:672:ILE:HG12	1:D:700:ASP:OD2	2.06	0.55
1:D:449[A]:HIS:HE1	5:D:1789:HOH:O	1.90	0.55
1:B:629:HIS:HD2	5:B:1054:HOH:O	1.89	0.55
1:D:127:VAL:HG22	3:D:761[B]:HDE:HMAB	1.88	0.54
2:C:760[A]:HDD:CBB	2:C:760[A]:HDD:CMB	2.85	0.54
1:A:73:LYS:HD2	5:C:3442:HOH:O	1.79	0.54
5:A:1788:HOH:O	1:C:449[A]:HIS:HE1	1.89	0.54
1:B:583:LYS:NZ	1:B:583:LYS:H	2.05	0.54
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.16	0.54
2:C:760[A]:HDD:CMC	2:C:760[A]:HDD:CBC	2.86	0.54
1:D:37:ARG:HD2	5:D:2157:HOH:O	2.08	0.54
2:D:760[A]:HDD:CBB	4:D:754[A]:H2S:S	2.96	0.53
1:A:725:ASP:H	1:A:728:PHE:HB3	1.72	0.53
1:D:748:ILE:O	1:D:751:ILE:HG22	2.08	0.53
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.39	0.53
1:A:29:LEU:HD23	5:C:3144:HOH:O	2.08	0.53
1:D:275:HIS:CE1	2:D:760[A]:HDD:HBB2	2.44	0.53
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.90	0.53
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.24	0.53
1:B:211:ALA:CB	1:B:410:GLY:HA3	2.38	0.53
1:A:214:PHE:CD2	3:A:761[B]:HDE:HAB	2.45	0.52
1:C:359:LEU:H	1:C:507:HIS:HD2	1.57	0.52
1:B:201:ASN:ND2	2:B:760[A]:HDD:CMB	2.72	0.52
1:C:700:ASP:HB2	5:C:3596:HOH:O	2.08	0.52
2:D:760[A]:HDD:HBB2	4:D:754[A]:H2S:S	2.49	0.52
1:B:36:HIS:HD1	1:B:36:HIS:H	1.58	0.52
3:B:761[B]:HDE:HMBB	3:B:761[B]:HDE:HBBB	1.92	0.52
1:A:274:CYS:CA	4:A:754[A]:H2S:S	2.99	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:634:TYR:O	1:C:653:THR:HA	2.10	0.51
5:B:3557:HOH:O	1:C:686:MET:HE1	2.08	0.51
2:B:760[A]:HDD:HBC1	2:B:760[A]:HDD:CMC	2.41	0.51
1:D:393:PRO:HD2	1:D:415:TYR:CG	2.45	0.51
2:B:760[A]:HDD:CBB	2:B:760[A]:HDD:CMB	2.90	0.50
1:C:199:VAL:HG12	3:C:761[B]:HDE:HHDA	1.93	0.50
1:A:748:ILE:O	1:A:751:ILE:HG13	2.13	0.49
1:A:73:LYS:CE	5:C:3442:HOH:O	2.40	0.49
2:C:760[A]:HDD:HBC1	2:C:760[A]:HDD:HMC2	1.93	0.49
3:D:761[B]:HDE:CMB	3:D:761[B]:HDE:CBB	2.91	0.49
1:B:115:THR:HG21	5:B:3420:HOH:O	2.11	0.48
1:B:201:ASN:OD1	2:B:760[A]:HDD:HMB1	2.11	0.48
1:B:521:ARG:NH2	1:B:745:ILE:HD13	2.29	0.48
1:B:578:ASP:HB2	5:B:2590:HOH:O	2.12	0.48
1:A:155:ASP:CG	5:A:3378:HOH:O	2.56	0.48
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.44	0.48
1:D:359:LEU:H	1:D:507:HIS:HD2	1.61	0.48
1:A:393:PRO:HD2	1:A:415:TYR:CG	2.48	0.48
1:A:451:MET:HE2	1:C:451:MET:CE	2.14	0.48
1:B:273:GLY:C	1:B:274:CYS:SG	2.96	0.48
3:D:761[B]:HDE:HMAA	3:D:761[B]:HDE:HAAA	1.67	0.48
1:A:128:HIS:HA	1:A:168:THR:O	2.14	0.48
3:B:761[B]:HDE:HMAB	3:B:761[B]:HDE:HAAA	1.59	0.47
1:C:201:ASN:ND2	2:C:760[A]:HDD:CMB	2.77	0.47
1:C:727:SER:O	1:C:731:GLU:HG3	2.13	0.47
1:D:341:ILE:CG1	5:D:3022:HOH:O	2.63	0.47
1:B:556:GLN:HG2	1:B:566:LEU:HD22	1.96	0.47
1:B:634:TYR:O	1:B:653:THR:HA	2.14	0.47
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.30	0.47
1:C:681:ALA:O	1:C:685:LEU:CD2	2.63	0.47
3:B:761[B]:HDE:HBBB	3:B:761[B]:HDE:CMB	2.44	0.47
1:C:685:LEU:HD22	1:C:685:LEU:H	1.76	0.47
1:D:278:ARG:HH12	1:D:487:GLU:CD	2.23	0.47
3:B:761[B]:HDE:HMBB	3:B:761[B]:HDE:HBBA	1.95	0.47
1:C:393:PRO:HD2	1:C:415:TYR:CG	2.50	0.47
1:C:685:LEU:N	1:C:685:LEU:CD2	2.73	0.47
1:D:273:GLY:C	1:D:274:CYS:SG	2.98	0.47
1:B:393:PRO:HD2	1:B:415:TYR:CG	2.50	0.46
1:D:341:ILE:HG13	5:D:3022:HOH:O	2.15	0.46
1:D:128:HIS:HA	1:D:168:THR:O	2.15	0.46
1:B:708:ILE:HG13	1:B:710:ILE:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:CYS:CA	4:C:754[A]:H2S:S	3.02	0.46
1:B:158:LYS:HG2	5:B:975:HOH:O	2.15	0.46
1:B:604:ALA:HB1	1:B:633:LEU:HD22	1.97	0.46
1:C:631:LYS:HG3	1:C:633:LEU:HD13	1.98	0.46
1:B:552:LEU:O	1:B:552:LEU:HD22	2.16	0.45
1:C:584:LYS:HB2	1:C:584:LYS:HE3	1.78	0.45
1:A:533:LYS:HE3	5:A:2410:HOH:O	2.17	0.45
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.32	0.45
3:A:761[B]:HDE:HMB	3:A:761[B]:HDE:HBBB	1.98	0.45
1:B:73:LYS:HD3	1:D:441:HIS:CD2	2.52	0.45
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.99	0.45
1:B:596:GLY:HA3	1:B:737:ALA:O	2.17	0.45
1:B:459:ASN:HD22	1:B:459:ASN:H	1.64	0.45
1:B:461:GLU:HA	1:B:462:PRO:C	2.41	0.45
5:B:983:HOH:O	1:D:52:PRO:HG3	2.17	0.45
1:D:672:ILE:CG1	1:D:700:ASP:OD2	2.65	0.45
1:A:38:PRO:HG2	1:A:51:ALA:HB2	1.99	0.44
1:D:201:ASN:OD1	2:D:760[A]:HDD:HMB1	2.16	0.44
1:B:201:ASN:ND2	2:B:760[A]:HDD:HMB3	2.32	0.44
1:A:414:SER:OG	3:A:761[B]:HDE:HBB	2.18	0.44
1:C:128:HIS:CE1	1:C:169:VAL:HG22	2.52	0.44
1:D:36:HIS:HD1	1:D:36:HIS:H	1.65	0.44
1:D:341:ILE:CD1	5:D:3022:HOH:O	2.62	0.44
1:A:690:LYS:HG3	1:A:751:ILE:HD11	1.99	0.44
1:B:411:ARG:HG2	3:B:761[B]:HDE:C3B	2.47	0.44
1:C:137:TYR:CB	1:C:159:ILE:HD11	2.41	0.44
1:B:207:PHE:O	1:B:249:THR:HA	2.17	0.44
1:D:404:ASN:O	1:D:405:ASP:C	2.60	0.44
1:B:407:LEU:HG	3:B:761[B]:HDE:HABA	1.99	0.44
1:A:29:LEU:N	1:A:29:LEU:HD12	2.33	0.43
1:B:583:LYS:O	1:B:584:LYS:HB3	2.18	0.43
2:B:760[A]:HDD:HMD2	2:B:760[A]:HDD:HAD2	1.65	0.43
2:B:760[A]:HDD:HBB1	2:B:760[A]:HDD:HMB2	1.99	0.43
3:B:761[B]:HDE:CBB	3:B:761[B]:HDE:CMB	2.93	0.43
1:A:29:LEU:HB2	5:C:2405:HOH:O	2.19	0.43
1:C:490:GLU:CD	1:D:488[B]:ARG:HH22	2.21	0.43
1:C:535:VAL:O	1:C:537:PRO:HD3	2.18	0.43
1:B:28:SER:HA	5:B:2571:HOH:O	2.18	0.43
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.34	0.43
1:C:583:LYS:O	1:C:584:LYS:CB	2.67	0.43
1:A:29:LEU:HD12	1:A:29:LEU:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:HIS:HA	1:C:168:THR:O	2.18	0.43
1:C:224:GLU:HB3	5:C:3120:HOH:O	2.19	0.43
1:D:201:ASN:CG	3:D:761[B]:HDE:HAC	2.43	0.43
5:B:3376:HOH:O	1:D:28:SER:HB3	2.19	0.43
1:A:459:ASN:HD22	1:A:459:ASN:C	2.25	0.43
1:C:461:GLU:HA	1:C:462:PRO:C	2.44	0.43
1:D:556:GLN:NE2	5:D:2773:HOH:O	2.52	0.43
1:B:115:THR:HG23	5:B:3420:HOH:O	2.17	0.42
1:B:682:ASN:HB3	1:B:707:THR:HG21	2.01	0.42
1:B:128:HIS:CE1	1:B:169:VAL:HG22	2.54	0.42
1:B:404:ASN:O	1:B:405:ASP:C	2.62	0.42
2:C:760[A]:HDD:HBB1	2:C:760[A]:HDD:HMB2	1.98	0.42
1:D:393:PRO:HD2	1:D:415:TYR:CD2	2.54	0.42
1:C:490:GLU:OE1	1:D:488[B]:ARG:NH2	2.28	0.42
1:D:552:LEU:HD22	1:D:552:LEU:HA	1.88	0.42
1:C:267:ARG:HH11	1:C:267:ARG:HD2	1.63	0.42
1:A:125:ARG:HG2	3:A:761[B]:HDE:HBA	2.02	0.42
1:B:583:LYS:H	1:B:583:LYS:HZ3	1.67	0.42
1:A:535:VAL:O	1:A:537:PRO:HD3	2.20	0.42
2:C:760[A]:HDD:CBB	2:C:760[A]:HDD:HMB3	2.49	0.42
3:A:761[B]:HDE:HABA	3:A:761[B]:HDE:HHCA	1.85	0.41
1:B:359:LEU:H	1:B:507:HIS:CD2	2.37	0.41
1:B:724:ALA:O	1:B:725:ASP:O	2.38	0.41
1:C:685:LEU:CD2	1:C:685:LEU:H	2.33	0.41
1:D:275:HIS:NE2	2:D:760[A]:HDD:CBB	2.83	0.41
1:A:83:ASN:HB3	1:C:429:HIS:CG	2.55	0.41
1:A:128:HIS:CE1	1:A:169:VAL:HG22	2.56	0.41
1:C:404:ASN:O	1:C:405:ASP:C	2.62	0.41
1:A:207:PHE:O	1:A:249:THR:HA	2.20	0.41
5:A:1058:HOH:O	1:C:451:MET:HE1	2.19	0.41
1:B:97:ALA:O	1:B:101:GLY:HA3	2.21	0.41
1:B:751:ILE:O	1:B:751:ILE:HG23	2.21	0.41
1:A:244:SER:HA	1:A:546[B]:GLN:NE2	2.36	0.41
1:B:521:ARG:HG3	5:B:3553:HOH:O	2.21	0.41
1:A:36:HIS:H	1:A:36:HIS:HD2	1.66	0.40
1:B:294:LYS:NZ	5:B:2778:HOH:O	2.53	0.40
1:C:507:HIS:HE1	5:C:926:HOH:O	2.04	0.40
1:D:369:ARG:CG	5:D:3574:HOH:O	2.68	0.40
1:A:83:ASN:HB3	1:C:429:HIS:CD2	2.56	0.40
1:B:364:LEU:HG	1:B:582:LEU:HD11	2.04	0.40
1:A:199:VAL:HG12	3:A:761[B]:HDE:HHDA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:751:ILE:O	1:A:751:ILE:CD1	2.64	0.40
2:B:760[A]:HDD:CMC	2:B:760[A]:HDD:CBC	2.99	0.40
1:C:631:LYS:HG3	1:C:633:LEU:CD1	2.51	0.40
1:D:207:PHE:O	1:D:249:THR:HA	2.21	0.40
1:A:162:VAL:HA	1:A:188:LYS:O	2.21	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]	1.92	0.28

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	729/753 (97%)	711 (98%)	17 (2%)	1 (0%)	48	23
1	B	729/753 (97%)	713 (98%)	14 (2%)	2 (0%)	36	17
1	C	728/753 (97%)	707 (97%)	20 (3%)	1 (0%)	48	23
1	D	732/753 (97%)	714 (98%)	17 (2%)	1 (0%)	48	23
All	All	2918/3012 (97%)	2845 (98%)	68 (2%)	5 (0%)	43	22

All (5) Ramachandran outliers are listed below:

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

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%)	599 (98%)	15 (2%)	43	14
1	B	614/634 (97%)	589 (96%)	25 (4%)	27	4
1	C	613/634 (97%)	587 (96%)	26 (4%)	26	4
1	D	617/634 (97%)	597 (97%)	20 (3%)	34	7
All	All	2458/2536 (97%)	2372 (96%)	86 (4%)	32	6

All (86) 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	205	ILE
1	A	252	ASN
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	584	LYS
1	A	610	GLU
1	A	617	LEU
1	A	707	THR
1	A	713	GLN
1	A	732	LEU
1	B	157	ASN
1	B	158	LYS
1	B	191	THR
1	B	205	ILE
1	B	252	ASN
1	B	274	CYS
1	B	285	LYS
1	B	344	GLU
1	B	370	VAL

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Mol	Chain	Res	Type
1	B	432	PRO
1	B	440	TYR
1	B	459	ASN
1	B	521	ARG
1	B	552	LEU
1	B	562	LEU
1	B	566	LEU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	594	PRO
1	B	616	LEU
1	B	633	LEU
1	B	703	LYS
1	B	713	GLN
1	B	750	LYS
1	C	159	ILE
1	C	191	THR
1	C	205	ILE
1	C	252	ASN
1	C	274	CYS
1	C	283	GLU
1	C	285	LYS
1	C	377	ARG
1	C	440[A]	TYR
1	C	440[B]	TYR
1	C	459	ASN
1	C	521	ARG
1	C	552	LEU
1	C	571	LEU
1	C	583	LYS
1	C	584	LYS
1	C	606	LEU
1	C	616	LEU
1	C	633	LEU
1	C	636	ARG
1	C	648	LEU
1	C	725	ASP
1	C	732	LEU
1	C	733	LEU
1	C	750	LYS
1	C	751	ILE

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Mol	Chain	Res	Type
1	D	32	GLU
1	D	48	GLN
1	D	73	LYS
1	D	191	THR
1	D	205	ILE
1	D	252	ASN
1	D	274	CYS
1	D	344	GLU
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 (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	139	GLN
1	A	201	ASN
1	A	252	ASN
1	A	459	ASN
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	546	GLN
1	C	556	GLN
1	C	629	HIS
1	C	682	ASN

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Mol	Chain	Res	Type
1	C	713	GLN
1	D	48	GLN
1	D	252	ASN
1	D	459	ASN
1	D	486	GLN
1	D	507	HIS
1	D	556	GLN
1	D	629	HIS

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 oligosaccharides 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	D	760[A]	5,1	49,52,52	2.50	13 (26%)	62,89,89	2.87	28 (45%)
3	HDE	C	761[B]	5,1	50,52,52	2.42	23 (46%)	60,89,89	2.38	22 (36%)
2	HDD	B	760[A]	5,1	49,52,52	2.00	14 (28%)	62,89,89	2.94	18 (29%)
2	HDD	A	760[A]	5,1	49,52,52	2.17	11 (22%)	62,89,89	2.37	15 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HDE	B	761[B]	5,1	50,52,52	2.41	20 (40%)	60,89,89	2.66	31 (51%)
3	HDE	D	761[B]	5,1	50,52,52	2.47	23 (46%)	60,89,89	2.31	26 (43%)
2	HDD	C	760[A]	5,1	49,52,52	2.03	11 (22%)	62,89,89	2.40	17 (27%)
3	HDE	A	761[B]	5,1	50,52,52	2.73	21 (42%)	60,89,89	2.86	26 (43%)

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	D	760[A]	5,1	1/1/8/14	5/9/89/89	0/1/9/9
3	HDE	C	761[B]	5,1	-	2/9/89/89	0/1/9/9
2	HDD	B	760[A]	5,1	1/1/8/14	2/9/89/89	0/1/9/9
2	HDD	A	760[A]	5,1	1/1/8/14	4/9/89/89	0/1/9/9
3	HDE	B	761[B]	5,1	-	2/9/89/89	0/1/9/9
3	HDE	D	761[B]	5,1	-	2/9/89/89	0/1/9/9
2	HDD	C	760[A]	5,1	1/1/8/14	2/9/89/89	0/1/9/9
3	HDE	A	761[B]	5,1	1/1/8/14	2/9/89/89	0/1/9/9

All (136) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	760[A]	HDD	FE-ND	9.29	2.23	1.94
2	C	760[A]	HDD	FE-ND	8.28	2.20	1.94
2	A	760[A]	HDD	FE-ND	7.92	2.19	1.94
2	D	760[A]	HDD	C1D-ND	7.31	1.40	1.35
3	A	761[B]	HDE	O1A-CGA	7.16	1.46	1.35
2	B	760[A]	HDD	FE-ND	6.93	2.16	1.94
3	A	761[B]	HDE	C3B-C2B	6.92	1.51	1.37
3	C	761[B]	HDE	C3B-C2B	6.33	1.50	1.37
3	D	761[B]	HDE	C3B-C2B	6.29	1.49	1.37
3	B	761[B]	HDE	C3B-C2B	5.91	1.49	1.37
3	A	761[B]	HDE	C3D-C2D	5.76	1.49	1.36
2	A	760[A]	HDD	FE-NB	5.47	2.11	1.94
2	B	760[A]	HDD	FE-NB	5.39	2.11	1.94
2	D	760[A]	HDD	CMD-C2D	5.20	1.60	1.53
3	C	761[B]	HDE	C3D-C2D	5.10	1.47	1.36
2	A	760[A]	HDD	OND-C2D	4.96	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	761[B]	HDE	FE-ND	4.83	2.09	1.94
3	A	761[B]	HDE	C1A-NA	4.74	1.45	1.37
3	B	761[B]	HDE	CHA-C4D	4.68	1.49	1.39
3	B	761[B]	HDE	FE-ND	4.66	2.09	1.94
3	D	761[B]	HDE	O1A-CGA	4.60	1.42	1.35
2	D	760[A]	HDD	FE-NB	4.60	2.09	1.94
3	C	761[B]	HDE	FE-ND	4.52	2.08	1.94
3	A	761[B]	HDE	CHA-C4D	4.46	1.49	1.39
2	C	760[A]	HDD	CMD-C2D	4.44	1.59	1.53
3	D	761[B]	HDE	CHA-C4D	4.39	1.49	1.39
3	C	761[B]	HDE	O1A-CGA	4.33	1.42	1.35
3	B	761[B]	HDE	CBB-CAB	4.18	1.50	1.30
3	D	761[B]	HDE	C3B-C4B	-4.15	1.36	1.44
3	A	761[B]	HDE	CHD-C1D	4.10	1.46	1.38
3	A	761[B]	HDE	CHB-C1B	4.04	1.48	1.39
2	A	760[A]	HDD	O1D-C3D	-4.00	1.40	1.46
3	A	761[B]	HDE	C3B-C4B	-4.00	1.37	1.44
2	A	760[A]	HDD	CMB-C2B	4.00	1.59	1.50
2	D	760[A]	HDD	CMC-C2C	3.96	1.58	1.50
3	C	761[B]	HDE	CBB-CAB	3.92	1.49	1.30
3	B	761[B]	HDE	O1A-CGA	3.88	1.41	1.35
3	B	761[B]	HDE	C4A-NA	3.87	1.44	1.37
3	A	761[B]	HDE	CHC-C4B	3.84	1.46	1.38
3	D	761[B]	HDE	C4A-NA	3.82	1.44	1.37
3	D	761[B]	HDE	C3D-C2D	3.81	1.45	1.36
3	A	761[B]	HDE	FE-ND	3.80	2.06	1.94
3	D	761[B]	HDE	CBB-CAB	3.80	1.48	1.30
2	D	760[A]	HDD	OND-C2D	3.79	1.49	1.42
3	C	761[B]	HDE	CHA-C4D	3.77	1.47	1.39
3	B	761[B]	HDE	C1A-NA	3.74	1.44	1.37
3	C	761[B]	HDE	C3B-C4B	-3.72	1.37	1.44
3	B	761[B]	HDE	CHC-C1C	3.70	1.47	1.39
2	B	760[A]	HDD	FE-NC	3.69	2.07	1.95
3	B	761[B]	HDE	C3D-C2D	3.66	1.44	1.36
3	B	761[B]	HDE	CHD-C4C	3.60	1.47	1.39
3	C	761[B]	HDE	CHD-C1D	3.56	1.45	1.38
3	A	761[B]	HDE	CBC-CAC	3.48	1.47	1.30
3	A	761[B]	HDE	FE-NC	3.44	2.06	1.95
3	A	761[B]	HDE	CBB-CAB	3.38	1.46	1.30
3	A	761[B]	HDE	C1C-NC	3.35	1.45	1.39
2	B	760[A]	HDD	CMD-C2D	3.32	1.57	1.53
3	D	761[B]	HDE	CMA-C3A	3.30	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	761[B]	HDE	CBC-CAC	3.27	1.46	1.30
3	B	761[B]	HDE	CBC-CAC	3.27	1.46	1.30
2	B	760[A]	HDD	CMC-C2C	3.24	1.57	1.50
3	D	761[B]	HDE	CBC-CAC	3.21	1.45	1.30
2	D	760[A]	HDD	CMA-C3A	3.20	1.57	1.50
3	D	761[B]	HDE	C1D-C2D	-3.18	1.38	1.44
3	D	761[B]	HDE	CHD-C1D	3.17	1.44	1.38
3	C	761[B]	HDE	C1A-NA	3.16	1.43	1.37
2	A	760[A]	HDD	CMC-C2C	3.12	1.57	1.50
2	C	760[A]	HDD	FE-NC	3.10	2.05	1.95
3	B	761[B]	HDE	C1C-NC	3.08	1.45	1.39
2	D	760[A]	HDD	CAC-C3C	3.07	1.55	1.47
2	C	760[A]	HDD	CAC-C3C	3.07	1.55	1.47
2	C	760[A]	HDD	O1D-C3D	-3.07	1.41	1.46
2	D	760[A]	HDD	FE-NC	3.06	2.05	1.95
3	C	761[B]	HDE	CMA-C3A	3.04	1.57	1.53
2	C	760[A]	HDD	FE-NB	3.02	2.04	1.94
2	C	760[A]	HDD	CMC-C2C	2.99	1.56	1.50
2	B	760[A]	HDD	C1D-ND	2.92	1.37	1.35
3	C	761[B]	HDE	C1C-NC	2.91	1.45	1.39
2	C	760[A]	HDD	C4A-C3A	2.90	1.49	1.43
2	D	760[A]	HDD	CAB-C3B	2.88	1.55	1.47
3	D	761[B]	HDE	C1D-ND	-2.85	1.35	1.40
3	B	761[B]	HDE	CHD-C1D	2.83	1.44	1.38
3	D	761[B]	HDE	CHC-C4B	2.80	1.44	1.38
3	B	761[B]	HDE	C3B-C4B	-2.77	1.39	1.44
3	D	761[B]	HDE	C1A-NA	2.77	1.42	1.37
3	A	761[B]	HDE	C4C-NC	2.77	1.44	1.39
3	D	761[B]	HDE	CHC-C1C	2.73	1.45	1.39
2	A	760[A]	HDD	CMD-C2D	2.73	1.56	1.53
3	D	761[B]	HDE	CHD-C4C	2.70	1.45	1.39
2	A	760[A]	HDD	FE-NC	2.69	2.04	1.95
3	C	761[B]	HDE	CHC-C4B	2.60	1.43	1.38
3	A	761[B]	HDE	CHC-C1C	2.60	1.45	1.39
3	B	761[B]	HDE	CHC-C4B	2.60	1.43	1.38
3	D	761[B]	HDE	C4D-C3D	2.58	1.49	1.45
3	B	761[B]	HDE	FE-NC	2.56	2.03	1.95
3	C	761[B]	HDE	CHC-C1C	2.55	1.45	1.39
3	D	761[B]	HDE	CHB-C1B	2.55	1.45	1.39
2	B	760[A]	HDD	C2A-C3A	-2.54	1.32	1.38
2	B	760[A]	HDD	CAC-C3C	2.53	1.54	1.47
3	A	761[B]	HDE	CHD-C4C	2.52	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	761[B]	HDE	FE-NB	2.52	2.02	1.94
3	C	761[B]	HDE	C1D-ND	-2.50	1.35	1.40
3	B	761[B]	HDE	CHB-C1B	2.48	1.44	1.39
3	A	761[B]	HDE	C3C-C2C	2.45	1.49	1.41
3	C	761[B]	HDE	CHD-C4C	2.44	1.44	1.39
2	B	760[A]	HDD	CMA-C3A	2.40	1.55	1.50
3	B	761[B]	HDE	C4D-C3D	2.34	1.49	1.45
2	A	760[A]	HDD	CAC-C3C	2.33	1.53	1.47
2	A	760[A]	HDD	FE-NA	2.31	2.02	1.95
3	D	761[B]	HDE	C1B-C2B	-2.31	1.39	1.44
3	C	761[B]	HDE	C4D-ND	-2.27	1.34	1.38
3	C	761[B]	HDE	FE-NC	2.26	2.02	1.95
3	C	761[B]	HDE	CHB-C1B	2.24	1.44	1.39
3	B	761[B]	HDE	C3C-C4C	2.22	1.49	1.42
2	B	760[A]	HDD	C4A-C3A	2.22	1.48	1.43
2	A	760[A]	HDD	CAB-C3B	2.21	1.53	1.47
3	D	761[B]	HDE	CAB-C3B	2.20	1.53	1.47
3	C	761[B]	HDE	C4A-NA	2.19	1.41	1.37
2	C	760[A]	HDD	CMB-C2B	2.18	1.55	1.50
3	A	761[B]	HDE	C1D-C2D	-2.18	1.40	1.44
3	A	761[B]	HDE	C3C-C4C	2.15	1.49	1.42
2	D	760[A]	HDD	C2A-C3A	-2.15	1.33	1.38
2	B	760[A]	HDD	CHB-C4A	-2.13	1.34	1.39
2	B	760[A]	HDD	C1B-NB	-2.12	1.36	1.40
2	D	760[A]	HDD	FE-NA	2.11	2.02	1.95
3	D	761[B]	HDE	ONA-C3A	2.10	1.46	1.42
2	C	760[A]	HDD	CAB-C3B	2.07	1.52	1.47
3	A	761[B]	HDE	O2D-CGD	-2.07	1.24	1.30
2	B	760[A]	HDD	CAA-C2A	2.06	1.56	1.51
2	D	760[A]	HDD	O1D-C3D	-2.06	1.43	1.46
2	C	760[A]	HDD	C2A-C3A	-2.05	1.33	1.38
3	C	761[B]	HDE	C4D-C3D	2.04	1.48	1.45
3	C	761[B]	HDE	C3C-C4C	2.03	1.48	1.42
3	D	761[B]	HDE	C3C-C2C	2.03	1.48	1.41
3	C	761[B]	HDE	C2A-C3A	-2.02	1.50	1.55
2	B	760[A]	HDD	CMB-C2B	2.01	1.54	1.50

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	760[A]	HDD	O1D-CGD-O2D	10.03	129.26	120.81
2	B	760[A]	HDD	O1D-CGD-CBD	-9.94	101.11	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	760[A]	HDD	O1D-CGD-O2D	9.02	128.41	120.81
2	B	760[A]	HDD	C3B-C4B-NB	-8.71	103.21	109.47
3	A	761[B]	HDE	O1A-CGA-O2A	8.11	127.64	120.81
2	C	760[A]	HDD	O1D-CGD-O2D	8.03	127.58	120.81
2	A	760[A]	HDD	C4D-ND-C1D	7.79	114.41	105.27
2	D	760[A]	HDD	O1D-CGD-CBD	-7.64	103.20	110.17
2	A	760[A]	HDD	CAD-CBD-CGD	-6.99	94.10	104.48
2	B	760[A]	HDD	C1B-NB-C4B	6.92	113.41	105.21
2	A	760[A]	HDD	C3B-C4B-NB	-6.79	104.59	109.47
3	D	761[B]	HDE	C2D-C1D-ND	6.51	117.32	109.84
2	D	760[A]	HDD	C3D-O1D-CGD	6.49	117.19	111.14
3	A	761[B]	HDE	C2A-O1A-CGA	6.45	117.16	111.14
2	C	760[A]	HDD	C3B-C4B-NB	-6.40	104.87	109.47
3	B	761[B]	HDE	C2D-C1D-ND	6.23	117.00	109.84
2	D	760[A]	HDD	C4D-ND-C1D	6.19	112.54	105.27
3	B	761[B]	HDE	C3C-C2C-C1C	-6.10	99.98	107.17
3	B	761[B]	HDE	CBC-CAC-C3C	-5.88	98.14	127.53
2	D	760[A]	HDD	C3B-C4B-NB	-5.72	105.36	109.47
3	C	761[B]	HDE	C2D-C1D-ND	5.64	116.33	109.84
3	D	761[B]	HDE	CBC-CAC-C3C	-5.59	99.58	127.53
3	A	761[B]	HDE	C2D-C1D-ND	5.58	116.25	109.84
3	D	761[B]	HDE	CBB-CAB-C3B	-5.29	101.07	127.53
3	C	761[B]	HDE	CBC-CAC-C3C	-5.28	101.16	127.53
3	A	761[B]	HDE	CBA-CAA-C2A	5.22	111.43	103.98
2	B	760[A]	HDD	C4D-ND-C1D	5.18	111.35	105.27
3	A	761[B]	HDE	O1A-CGA-CBA	-5.18	105.45	110.17
2	B	760[A]	HDD	C3D-O1D-CGD	5.16	115.95	111.14
3	C	761[B]	HDE	C3C-C2C-C1C	-5.08	101.18	107.17
2	A	760[A]	HDD	CMB-C2B-C1B	4.96	132.79	125.03
3	A	761[B]	HDE	CHC-C1C-NC	-4.95	114.88	123.86
3	B	761[B]	HDE	C3B-C2B-C1B	-4.92	102.71	106.41
2	D	760[A]	HDD	C4B-C3B-C2B	4.66	111.56	107.28
3	B	761[B]	HDE	CAD-CBD-CGD	-4.64	101.35	113.67
2	C	760[A]	HDD	CHD-C4C-NC	4.64	129.50	124.45
3	A	761[B]	HDE	CAD-CBD-CGD	-4.62	101.41	113.67
3	C	761[B]	HDE	CMA-C3A-C4A	-4.62	104.86	112.68
3	C	761[B]	HDE	CBB-CAB-C3B	-4.61	104.52	127.53
2	D	760[A]	HDD	C3C-C2C-C1C	4.58	111.38	107.05
3	D	761[B]	HDE	C3B-C2B-C1B	-4.56	102.99	106.41
3	B	761[B]	HDE	C2B-C1B-NB	4.54	115.15	109.90
2	C	760[A]	HDD	C4B-C3B-C2B	4.54	111.45	107.28
2	C	760[A]	HDD	O1D-CGD-CBD	-4.53	106.04	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	761[B]	HDE	CBC-CAC-C3C	-4.51	105.00	127.53
2	A	760[A]	HDD	CHC-C4B-NB	4.48	129.25	124.42
3	C	761[B]	HDE	C4B-C3B-C2B	-4.46	103.18	107.28
2	C	760[A]	HDD	CHC-C4B-NB	4.46	129.22	124.42
2	D	760[A]	HDD	CHC-C1C-NC	4.44	129.29	124.45
3	B	761[B]	HDE	CAD-C3D-C4D	4.41	132.38	124.70
2	B	760[A]	HDD	CAA-CBA-CGA	-4.37	102.07	113.67
3	A	761[B]	HDE	C3C-C4C-NC	4.34	113.45	109.80
3	D	761[B]	HDE	C3A-C4A-CHB	-4.27	117.63	124.27
2	D	760[A]	HDD	C2A-C1A-NA	-4.24	105.44	110.15
3	C	761[B]	HDE	C3D-C4D-ND	4.23	114.44	110.35
3	A	761[B]	HDE	C2C-C1C-NC	4.23	116.92	110.14
3	C	761[B]	HDE	C2C-C1C-NC	4.23	116.92	110.14
2	C	760[A]	HDD	OND-C2D-CMD	-4.20	101.34	109.45
3	B	761[B]	HDE	O1A-CGA-CBA	4.10	113.91	110.17
2	D	760[A]	HDD	CHD-C4C-NC	4.09	128.91	124.45
3	B	761[B]	HDE	CBB-CAB-C3B	-4.00	107.55	127.53
2	D	760[A]	HDD	CBB-CAB-C3B	-3.98	107.65	127.53
3	B	761[B]	HDE	C4B-NB-C1B	-3.96	100.52	105.21
3	B	761[B]	HDE	C2C-C1C-NC	3.94	116.46	110.14
3	A	761[B]	HDE	CMC-C2C-C1C	3.87	131.31	125.42
2	A	760[A]	HDD	C4B-C3B-C2B	3.82	110.79	107.28
2	B	760[A]	HDD	CHC-C4B-NB	3.82	128.53	124.42
2	A	760[A]	HDD	CBB-CAB-C3B	-3.80	108.53	127.53
2	C	760[A]	HDD	CBC-CAC-C3C	-3.79	108.60	127.53
2	C	760[A]	HDD	C3D-O1D-CGD	3.78	114.67	111.14
3	A	761[B]	HDE	C3D-C4D-ND	3.75	113.97	110.35
2	B	760[A]	HDD	C2B-C1B-NB	-3.72	105.56	109.84
3	C	761[B]	HDE	C4D-C3D-C2D	-3.68	101.54	106.89
3	A	761[B]	HDE	CBB-CAB-C3B	-3.67	109.21	127.53
2	D	760[A]	HDD	CAA-CBA-CGA	-3.65	103.99	113.67
3	B	761[B]	HDE	CBA-CAA-C2A	3.63	109.16	103.98
2	A	760[A]	HDD	C1B-NB-C4B	3.62	109.49	105.21
3	A	761[B]	HDE	CMA-C3A-C4A	-3.60	106.58	112.68
2	C	760[A]	HDD	CBB-CAB-C3B	-3.60	109.53	127.53
2	B	760[A]	HDD	C4B-C3B-C2B	3.58	110.57	107.28
2	C	760[A]	HDD	C4D-ND-C1D	3.58	109.47	105.27
2	A	760[A]	HDD	CAA-CBA-CGA	-3.56	104.21	113.67
3	A	761[B]	HDE	C3C-C2C-C1C	-3.54	103.00	107.17
2	B	760[A]	HDD	OND-C2D-CMD	-3.47	102.74	109.45
2	A	760[A]	HDD	C2D-C1D-CHD	3.37	128.59	123.28
3	A	761[B]	HDE	C4C-NC-C1C	-3.35	100.35	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	761[B]	HDE	CMC-C2C-C1C	3.33	130.49	125.42
3	A	761[B]	HDE	ONA-C3A-CMA	-3.32	103.04	109.45
2	D	760[A]	HDD	CBD-CAD-C3D	-3.27	99.32	103.98
2	C	760[A]	HDD	CAA-CBA-CGA	-3.25	105.04	113.67
3	D	761[B]	HDE	O1A-CGA-O2A	3.23	123.53	120.81
3	A	761[B]	HDE	CAD-C3D-C2D	3.21	133.88	127.87
3	D	761[B]	HDE	CHB-C4A-NA	3.19	128.69	124.28
3	C	761[B]	HDE	CAD-CBD-CGD	-3.19	105.21	113.67
3	A	761[B]	HDE	CHD-C1D-C2D	-3.19	117.89	126.95
3	B	761[B]	HDE	C4C-C3C-C2C	3.18	111.26	107.30
3	C	761[B]	HDE	C3A-C4A-CHB	-3.16	119.35	124.27
2	A	760[A]	HDD	CHB-C4A-NA	3.14	129.55	123.86
2	C	760[A]	HDD	C3C-C2C-C1C	3.12	110.00	107.05
2	B	760[A]	HDD	CBC-CAC-C3C	-3.12	111.95	127.53
2	A	760[A]	HDD	CMB-C2B-C3B	-3.10	120.91	128.43
3	D	761[B]	HDE	C3C-C2C-C1C	-3.07	103.55	107.17
3	D	761[B]	HDE	CMA-C3A-C4A	-3.06	107.50	112.68
3	A	761[B]	HDE	C4B-C3B-C2B	-3.02	104.50	107.28
3	A	761[B]	HDE	C4D-C3D-C2D	-3.02	102.50	106.89
3	A	761[B]	HDE	C1D-C2D-C3D	-3.02	103.81	106.98
2	D	760[A]	HDD	C3B-C2B-C1B	-3.01	104.15	106.41
2	D	760[A]	HDD	C1B-NB-C4B	2.96	108.71	105.21
3	D	761[B]	HDE	CAD-CBD-CGD	-2.92	105.93	113.67
2	B	760[A]	HDD	CHD-C4C-NC	2.91	127.62	124.45
3	B	761[B]	HDE	CMD-C2D-C1D	2.91	129.58	125.03
3	D	761[B]	HDE	C2C-C1C-NC	2.91	114.80	110.14
3	D	761[B]	HDE	C2B-C1B-NB	2.89	113.24	109.90
2	B	760[A]	HDD	CBB-CAB-C3B	-2.86	113.24	127.53
2	C	760[A]	HDD	C1B-NB-C4B	2.85	108.58	105.21
3	D	761[B]	HDE	C4D-C3D-C2D	-2.83	102.77	106.89
2	D	760[A]	HDD	CHB-C4A-NA	2.80	128.94	123.86
3	C	761[B]	HDE	O1A-C2A-CAA	2.80	108.23	103.06
3	B	761[B]	HDE	C3A-C4A-CHB	-2.79	119.93	124.27
2	A	760[A]	HDD	C4C-CHD-C1D	2.79	130.50	125.99
3	D	761[B]	HDE	CBA-CAA-C2A	2.79	107.95	103.98
2	D	760[A]	HDD	CMB-C2B-C1B	2.78	129.38	125.03
3	B	761[B]	HDE	C1D-C2D-C3D	-2.73	104.11	106.98
3	B	761[B]	HDE	CAA-CBA-CGA	-2.72	100.44	104.48
2	A	760[A]	HDD	CHD-C4C-NC	2.69	127.39	124.45
2	B	760[A]	HDD	CHB-C4A-NA	2.69	128.74	123.86
3	C	761[B]	HDE	C1D-C2D-C3D	-2.68	104.16	106.98
3	D	761[B]	HDE	CAD-C3D-C4D	2.67	129.36	124.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	761[B]	HDE	O1A-CGA-O2A	2.67	123.06	120.81
2	C	760[A]	HDD	CHB-C4A-NA	2.65	128.67	123.86
3	B	761[B]	HDE	ONA-C3A-CMA	-2.64	104.35	109.45
3	C	761[B]	HDE	C2A-O1A-CGA	-2.64	108.68	111.14
2	B	760[A]	HDD	CBD-CAD-C3D	-2.63	100.23	103.98
2	D	760[A]	HDD	O2A-CGA-CBA	2.58	122.14	114.00
3	C	761[B]	HDE	CHA-C4D-ND	-2.56	121.67	124.42
2	D	760[A]	HDD	C3A-C4A-NA	-2.52	106.11	110.14
3	D	761[B]	HDE	CHC-C1C-NC	-2.51	119.30	123.86
2	B	760[A]	HDD	C3C-C2C-C1C	2.51	109.42	107.05
3	D	761[B]	HDE	CHD-C1D-C2D	-2.50	119.85	126.95
3	D	761[B]	HDE	ONA-C3A-CMA	2.48	114.25	109.45
3	C	761[B]	HDE	CMB-C2B-C1B	-2.47	121.17	125.03
2	D	760[A]	HDD	CMC-C2C-C3C	-2.46	122.48	128.43
2	D	760[A]	HDD	C4A-NA-C1A	2.46	109.83	105.82
2	D	760[A]	HDD	CBC-CAC-C3C	-2.46	115.25	127.53
3	D	761[B]	HDE	CHA-C1A-NA	2.46	127.67	124.28
3	C	761[B]	HDE	CHD-C1D-C2D	-2.45	119.98	126.95
2	C	760[A]	HDD	C2D-C1D-CHD	2.41	127.08	123.28
3	C	761[B]	HDE	CHC-C1C-NC	-2.39	119.52	123.86
2	D	760[A]	HDD	OND-C2D-CMD	-2.39	104.83	109.45
3	B	761[B]	HDE	C3C-C4C-NC	-2.38	107.80	109.80
3	B	761[B]	HDE	CHC-C1C-NC	-2.33	119.63	123.86
3	B	761[B]	HDE	C2A-O1A-CGA	-2.31	108.99	111.14
2	D	760[A]	HDD	C4C-NC-C1C	2.31	109.59	105.82
2	D	760[A]	HDD	C2C-C1C-NC	-2.31	105.36	109.64
3	C	761[B]	HDE	CHA-C1A-NA	2.29	127.44	124.28
3	D	761[B]	HDE	CMC-C2C-C1C	2.29	128.91	125.42
2	A	760[A]	HDD	C1A-CHA-C4D	2.28	130.08	125.87
3	B	761[B]	HDE	CHB-C1B-NB	-2.28	121.97	124.42
3	D	761[B]	HDE	CMB-C2B-C3B	2.27	133.93	128.43
2	D	760[A]	HDD	O1A-CGA-CBA	-2.26	115.92	123.09
3	A	761[B]	HDE	CMB-C2B-C1B	-2.26	121.51	125.03
3	A	761[B]	HDE	C4C-CHD-C1D	-2.24	120.98	126.25
3	B	761[B]	HDE	C1D-ND-C4D	-2.23	102.56	105.21
3	D	761[B]	HDE	C1D-C2D-C3D	-2.23	104.64	106.98
3	C	761[B]	HDE	C2B-C1B-NB	2.20	112.44	109.90
3	B	761[B]	HDE	CAD-C3D-C2D	-2.20	123.75	127.87
3	B	761[B]	HDE	C4B-C3B-C2B	-2.19	105.26	107.28
2	D	760[A]	HDD	CAA-C2A-C1A	-2.19	120.66	124.94
3	B	761[B]	HDE	CHD-C1D-ND	-2.19	121.66	124.37
2	C	760[A]	HDD	C3A-C4A-NA	-2.19	106.64	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	760[A]	HDD	CHC-C4B-C3B	2.18	129.42	125.07
3	B	761[B]	HDE	C3D-C4D-ND	2.17	112.45	110.35
3	D	761[B]	HDE	C4C-CHD-C1D	-2.14	121.21	126.25
3	C	761[B]	HDE	C4C-NC-C1C	-2.13	102.35	105.82
3	D	761[B]	HDE	CHD-C4C-NC	2.13	127.72	123.86
3	B	761[B]	HDE	O1A-CGA-O2A	-2.11	119.03	120.81
3	B	761[B]	HDE	C4D-C3D-C2D	-2.09	103.85	106.89
3	D	761[B]	HDE	O1A-C2A-CAA	2.03	106.82	103.06
3	D	761[B]	HDE	CHB-C1B-C2B	-2.03	121.82	125.03
3	B	761[B]	HDE	CHC-C4B-NB	-2.03	121.85	124.37
3	A	761[B]	HDE	CMB-C2B-C3B	2.03	133.33	128.43
3	A	761[B]	HDE	CAB-C3B-C2B	2.02	134.99	128.43
2	B	760[A]	HDD	C4C-NC-C1C	2.01	109.10	105.82

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	760[A]	HDD	NC
2	B	760[A]	HDD	NC
2	C	760[A]	HDD	NC
2	D	760[A]	HDD	NC
3	A	761[B]	HDE	NA

All (21) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
2	B	760[A]	HDD	CAA-CBA-CGA-O1A
3	B	761[B]	HDE	CAD-CBD-CGD-O1D
3	D	761[B]	HDE	CAD-CBD-CGD-O1D
2	D	760[A]	HDD	CAA-CBA-CGA-O2A
2	D	760[A]	HDD	C2C-C3C-CAC-CBC

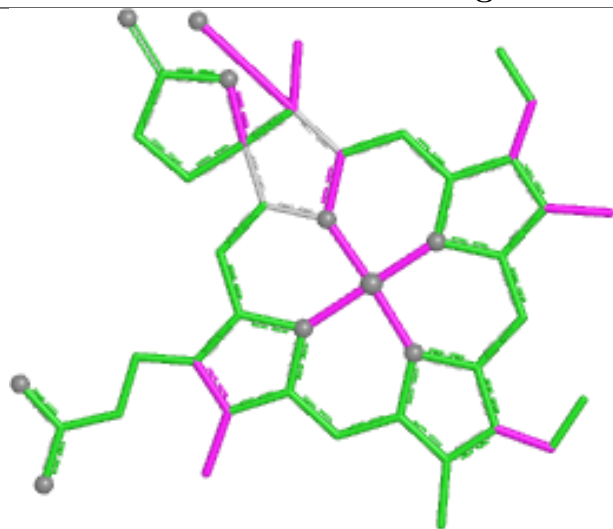
There are no ring outliers.

8 monomers are involved in 76 short contacts:

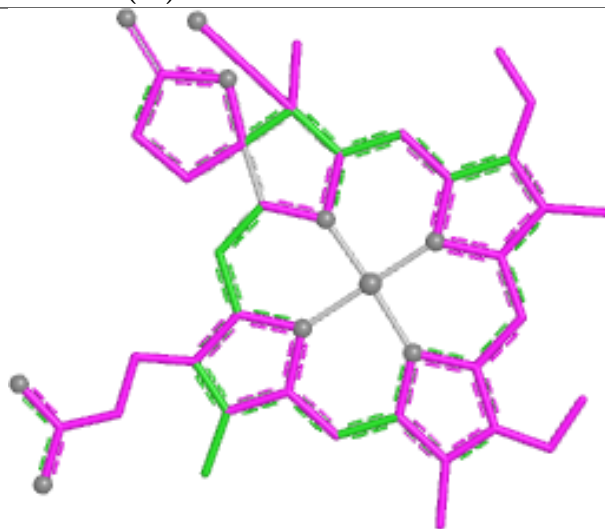
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	760[A]	HDD	7	0
3	C	761[B]	HDE	6	0
2	B	760[A]	HDD	13	0
2	A	760[A]	HDD	6	0
3	B	761[B]	HDE	14	0
3	D	761[B]	HDE	9	0
2	C	760[A]	HDD	12	0
3	A	761[B]	HDE	9	0

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

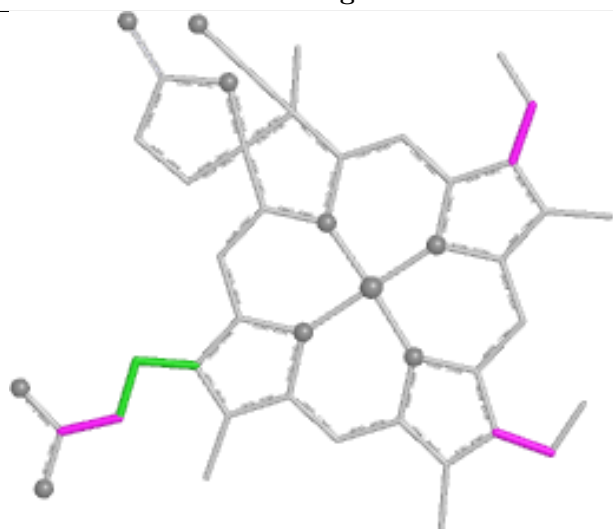
Ligand HDD D 760 (A)



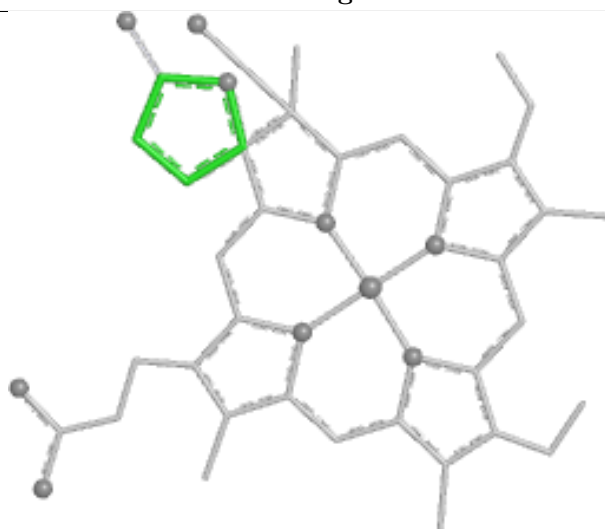
Bond lengths



Bond angles

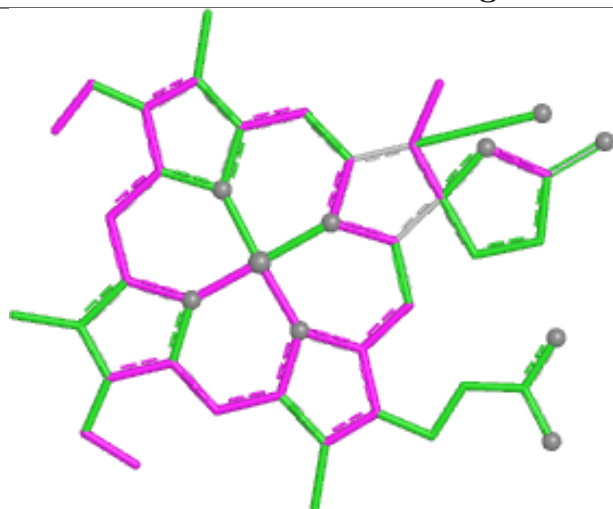


Torsions

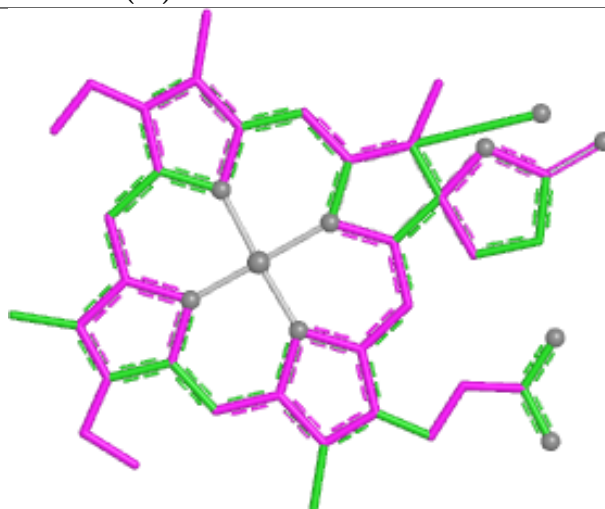


Rings

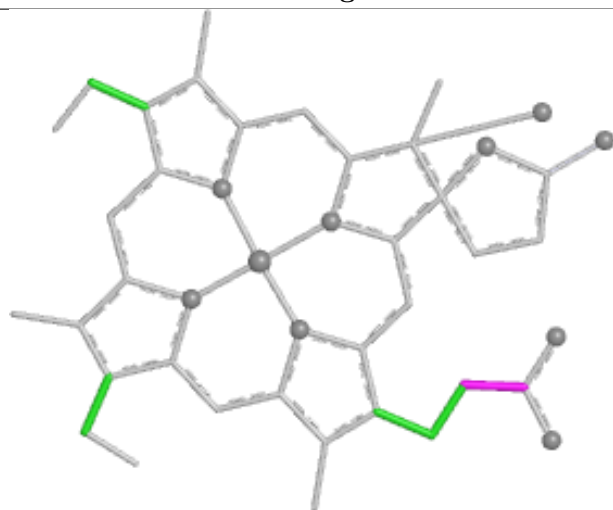
Ligand HDE C 761 (B)



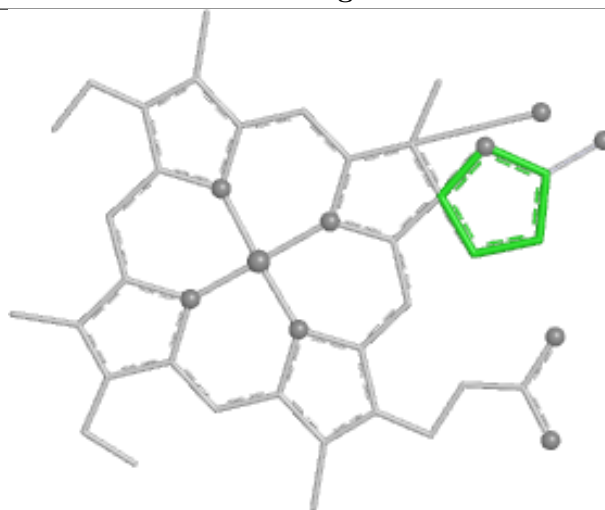
Bond lengths



Bond angles

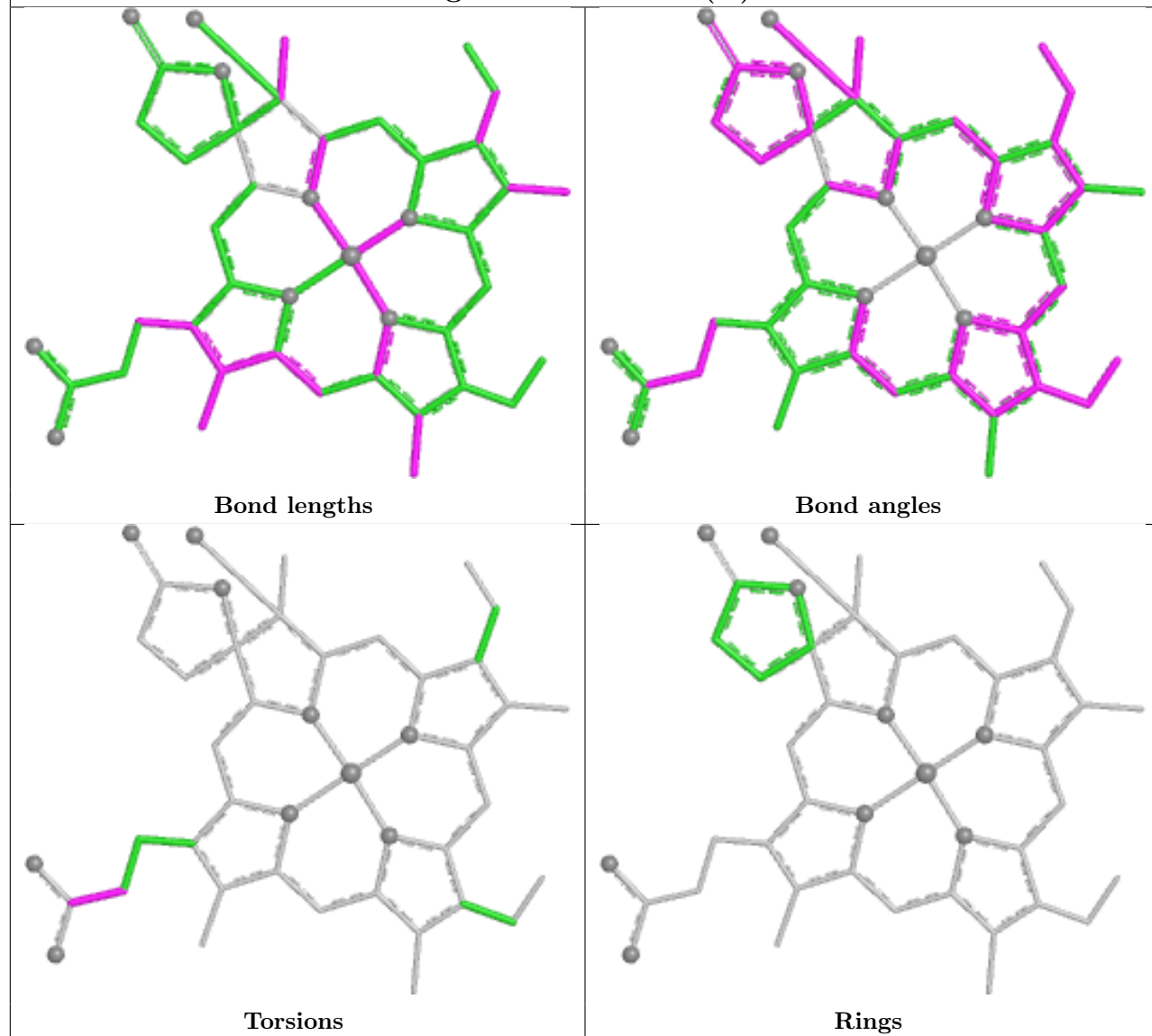


Torsions

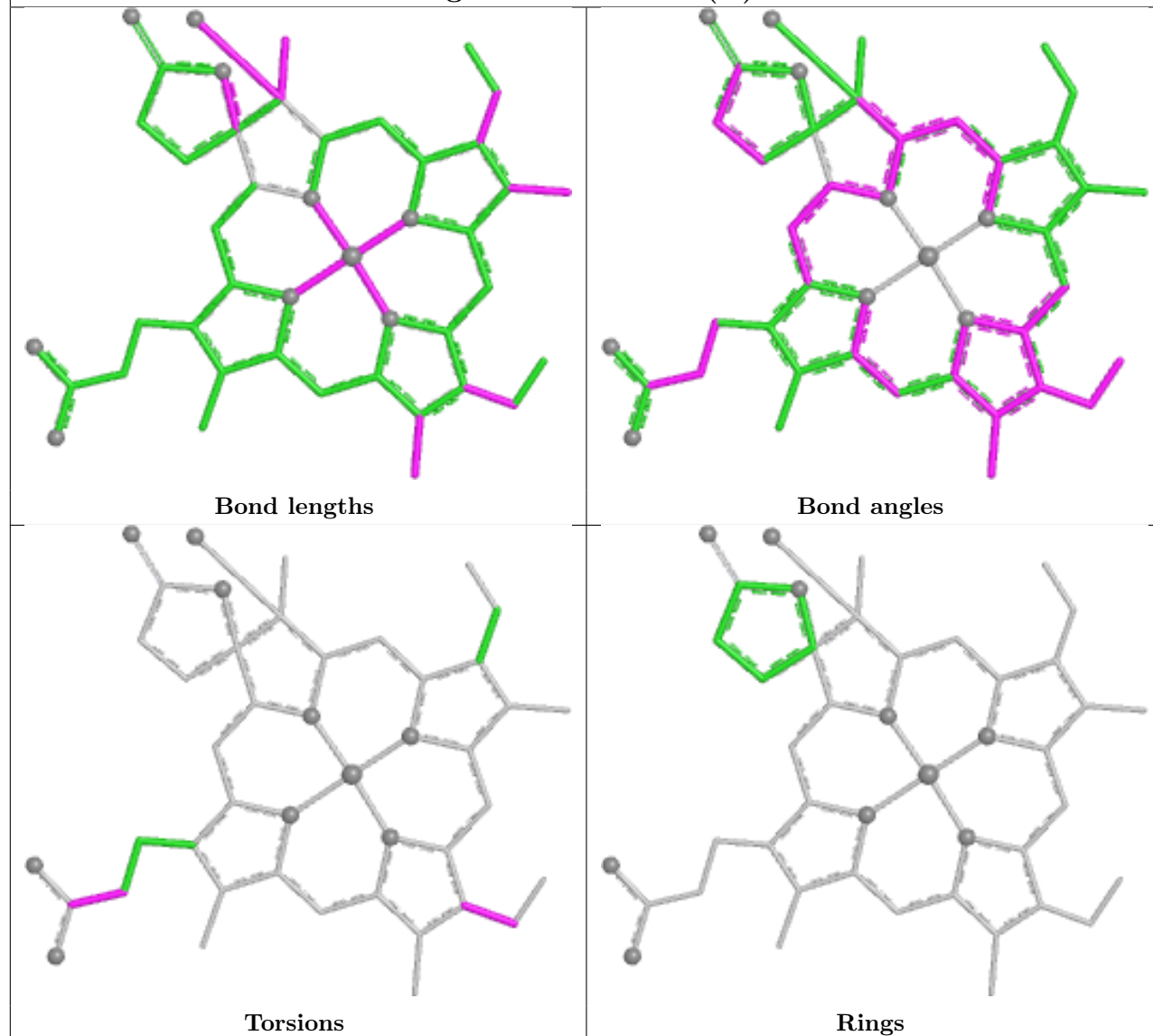


Rings

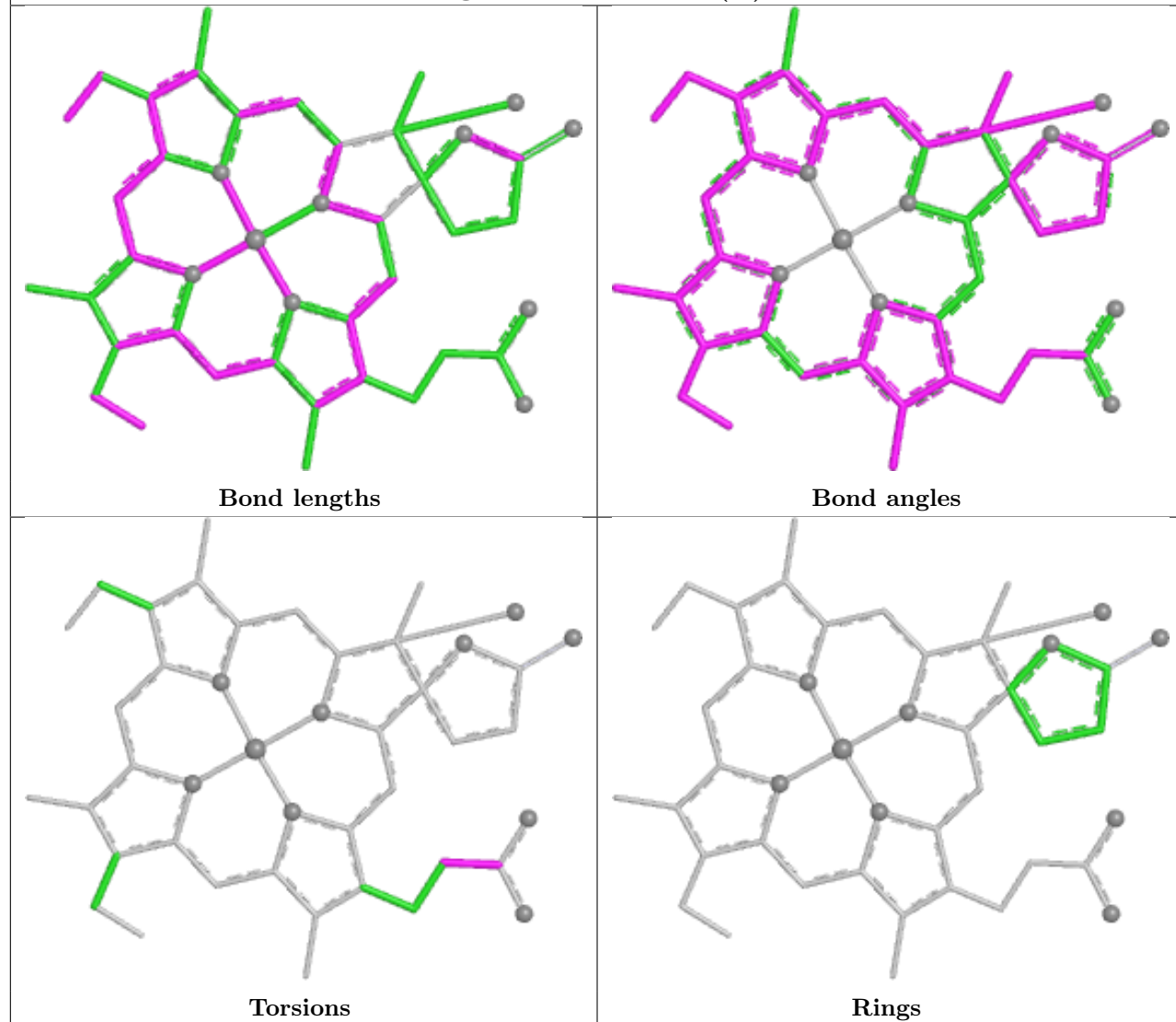
Ligand HDD B 760 (A)



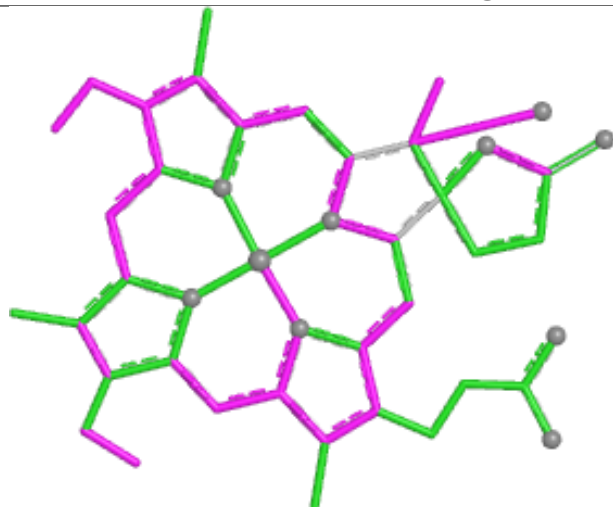
Ligand HDD A 760 (A)



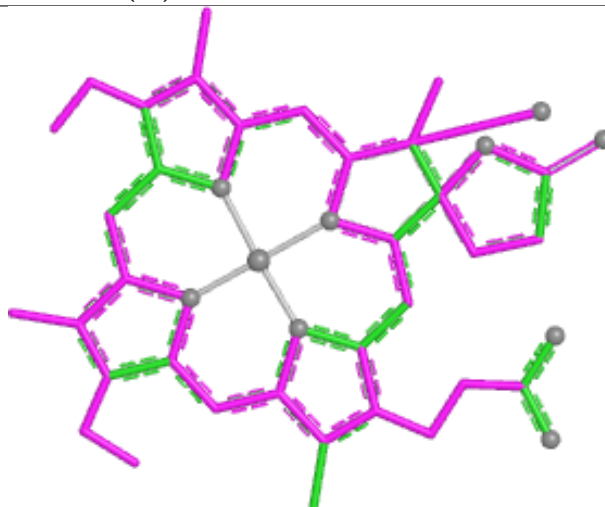
Ligand HDE B 761 (B)



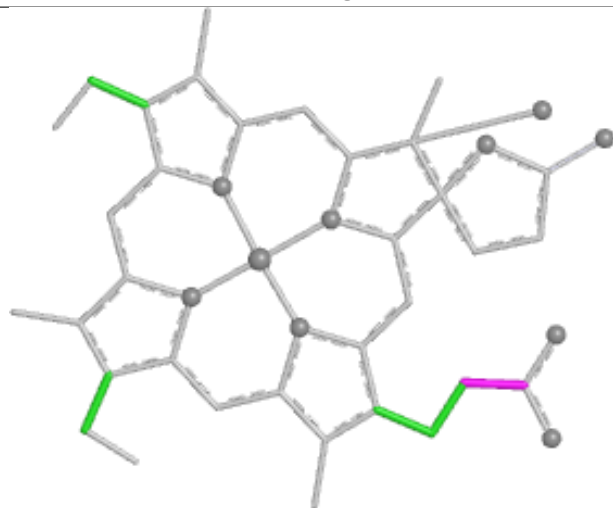
Ligand HDE D 761 (B)



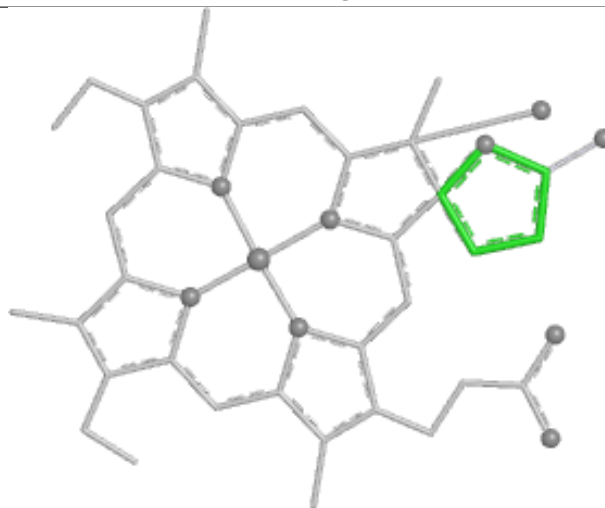
Bond lengths



Bond angles

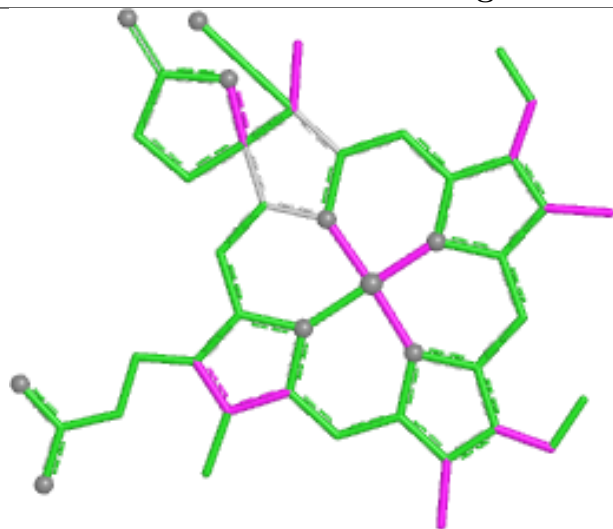


Torsions

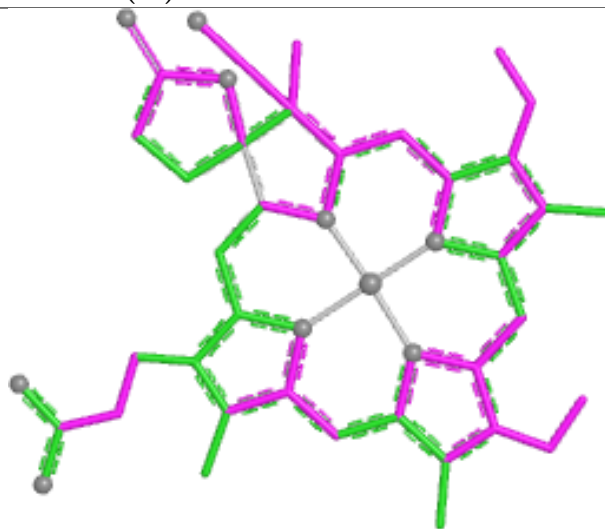


Rings

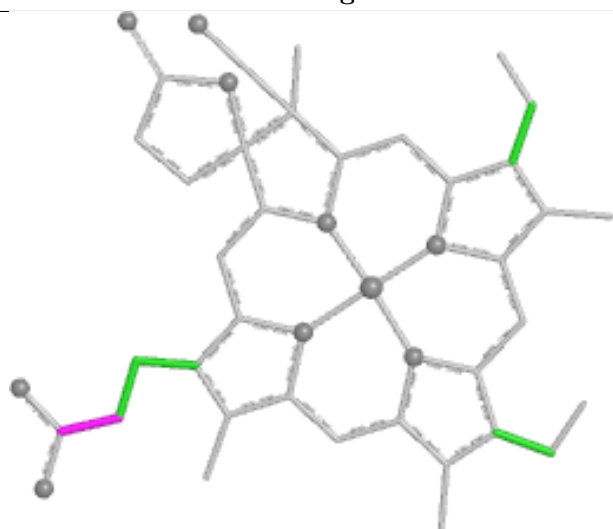
Ligand HDD C 760 (A)



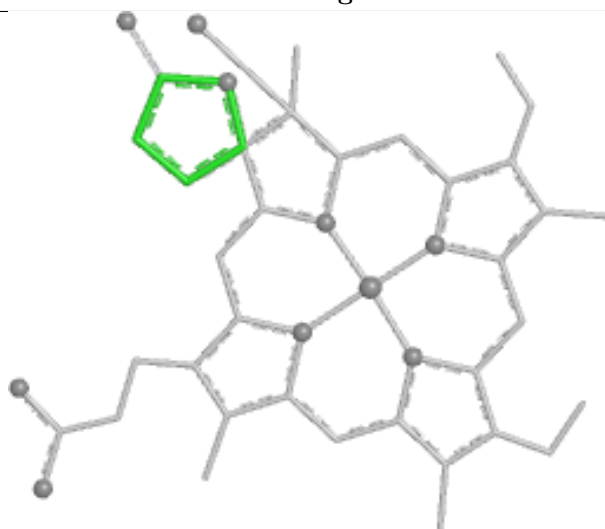
Bond lengths



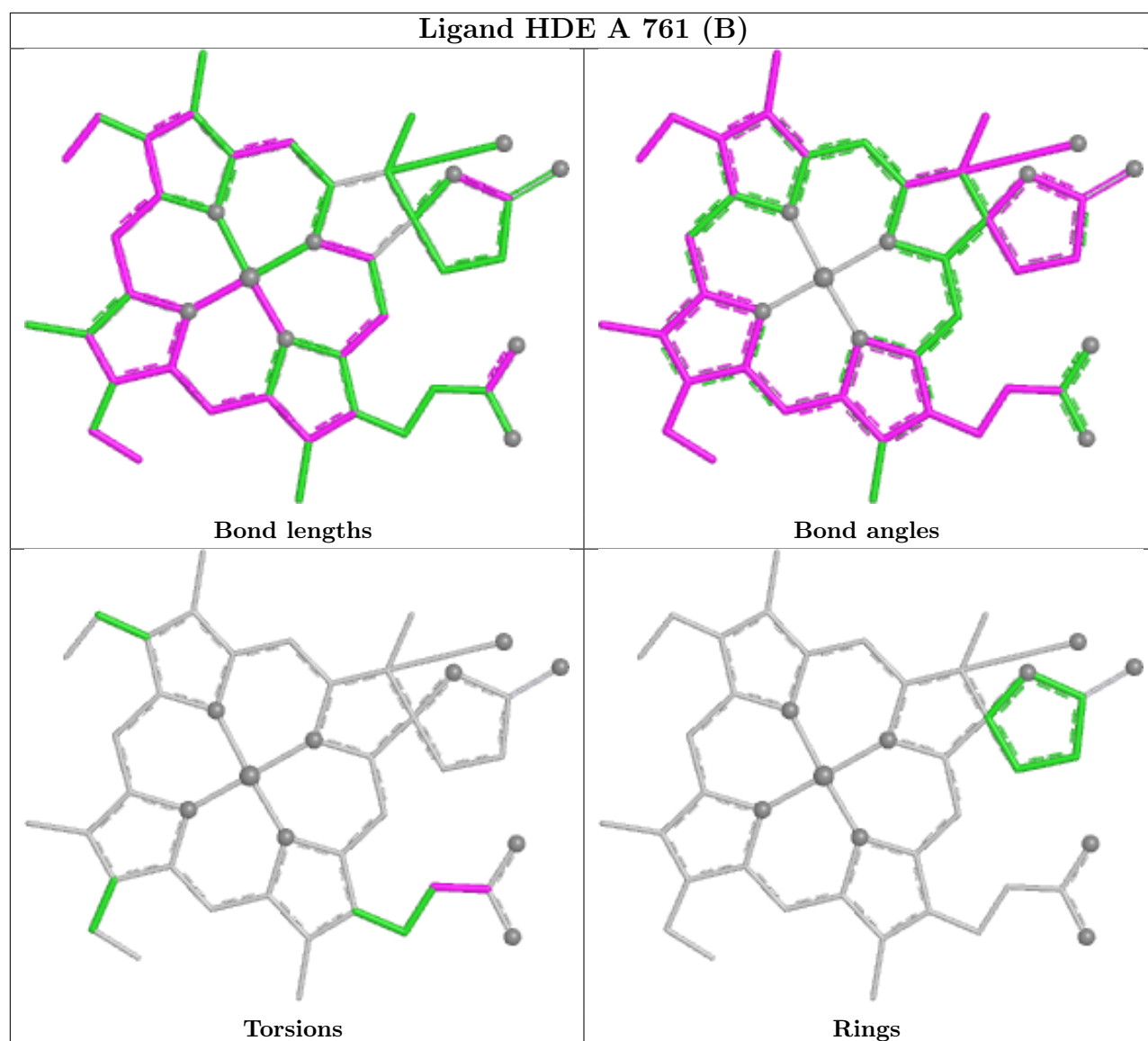
Bond angles



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 [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%)	-0.72	4 (0%) 85 89	3, 10, 25, 45	7 (0%)
1	B	726/753 (96%)	-0.56	6 (0%) 82 86	3, 12, 32, 47	7 (0%)
1	C	726/753 (96%)	-0.61	4 (0%) 85 89	3, 12, 31, 46	6 (0%)
1	D	726/753 (96%)	-0.71	3 (0%) 88 91	3, 10, 26, 45	9 (1%)
All	All	2904/3012 (96%)	-0.65	17 (0%) 85 89	3, 11, 29, 47	29 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	SER	4.9
1	D	28	SER	3.6
1	B	726	GLY	3.0
1	A	713	GLN	2.6
1	B	725	ASP	2.6
1	B	751	ILE	2.4
1	C	724	ALA	2.4
1	D	751	ILE	2.3
1	A	29	LEU	2.3
1	B	583	LYS	2.2
1	B	673	ALA	2.2
1	A	751	ILE	2.1
1	C	725	ASP	2.1
1	B	710	ILE	2.1
1	D	700	ASP	2.1
1	C	750	LYS	2.0
1	C	595	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

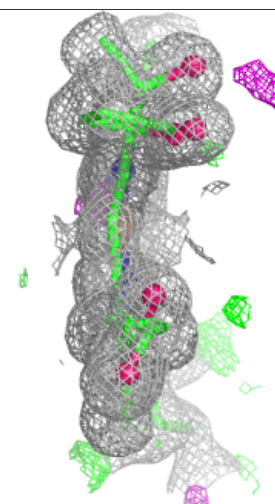
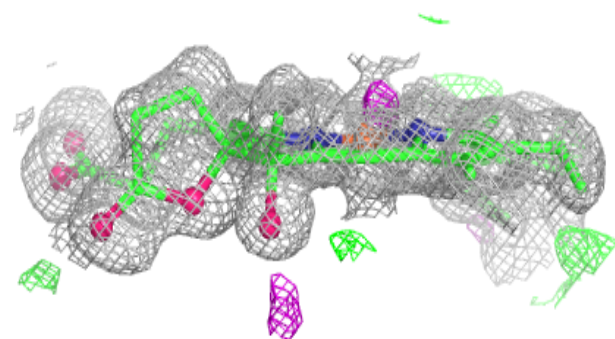
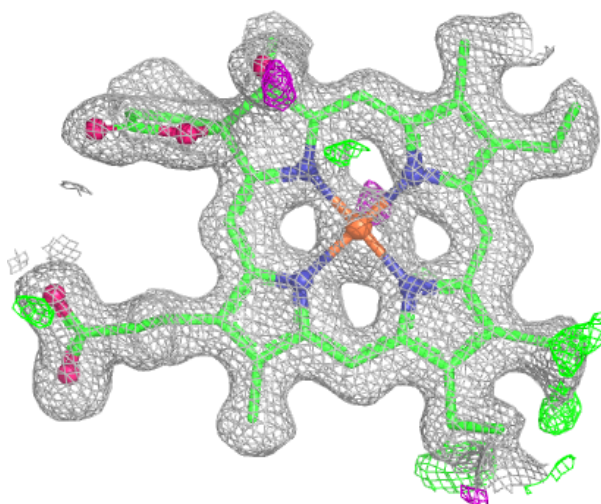
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	H2S	C	754[A]	1/1	0.90	0.11	21,21,21,21	1
4	H2S	D	754[A]	1/1	0.92	0.13	23,23,23,23	1
4	H2S	B	754[A]	1/1	0.93	0.07	22,22,22,22	1
4	H2S	A	754[A]	1/1	0.95	0.08	21,21,21,21	1
3	HDE	A	761[B]	44/44	0.98	0.05	4,10,13,14	44
3	HDE	B	761[B]	44/44	0.98	0.06	2,11,15,18	44
3	HDE	C	761[B]	44/44	0.98	0.05	4,11,14,15	44
3	HDE	D	761[B]	44/44	0.98	0.05	4,11,15,19	44
2	HDD	A	760[A]	44/44	0.99	0.04	2,3,10,14	44
2	HDD	B	760[A]	44/44	0.99	0.04	2,4,8,12	44
2	HDD	C	760[A]	44/44	0.99	0.04	2,5,12,17	44
2	HDD	D	760[A]	44/44	0.99	0.04	2,4,10,15	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.

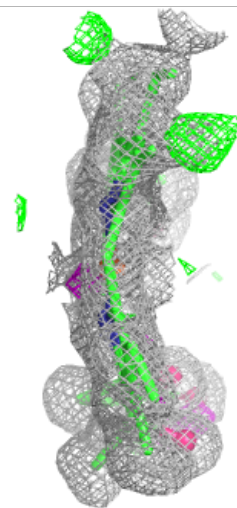
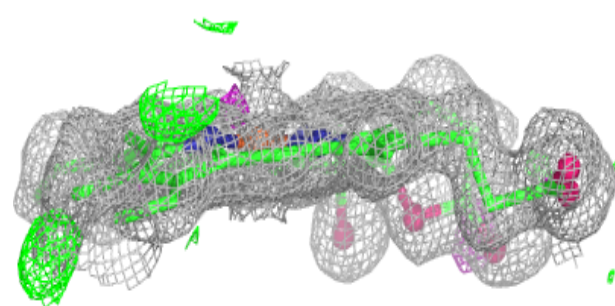
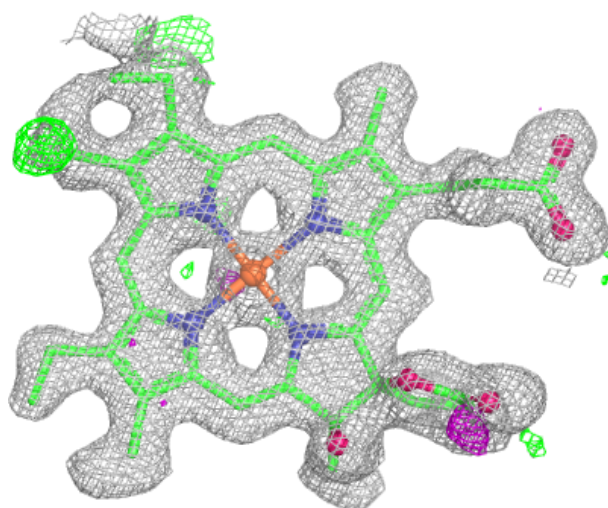
Electron density around HDE A 761 (B):

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



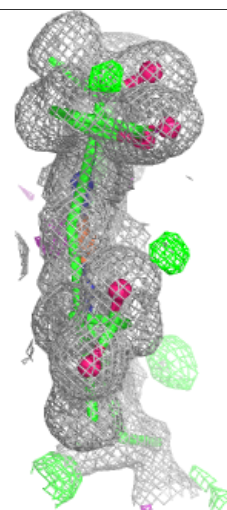
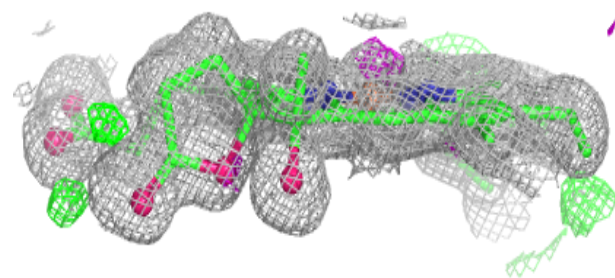
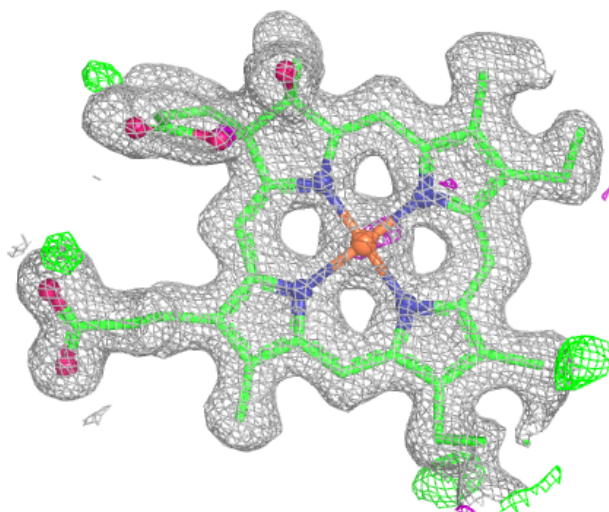
Electron density around HDE B 761 (B):

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



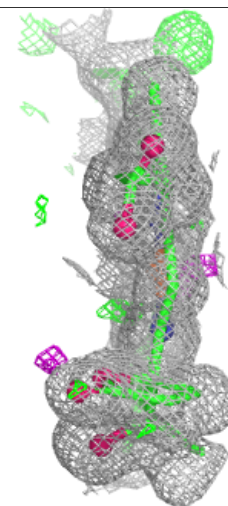
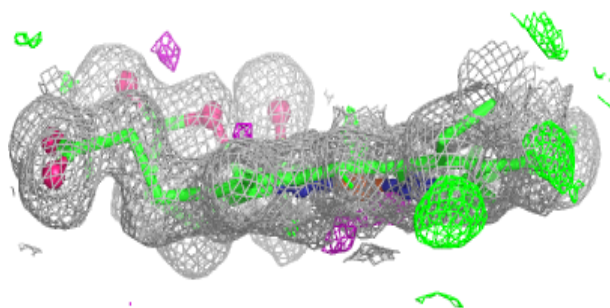
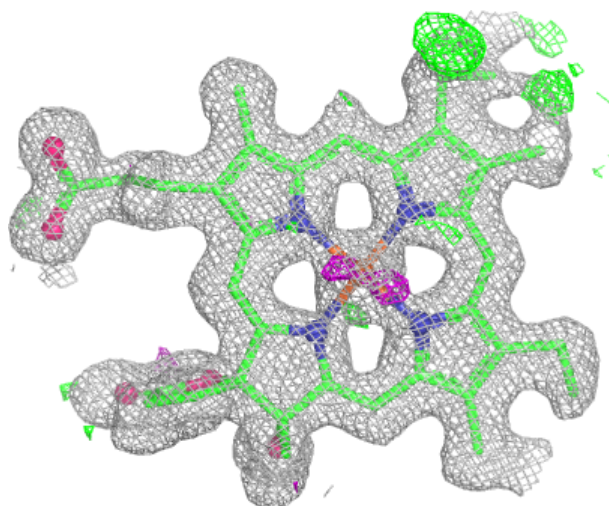
Electron density around HDE C 761 (B):

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



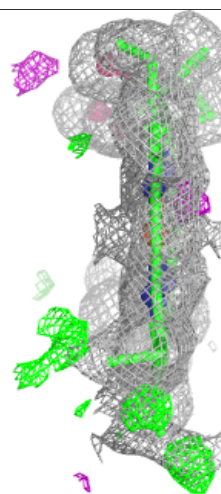
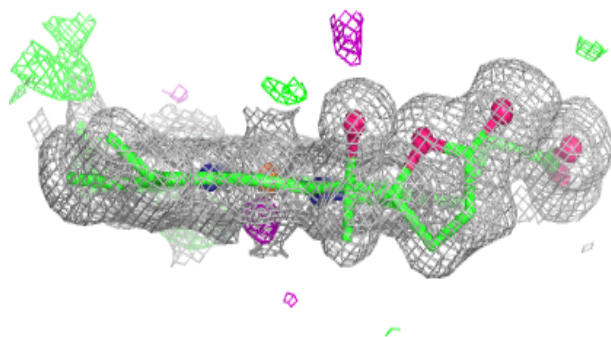
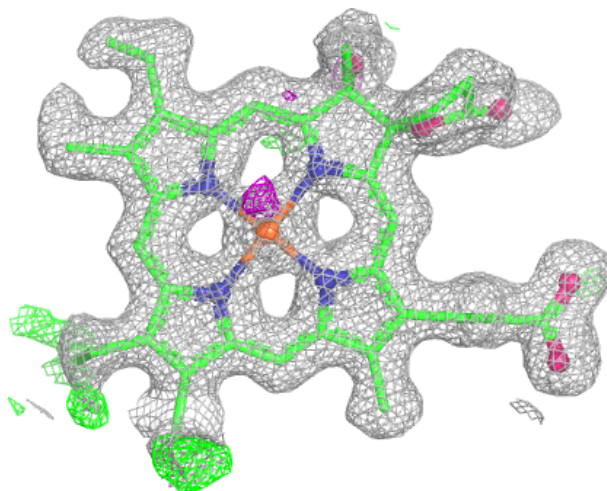
Electron density around HDE D 761 (B):

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



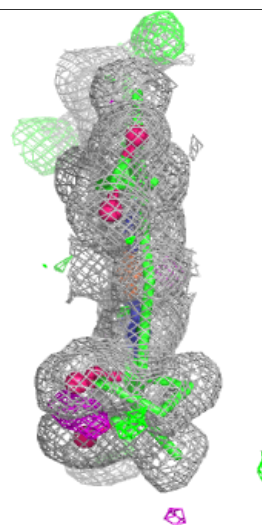
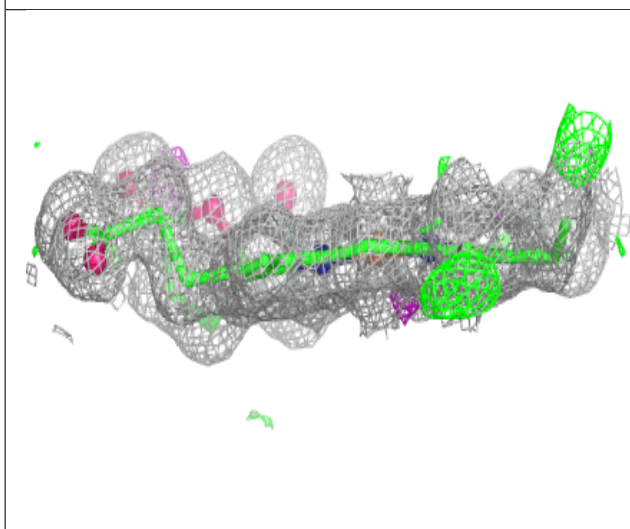
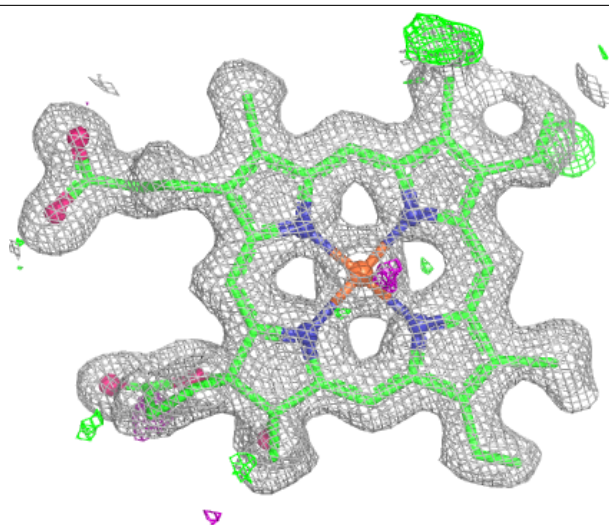
Electron density around HDD A 760 (A):

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



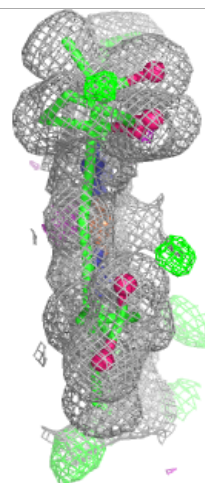
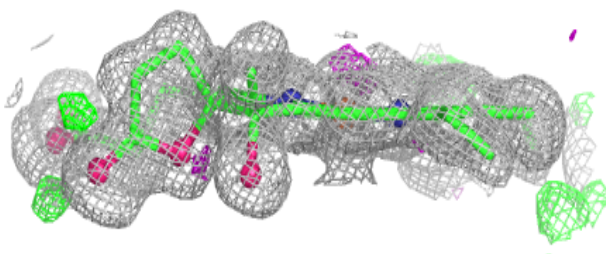
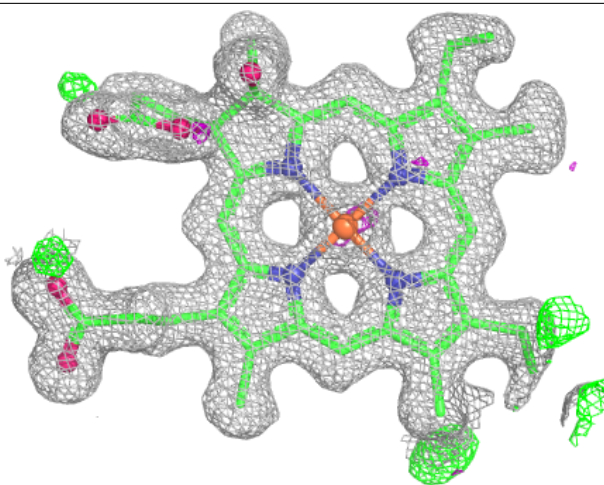
Electron density around HDD B 760 (A):

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and green (positive)



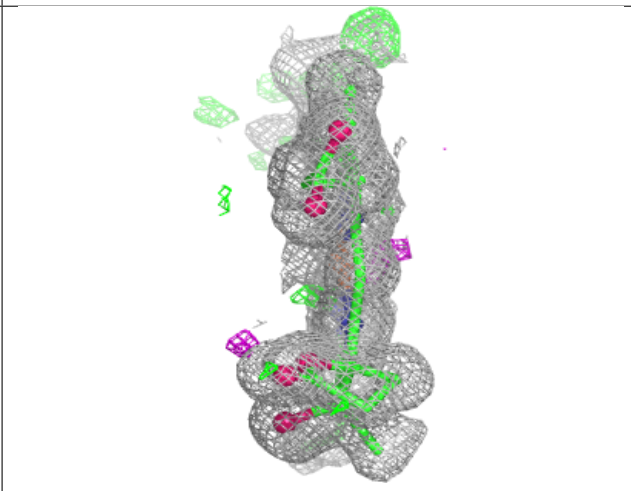
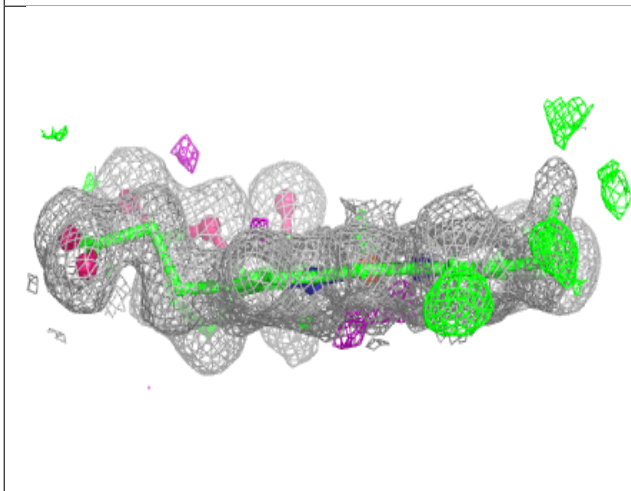
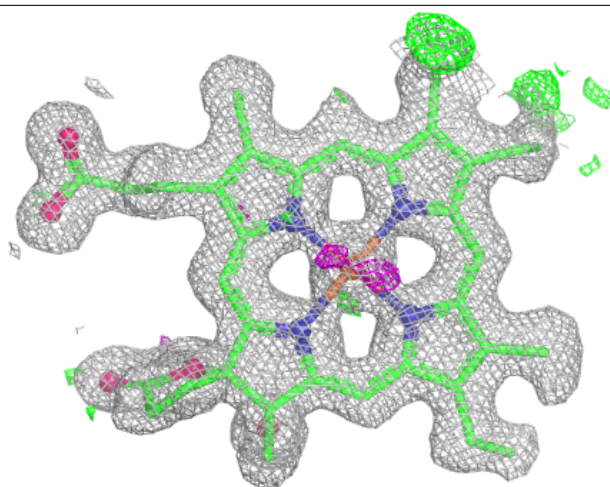
Electron density around HDD C 760 (A):

$2mF_o-DF_c$ (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.