



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 03:44 am BST

PDB ID : 3PQ4
Title : Structure of I274C variant of E. coli KatE[] - Images 13-18
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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

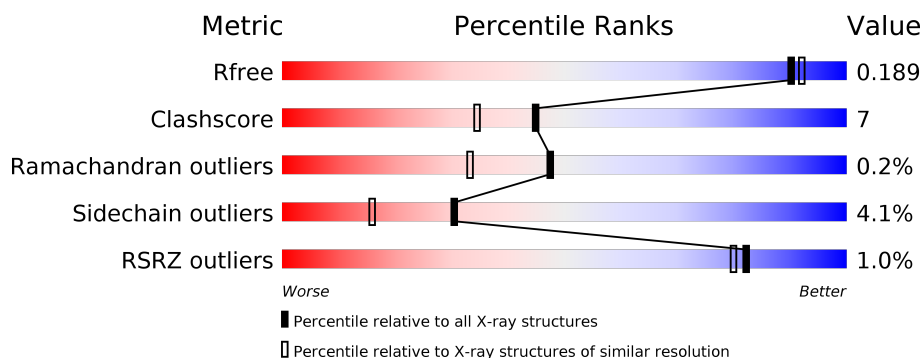
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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 on 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	<div> <div>86%</div> <div>9%</div> <div>• •</div> </div>
1	B	753	<div> <div>2%</div> <div>85%</div> <div>10%</div> <div>• •</div> </div>
1	C	753	<div> <div>%</div> <div>84%</div> <div>10%</div> <div>• •</div> </div>
1	D	753	<div> <div>%</div> <div>86%</div> <div>10%</div> <div>• •</div> </div>

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 crite-

ria:

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

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26821 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.

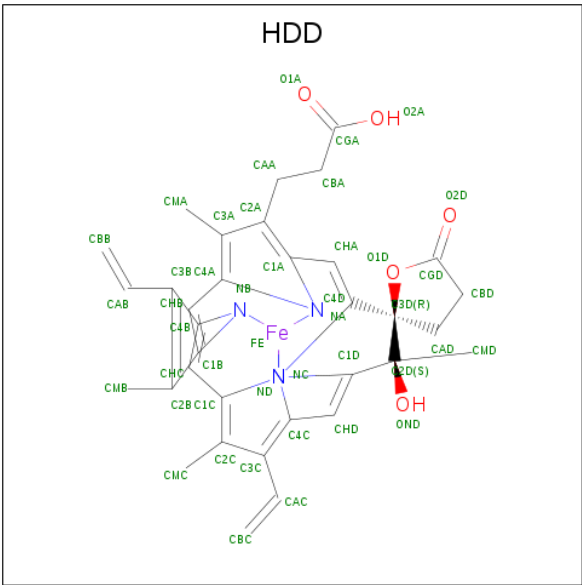
- Molecule 1 is a protein called Catalase HPIL.

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	2	0
			5747	3649	1007	1080	11			
1	D	726	Total	C	N	O	S	0	9	0
			5771	3662	1013	1085	11			

There are 12 discrepancies between the modelled and reference sequences:

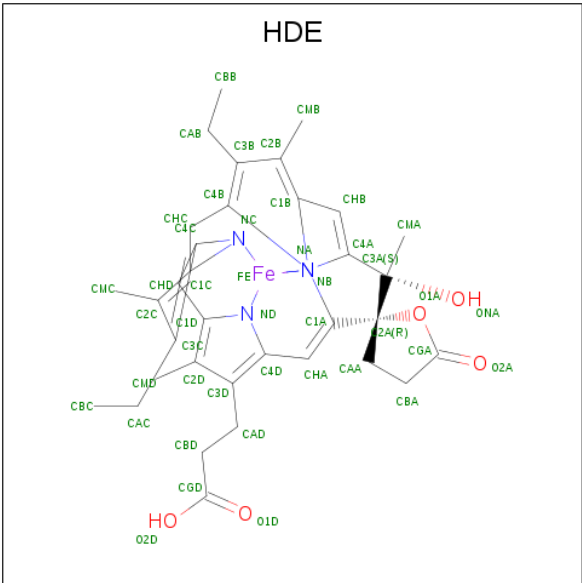
Chain	Residue	Modelled	Actual	Comment	Reference
A	274	CYS	ILE	ENGINEERED MUTATION	UNP P21179
A	438	ALA	CYS	ENGINEERED MUTATION	UNP P21179
A	669	ALA	CYS	ENGINEERED MUTATION	UNP P21179
B	274	CYS	ILE	ENGINEERED MUTATION	UNP P21179
B	438	ALA	CYS	ENGINEERED MUTATION	UNP P21179
B	669	ALA	CYS	ENGINEERED MUTATION	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: C₃₄H₃₂FeN₄O₅).



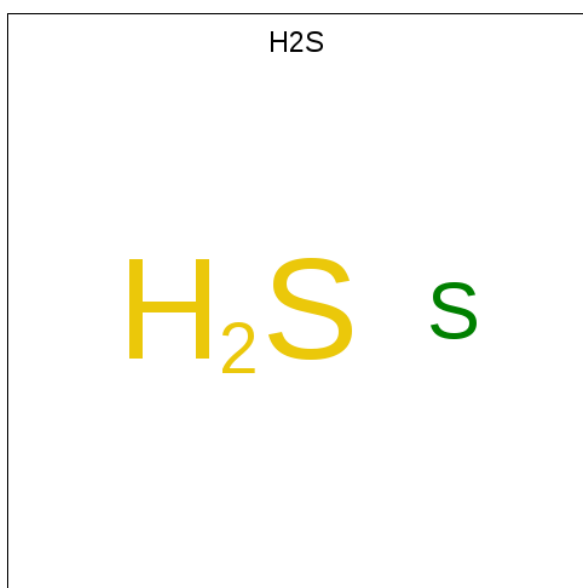
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
2	B	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
2	C	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
2	D	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		

- Molecule 3 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE 17R, 18S (three-letter code: HDE) (formula: C₃₄H₃₈FeN₄O₅).



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: H₂S).



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	896	Total	O	0	0
			896	896		
5	B	788	Total	O	0	0
			788	788		

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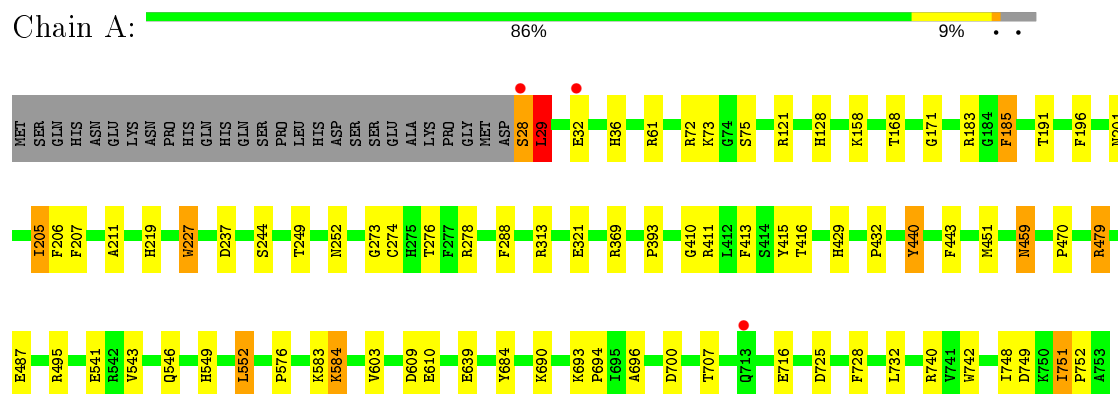
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	838	Total 838	O 838	0	0
5	D	913	Total 913	O 913	0	0

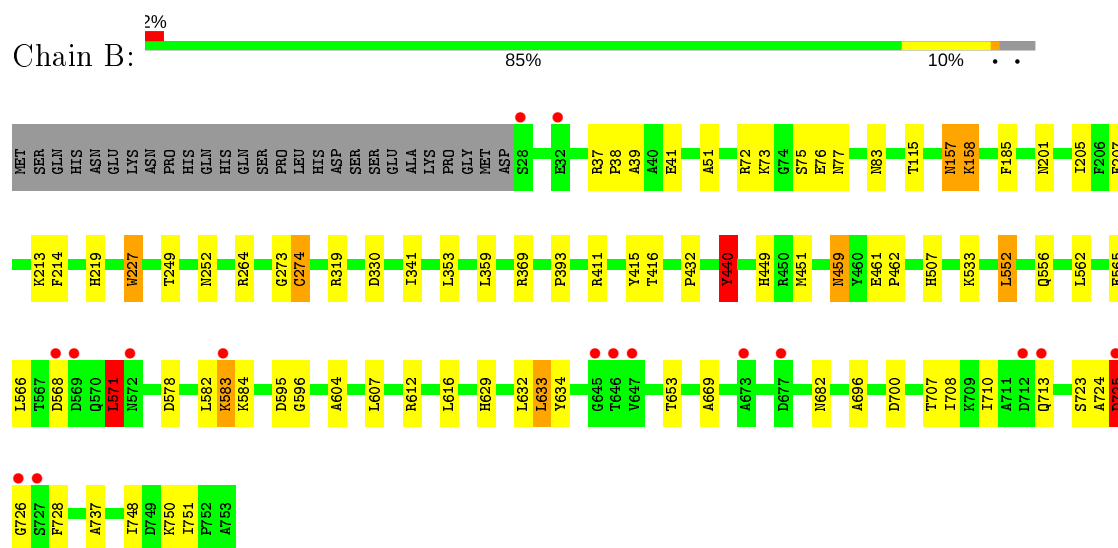
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

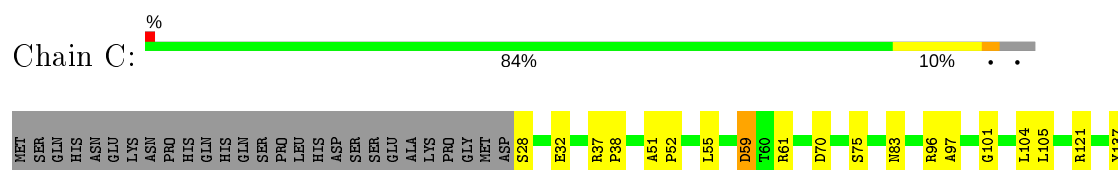
• Molecule 1: Catalase HP1I



• Molecule 1: Catalase HP1I



• Molecule 1: Catalase HP1I





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.51Å 133.03Å 122.65Å 90.00° 109.39° 90.00°	Depositor
Resolution (Å)	35.19 – 1.79 35.19 – 1.79	Depositor EDS
% Data completeness (in resolution range)	92.0 (35.19-1.79) 92.1 (35.19-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 1.79Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.141 , 0.189 0.141 , 0.189	Depositor DCC
R_{free} test set	12136 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	11.7	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	26821	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 3.21% 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	1.18	9/5932 (0.2%)	0.96	10/8064 (0.1%)
1	B	1.11	2/5931 (0.0%)	0.94	5/8062 (0.1%)
1	C	1.14	3/5908 (0.1%)	0.97	12/8033 (0.1%)
1	D	1.19	7/5966 (0.1%)	0.97	14/8109 (0.2%)
All	All	1.15	21/23737 (0.1%)	0.96	41/32268 (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 (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	272	PHE	CE2-CZ	7.73	1.52	1.37
1	D	333	GLU	CD-OE2	-7.34	1.17	1.25
1	A	684	TYR	CD2-CE2	6.67	1.49	1.39
1	A	603	VAL	CB-CG1	-6.55	1.39	1.52
1	D	334	TYR	CD2-CE2	5.89	1.48	1.39
1	D	317	PHE	CE2-CZ	5.78	1.48	1.37
1	C	443	PHE	CE1-CZ	5.73	1.48	1.37
1	D	270	GLU	CD-OE2	-5.70	1.19	1.25
1	A	196	PHE	CE1-CZ	5.51	1.47	1.37
1	B	440	TYR	CE1-CZ	5.50	1.45	1.38
1	A	171	GLY	C-O	5.50	1.32	1.23
1	C	402	PHE	CE1-CZ	5.38	1.47	1.37
1	A	321	GLU	CB-CG	-5.35	1.42	1.52
1	D	206	PHE	CD1-CE1	5.34	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	227	TRP	CB-CG	5.28	1.59	1.50
1	A	29	LEU	N-CA	-5.22	1.35	1.46
1	A	440	TYR	CE1-CZ	5.12	1.45	1.38
1	A	742	TRP	CE3-CZ3	5.10	1.47	1.38
1	D	166	PHE	CE1-CZ	5.06	1.47	1.37
1	C	413	PHE	CE2-CZ	5.04	1.47	1.37
1	A	206	PHE	CE2-CZ	5.00	1.46	1.37

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	636	ARG	NE-CZ-NH1	13.18	126.89	120.30
1	C	636	ARG	NE-CZ-NH2	-12.14	114.23	120.30
1	A	740	ARG	NE-CZ-NH1	7.97	124.29	120.30
1	B	72	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	C	59	ASP	CB-CG-OD1	7.66	125.19	118.30
1	D	521	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	D	582	LEU	CB-CG-CD1	7.40	123.59	111.00
1	C	121	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	C	37	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	479	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	B	72	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	C	70	ASP	CB-CG-OD2	6.45	124.10	118.30
1	C	159	ILE	CB-CG1-CD1	-6.36	96.10	113.90
1	D	495	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	D	377	ARG	NE-CZ-NH1	-6.07	117.27	120.30
1	B	571	LEU	CA-CB-CG	5.85	128.76	115.30
1	A	552	LEU	CB-CG-CD1	5.82	120.90	111.00
1	C	725	ASP	N-CA-C	5.82	126.72	111.00
1	A	313	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	A	72	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	D	155	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	495	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	D	111	ARG	NE-CZ-NH1	-5.69	117.45	120.30
1	C	267	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	B	264	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	B	595	ASP	CB-CG-OD1	-5.46	113.38	118.30
1	C	733	LEU	CA-CB-CG	5.41	127.74	115.30
1	A	185	PHE	CB-CG-CD2	-5.40	117.02	120.80
1	A	121	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	D	183	ARG	NE-CZ-NH1	-5.29	117.65	120.30
1	D	700	ASP	CB-CG-OD1	5.28	123.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	422	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	D	612	ARG	NE-CZ-NH2	5.23	122.92	120.30
1	D	350	ASP	CB-CG-OD1	-5.22	113.60	118.30
1	A	609	ASP	CB-CG-OD2	5.12	122.90	118.30
1	C	96	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	D	377	ARG	NH1-CZ-NH2	5.05	124.95	119.40
1	D	377	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	183	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	D	290	ARG	NE-CZ-NH1	-5.01	117.79	120.30
1	D	61	ARG	NE-CZ-NH1	-5.01	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

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	66	0
1	B	5757	0	5587	68	0
1	C	5747	0	5577	68	1
1	D	5771	0	5598	49	0
2	A	44	0	31	12	0
2	B	44	0	31	15	0
2	C	44	0	30	15	0
2	D	44	0	31	10	0
3	A	44	0	36	11	0
3	B	44	0	36	14	0
3	C	44	0	36	14	0
3	D	44	0	36	11	0
4	A	1	0	0	8	0
4	B	1	0	0	5	0
4	C	1	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1	0	0	7	0
5	A	896	0	0	14	2
5	B	788	0	0	14	0
5	C	838	0	0	18	0
5	D	913	0	0	25	2
All	All	26821	0	22611	300	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (300) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:CYS:HB3	4:A:754:H2S:S	1.24	1.67
1:C:274:CYS:HB3	4:C:754:H2S:S	1.33	1.67
1:D:274:CYS:HB3	4:D:754:H2S:S	1.36	1.64
2:B:760[A]:HDD:HBB2	4:B:754:H2S:S	1.42	1.56
1:B:274:CYS:HB3	4:B:754:H2S:S	1.51	1.49
2:A:760[A]:HDD:HBB2	4:A:754:H2S:S	1.51	1.49
2:C:760[A]:HDD:CBB	4:C:754:H2S:S	2.06	1.43
2:D:760[A]:HDD:HBB2	4:D:754:H2S:S	1.66	1.35
1:A:274:CYS:CB	4:A:754:H2S:S	2.19	1.30
2:A:760[A]:HDD:CBB	4:A:754:H2S:S	2.19	1.29
1:B:449[A]:HIS:CD2	5:B:3614:HOH:O	1.67	1.26
1:D:449[B]:HIS:CE1	5:D:3616:HOH:O	1.65	1.25
1:C:274:CYS:CB	4:C:754:H2S:S	2.25	1.24
2:B:760[A]:HDD:CBB	4:B:754:H2S:S	2.26	1.23
1:D:274:CYS:CB	4:D:754:H2S:S	2.29	1.19
3:D:761[B]:HDE:HMC	3:D:761[B]:HDE:HBCB	1.20	1.19
3:B:761[B]:HDE:CBC	3:B:761[B]:HDE:HMC	1.73	1.18
2:C:760[A]:HDD:CMB	2:C:760[A]:HDD:HBB1	1.73	1.18
1:B:451:MET:SD	5:B:3614:HOH:O	2.00	1.16
1:D:451:MET:SD	5:D:3617:HOH:O	2.00	1.16
2:D:760[A]:HDD:CBB	4:D:754:H2S:S	2.34	1.15
1:B:274:CYS:CB	4:B:754:H2S:S	2.36	1.13
1:C:578:ASP:HB3	5:C:2919:HOH:O	1.48	1.13
3:B:761[B]:HDE:HBCA	3:B:761[B]:HDE:HMC	1.22	1.09
1:A:716:GLU:HG2	5:A:3090:HOH:O	1.52	1.09
3:A:761[B]:HDE:HBCB	3:A:761[B]:HDE:HMC	1.28	1.09
3:C:761[B]:HDE:HBCB	3:C:761[B]:HDE:HMC	1.11	1.06
1:C:267:ARG:HG3	5:C:2916:HOH:O	1.56	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ASN:CG	2:A:760[A]:HDD:HMB2	1.76	1.04
1:B:416:THR:HG21	5:D:2464:HOH:O	1.56	1.04
3:C:761[B]:HDE:CBC	3:C:761[B]:HDE:HMC	1.86	1.03
2:C:760[A]:HDD:CBB	2:C:760[A]:HDD:HMB1	1.82	1.02
1:C:451:MET:SD	5:C:3612:HOH:O	2.17	1.02
3:C:761[B]:HDE:CBB	3:C:761[B]:HDE:HMB	1.90	1.01
1:C:201:ASN:CG	2:C:760[A]:HDD:HMB2	1.83	1.00
1:D:201:ASN:CG	2:D:760[A]:HDD:HMB2	1.82	0.99
1:B:201:ASN:CG	2:B:760[A]:HDD:HMB2	1.84	0.98
1:B:449[A]:HIS:NE2	5:B:3614:HOH:O	1.67	0.96
3:C:761[B]:HDE:CMC	3:C:761[B]:HDE:HBCB	1.90	0.96
3:B:761[B]:HDE:CMC	3:B:761[B]:HDE:HBCA	1.93	0.95
3:C:761[B]:HDE:HBBA	3:C:761[B]:HDE:HMB	1.48	0.94
1:A:610:GLU:HG2	5:A:3555:HOH:O	1.65	0.93
1:A:274:CYS:SG	2:A:760[A]:HDD:CMB	2.55	0.93
3:B:761[B]:HDE:CBB	3:B:761[B]:HDE:HMB	1.99	0.93
2:C:760[A]:HDD:HBB1	2:C:760[A]:HDD:HMB1	0.93	0.93
1:A:416[A]:THR:HG21	5:C:3313:HOH:O	1.69	0.92
1:A:274:CYS:SG	2:A:760[A]:HDD:HMB3	2.11	0.90
3:B:761[B]:HDE:HBBB	3:B:761[B]:HDE:HMB	1.50	0.90
3:A:761[B]:HDE:CBC	3:A:761[B]:HDE:HMC	2.00	0.90
1:A:201:ASN:ND2	2:A:760[A]:HDD:HMB2	1.88	0.88
1:A:541:GLU:OE2	5:A:2550:HOH:O	1.91	0.88
1:D:274:CYS:SG	2:D:760[A]:HDD:CMB	2.61	0.88
1:A:28:SER:OG	1:A:28:SER:O	1.85	0.86
1:C:274:CYS:SG	2:C:760[A]:HDD:HMB3	2.16	0.86
1:C:274:CYS:SG	2:C:760[A]:HDD:CMB	2.64	0.85
1:C:713:GLN:HB3	5:C:3004:HOH:O	1.76	0.84
3:B:761[B]:HDE:CMC	3:B:761[B]:HDE:CBC	2.45	0.84
3:D:761[B]:HDE:CMC	3:D:761[B]:HDE:HBCB	2.01	0.83
1:A:274:CYS:SG	2:A:760[A]:HDD:HMB1	2.18	0.82
1:D:274:CYS:SG	2:D:760[A]:HDD:HMB1	2.19	0.82
3:B:761[B]:HDE:HBCB	3:B:761[B]:HDE:HMC	1.61	0.82
1:C:440:TYR:HD1	5:C:3454:HOH:O	1.62	0.81
3:C:761[B]:HDE:CMC	3:C:761[B]:HDE:CBC	2.55	0.80
1:D:274:CYS:SG	2:D:760[A]:HDD:HMB3	2.22	0.80
1:D:267:ARG:HG3	5:D:1920:HOH:O	1.85	0.76
3:C:761[B]:HDE:HBBB	3:C:761[B]:HDE:HMB	1.65	0.76
1:A:751:ILE:O	1:A:751:ILE:HD13	1.86	0.76
3:D:761[B]:HDE:HMC	4:D:754:H2S:S	2.26	0.75
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:GLU:CG	5:A:3555:HOH:O	2.30	0.75
3:D:761[B]:HDE:HMC	3:D:761[B]:HDE:CBC	2.10	0.75
1:A:451:MET:SD	5:A:3609:HOH:O	2.44	0.74
1:D:201:ASN:ND2	2:D:760[A]:HDD:HMB2	2.02	0.74
1:C:201:ASN:ND2	2:C:760[A]:HDD:HMB2	2.03	0.73
1:D:731:GLU:OE2	5:D:3028:HOH:O	2.06	0.73
1:A:29:LEU:HD22	5:C:2405:HOH:O	1.88	0.72
1:D:449[A]:HIS:HD2	5:D:3615:HOH:O	1.72	0.71
1:C:578:ASP:HB2	1:C:582:LEU:O	1.91	0.70
1:B:700:ASP:HB2	5:B:3595:HOH:O	1.92	0.69
1:B:201:ASN:ND2	2:B:760[A]:HDD:HMB2	2.08	0.69
1:D:703:LYS:NZ	5:D:2744:HOH:O	2.25	0.68
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.77	0.68
1:C:274:CYS:HB3	2:C:760[A]:HDD:CBB	2.24	0.67
1:A:274:CYS:HB3	2:A:760[A]:HDD:CBB	2.24	0.67
1:B:449[B]:HIS:HD2	5:B:3613:HOH:O	1.76	0.67
1:B:274:CYS:SG	2:B:760[A]:HDD:CMB	2.84	0.66
1:C:274:CYS:SG	2:C:760[A]:HDD:HMB1	2.30	0.66
1:C:274:CYS:SG	2:C:760[A]:HDD:HBB1	2.34	0.66
1:D:556:GLN:NE2	5:D:2773:HOH:O	2.29	0.66
1:A:639:GLU:HG3	5:A:2414:HOH:O	1.96	0.66
3:C:761[B]:HDE:HMC	4:C:754:H2S:S	2.37	0.65
1:A:29:LEU:HB2	5:C:2405:HOH:O	1.97	0.65
1:D:639:GLU:OE1	5:D:2189:HOH:O	2.14	0.64
1:A:36:HIS:HE1	5:A:1872:HOH:O	1.80	0.64
3:B:761[B]:HDE:CMC	3:B:761[B]:HDE:HBCB	2.21	0.64
1:B:724:ALA:O	1:B:725:ASP:O	2.14	0.64
1:B:274:CYS:SG	2:B:760[A]:HDD:HMB3	2.37	0.64
1:D:449[B]:HIS:NE2	5:D:3616:HOH:O	1.93	0.64
1:B:115:THR:HG21	5:B:3420:HOH:O	1.98	0.64
1:A:274:CYS:CB	2:A:760[A]:HDD:CBB	2.76	0.64
1:C:725:ASP:O	5:C:2403:HOH:O	2.15	0.63
1:D:28:SER:HA	5:D:2467:HOH:O	1.99	0.63
1:B:748:ILE:O	1:B:751:ILE:HG22	1.99	0.62
1:A:416[B]:THR:HG22	5:A:900:HOH:O	2.00	0.61
3:C:761[B]:HDE:CMB	3:C:761[B]:HDE:HBBA	2.26	0.61
1:A:61:ARG:HD2	5:A:3208:HOH:O	2.00	0.61
3:B:761[B]:HDE:HBBA	3:B:761[B]:HDE:HMB	1.80	0.61
1:A:610:GLU:CD	5:A:3555:HOH:O	2.39	0.61
1:B:449[B]:HIS:HE1	5:D:1789:HOH:O	1.83	0.61
3:A:761[B]:HDE:CBC	3:A:761[B]:HDE:CMC	2.73	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:636:ARG:HD3	5:C:2717:HOH:O	2.00	0.60
3:A:761[B]:HDE:CBB	3:A:761[B]:HDE:HMB	2.31	0.60
1:B:726:GLY:HA2	5:B:3590:HOH:O	2.00	0.60
1:B:583:LYS:O	1:B:584:LYS:HB3	2.02	0.60
1:D:629:HIS:HD2	5:D:1554:HOH:O	1.83	0.60
1:C:59:ASP:OD2	5:C:2529:HOH:O	2.16	0.60
1:B:533[A]:LYS:HE2	5:B:3100:HOH:O	2.00	0.59
1:C:629:HIS:HD2	5:C:1129:HOH:O	1.84	0.59
1:A:244:SER:HA	1:A:546[B]:GLN:NE2	2.17	0.59
1:A:201:ASN:ND2	2:A:760[A]:HDD:CMB	2.64	0.59
2:A:760[A]:HDD:CAB	4:A:754:H2S:S	2.88	0.58
1:D:748:ILE:O	1:D:751:ILE:HG22	2.02	0.58
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.84	0.58
1:C:521:ARG:NH1	1:C:521:ARG:HG2	2.18	0.58
1:D:509:ARG:HD2	1:D:576:PRO:HD2	1.85	0.57
3:D:761[B]:HDE:CMC	3:D:761[B]:HDE:CBC	2.76	0.57
3:B:761[B]:HDE:HMC	4:B:754:H2S:S	2.44	0.57
1:C:449[A]:HIS:HD2	5:C:3611:HOH:O	1.86	0.57
1:B:274:CYS:SG	2:B:760[A]:HDD:HMB1	2.45	0.57
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.87	0.56
3:A:761[B]:HDE:HBCB	3:A:761[B]:HDE:CMC	2.14	0.56
1:B:708:ILE:HG13	1:B:710:ILE:HG12	1.88	0.56
1:C:704:PHE:O	1:C:707:THR:HG22	2.06	0.56
2:B:760[A]:HDD:HBB1	2:B:760[A]:HDD:HMB1	1.88	0.56
1:A:690:LYS:HG3	1:A:751:ILE:HD11	1.87	0.55
1:A:29:LEU:HD23	5:C:3144:HOH:O	2.07	0.55
1:A:479:ARG:NH2	5:A:2607:HOH:O	2.30	0.55
1:C:359:LEU:H	1:C:507:HIS:HD2	1.55	0.55
1:B:73:LYS:CD	5:D:3517:HOH:O	2.55	0.55
1:C:214:PHE:CD2	2:C:760[A]:HDD:HMC2	2.42	0.55
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.10	0.55
1:C:634:TYR:O	1:C:653:THR:HA	2.07	0.55
3:D:761[B]:HDE:HMB	3:D:761[B]:HDE:CBB	2.36	0.55
1:D:552:LEU:HD11	1:D:571:LEU:HA	1.88	0.54
3:D:761[B]:HDE:HBCB	4:D:754:H2S:S	2.48	0.54
2:D:760[A]:HDD:CAB	4:D:754:H2S:S	2.95	0.54
3:B:761[B]:HDE:CMB	3:B:761[B]:HDE:CBB	2.75	0.54
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.23	0.53
1:B:73:LYS:HE3	5:D:3517:HOH:O	2.08	0.53
1:B:359:LEU:H	1:B:507:HIS:HD2	1.55	0.53
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:TYR:O	1:D:73[B]:LYS:HE3	2.08	0.53
1:B:115:THR:CG2	5:B:3420:HOH:O	2.54	0.53
3:A:761[B]:HDE:HBCB	4:A:754:H2S:S	2.49	0.52
2:C:760[A]:HDD:HMD1	2:C:760[A]:HDD:HBD2	1.91	0.52
1:B:583:LYS:NZ	1:B:583:LYS:H	2.08	0.52
1:A:748:ILE:O	1:A:751:ILE:HD12	2.09	0.52
1:A:751:ILE:HD13	1:A:751:ILE:C	2.30	0.52
1:C:368:GLN:NE2	5:C:1787:HOH:O	2.26	0.52
1:A:725:ASP:H	1:A:728:PHE:HB3	1.76	0.51
1:C:359:LEU:H	1:C:507:HIS:CD2	2.29	0.51
1:D:677:ASP:HB2	5:D:3257:HOH:O	2.10	0.51
1:C:274:CYS:CB	2:C:760[A]:HDD:CBB	2.88	0.51
2:A:760[A]:HDD:HMC1	2:A:760[A]:HDD:CBC	2.41	0.51
3:A:761[B]:HDE:HBBA	3:A:761[B]:HDE:HMB	1.92	0.51
1:B:596:GLY:HA3	1:B:737:ALA:O	2.11	0.51
1:C:38:PRO:HG2	1:C:51:ALA:HB2	1.93	0.51
1:A:274:CYS:CA	4:A:754:H2S:S	2.96	0.50
1:B:629:HIS:HD2	5:B:1053:HOH:O	1.93	0.50
5:A:1788:HOH:O	1:C:449[A]:HIS:HE1	1.92	0.50
1:B:201:ASN:ND2	2:B:760[A]:HDD:CMB	2.74	0.50
1:A:751:ILE:O	1:A:751:ILE:CD1	2.58	0.49
3:B:761[B]:HDE:CMB	3:B:761[B]:HDE:HBBB	2.30	0.49
1:B:39:ALA:HB1	1:B:41:GLU:HG2	1.94	0.49
1:B:73:LYS:CE	5:D:3517:HOH:O	2.60	0.49
1:B:411:ARG:HG2	3:B:761[B]:HDE:C3B	2.42	0.49
1:A:696:ALA:HB1	1:A:728:PHE:CZ	2.47	0.49
1:A:73:LYS:HE3	1:C:440:TYR:O	2.13	0.49
1:B:76:GLU:O	1:B:77:ASN:HB2	2.13	0.49
3:D:761[B]:HDE:HBBB	3:D:761[B]:HDE:HMB	1.95	0.48
1:B:578:ASP:HB3	1:B:582:LEU:O	2.12	0.48
1:D:449[A]:HIS:HE1	5:D:1789:HOH:O	1.96	0.48
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.97	0.48
1:D:574:THR:HG23	5:D:1614:HOH:O	2.13	0.48
1:A:273:GLY:C	1:A:274:CYS:SG	2.92	0.48
1:C:583:LYS:O	1:C:584:LYS:HB3	2.12	0.48
1:C:556:GLN:HG3	1:C:566:LEU:CD1	2.44	0.48
1:C:578:ASP:CB	1:C:582:LEU:O	2.62	0.48
1:C:199:VAL:HG12	3:C:761[B]:HDE:HHDA	1.96	0.47
1:B:369:ARG:HG2	5:B:1639:HOH:O	2.13	0.47
1:C:556:GLN:CG	1:C:566:LEU:HD12	2.44	0.47
1:A:205:ILE:H	1:A:205:ILE:HD13	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:ARG:HG2	3:C:761[B]:HDE:C3B	2.44	0.47
1:B:201:ASN:OD1	2:B:760[A]:HDD:HMB2	2.14	0.47
1:C:748:ILE:O	1:C:751:ILE:HG22	2.15	0.47
1:B:37:ARG:HD3	5:B:2886:HOH:O	2.14	0.47
1:B:157:ASN:HD22	1:B:157:ASN:C	2.18	0.47
2:B:760[A]:HDD:CBB	2:B:760[A]:HDD:HMB1	2.45	0.47
1:C:556:GLN:HG3	1:C:566:LEU:HD12	1.96	0.47
1:B:157:ASN:HD22	1:B:158:LYS:N	2.13	0.47
1:A:543:VAL:HA	1:A:546[B]:GLN:HE21	1.79	0.46
2:B:760[A]:HDD:CMB	2:B:760[A]:HDD:HBB1	2.46	0.46
1:D:359:LEU:HD21	5:D:2971:HOH:O	2.15	0.46
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.31	0.46
1:C:52:PRO:HG2	1:C:55:LEU:HD12	1.98	0.46
1:A:700:ASP:HB2	5:A:3594:HOH:O	2.15	0.46
1:D:260:ARG:HD3	1:D:590:LEU:HD21	1.99	0.45
1:C:28:SER:HA	5:C:2891:HOH:O	2.16	0.45
1:C:696:ALA:HB1	1:C:728:PHE:CZ	2.52	0.45
1:C:359:LEU:C	1:C:359:LEU:HD12	2.37	0.45
1:B:393:PRO:HD2	1:B:415:TYR:CG	2.52	0.45
1:D:201:ASN:ND2	2:D:760[A]:HDD:CMB	2.77	0.45
1:B:274:CYS:SG	2:B:760[A]:HDD:HBB1	2.57	0.44
1:D:359:LEU:H	1:D:507:HIS:HD2	1.65	0.44
1:B:634:TYR:O	1:B:653:THR:HA	2.18	0.44
1:C:578:ASP:CB	5:C:2919:HOH:O	2.31	0.44
1:A:393:PRO:HD2	1:A:415:TYR:CG	2.52	0.44
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.32	0.44
3:B:761[B]:HDE:HMAA	3:B:761[B]:HDE:HAAA	1.80	0.44
3:C:761[B]:HDE:CMB	3:C:761[B]:HDE:CBB	2.68	0.44
1:A:751:ILE:HA	1:A:752:PRO:HD3	1.90	0.44
1:B:359:LEU:H	1:B:507:HIS:CD2	2.33	0.44
1:C:184:GLY:HA3	2:C:760[A]:HDD:HMA2	2.00	0.44
1:B:83:ASN:HB3	1:D:429:HIS:CG	2.53	0.44
3:A:761[B]:HDE:HBBB	3:A:761[B]:HDE:HMB	1.99	0.44
1:A:36:HIS:CD2	1:A:36:HIS:H	2.36	0.44
1:B:319:ARG:HD3	1:C:227:TRP:O	2.17	0.44
1:D:490:GLU:OE1	5:D:2308:HOH:O	2.21	0.44
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.48	0.43
1:B:696:ALA:HB1	1:B:728:PHE:CZ	2.53	0.43
1:D:274:CYS:CB	2:D:760[A]:HDD:CBB	2.96	0.43
1:A:443:PHE:CZ	1:A:470:PRO:HD2	2.54	0.43
1:A:549:HIS:O	1:A:576:PRO:HD3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:GLU:HA	1:B:462:PRO:C	2.37	0.43
1:C:488:ARG:NH1	5:C:2379:HOH:O	2.23	0.43
1:C:521:ARG:CG	1:C:521:ARG:HH11	2.29	0.43
1:A:207:PHE:O	1:A:249:THR:HA	2.17	0.43
1:D:416[B]:THR:HG22	5:D:1415:HOH:O	2.18	0.43
1:A:128:HIS:HA	1:A:168:THR:O	2.19	0.43
1:B:37:ARG:HA	1:B:38:PRO:HD3	1.89	0.43
1:A:413:PHE:HB2	1:C:105:LEU:HD11	2.00	0.43
1:D:751:ILE:HG23	1:D:751:ILE:O	2.18	0.43
1:B:612:ARG:NH2	1:B:723:SER:HA	2.34	0.43
1:D:670:GLY:O	1:D:700:ASP:OD2	2.37	0.43
3:A:761[B]:HDE:HMC	4:A:754:H2S:S	2.59	0.43
1:B:214:PHE:CD2	2:B:760[A]:HDD:HMC2	2.54	0.43
1:D:440:TYR:CZ	5:D:3517:HOH:O	2.55	0.43
1:C:199:VAL:O	3:C:761[B]:HDE:HACA	2.18	0.42
1:A:211:ALA:HA	3:A:761[B]:HDE:HBB	2.02	0.42
1:C:443:PHE:CZ	1:C:470:PRO:HD2	2.54	0.42
1:B:274:CYS:HB3	2:B:760[A]:HDD:CBB	2.49	0.42
1:C:273:GLY:C	1:C:274:CYS:SG	2.98	0.42
1:A:276:THR:CG2	1:A:288:PHE:HB3	2.49	0.42
1:C:509:ARG:HD2	1:C:576:PRO:HD2	2.02	0.42
1:D:393:PRO:HD2	1:D:415:TYR:CG	2.54	0.42
1:B:273:GLY:C	1:B:274:CYS:SG	2.98	0.42
1:B:341:ILE:HG21	1:B:353:LEU:HD11	2.01	0.42
5:A:1016:HOH:O	1:C:104:LEU:HB3	2.20	0.42
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.50	0.42
1:A:583:LYS:O	1:A:584:LYS:HB3	2.19	0.42
1:B:604:ALA:HB1	1:B:633:LEU:HD22	2.01	0.42
1:C:299:LYS:HB2	1:C:299:LYS:HE3	1.90	0.42
3:C:761[B]:HDE:HMAA	3:C:761[B]:HDE:HAAA	1.84	0.42
1:A:693:LYS:HA	1:A:694:PRO:HD3	1.92	0.42
1:B:612:ARG:HH21	1:B:723:SER:HA	1.85	0.42
1:C:97:ALA:O	1:C:101:GLY:HA3	2.20	0.41
1:C:207:PHE:O	1:C:249:THR:HA	2.20	0.41
1:D:634:TYR:O	1:D:653:THR:HA	2.19	0.41
1:C:211:ALA:CB	1:C:410:GLY:HA3	2.51	0.41
1:C:686:MET:HB3	1:C:751:ILE:HD11	2.03	0.41
1:D:244:SER:HA	1:D:546[B]:GLN:NE2	2.35	0.41
1:B:207:PHE:O	1:B:249:THR:HA	2.19	0.41
1:B:556:GLN:NE2	1:B:571:LEU:HD11	2.35	0.41
1:C:356:PRO:HG3	1:C:407:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:ARG:HG3	1:D:660:LEU:HD12	2.02	0.41
1:C:602[B]:VAL:HG13	1:C:662:VAL:HA	2.02	0.41
1:D:273:GLY:C	1:D:274:CYS:SG	2.99	0.41
3:D:761[B]:HDE:HMAA	3:D:761[B]:HDE:HAAA	1.84	0.41
1:A:227:TRP:O	1:D:319:ARG:HD3	2.20	0.41
1:B:607:LEU:HD11	1:B:632:LEU:HB3	2.01	0.41
1:A:205:ILE:HD13	1:A:205:ILE:N	2.35	0.41
1:D:37:ARG:HG3	5:D:3415:HOH:O	2.20	0.41
1:D:696:ALA:HB1	1:D:728:PHE:CZ	2.56	0.41
1:B:157:ASN:HB3	5:B:3138:HOH:O	2.21	0.41
1:A:429:HIS:CG	1:C:83:ASN:HB3	2.55	0.41
1:D:411:ARG:HG2	3:D:761[B]:HDE:C3B	2.51	0.41
3:D:761[B]:HDE:HBBA	3:D:761[B]:HDE:HMB	2.03	0.40
1:A:393:PRO:HD2	1:A:415:TYR:CD2	2.56	0.40
1:A:411:ARG:HG2	3:A:761[B]:HDE:C3B	2.51	0.40
1:B:213:LYS:HE3	1:B:213:LYS:HB3	1.83	0.40
1:B:669:ALA:HB1	5:B:3595:HOH:O	2.20	0.40
1:B:38:PRO:HG2	1:B:51:ALA:HB2	2.04	0.40
1:C:724:ALA:O	1:C:725:ASP:HB2	2.22	0.40
1:D:29:LEU:N	5:D:2467:HOH:O	2.35	0.40
1:B:682:ASN:HB3	1:B:707:THR:HG21	2.04	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:2178:HOH:O	5:D:2976:HOH:O[1_655]	2.00	0.20
1:C:584:LYS:NZ	5:A:1624:HOH:O[1_554]	2.06	0.14
5:A:3241:HOH:O	5:D:2457:HOH:O[2_646]	2.15	0.05

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%)	707 (97%)	21 (3%)	1 (0%)	51	36
1	B	729/753 (97%)	709 (97%)	18 (2%)	2 (0%)	41	27
1	C	726/753 (96%)	702 (97%)	22 (3%)	2 (0%)	41	27
1	D	733/753 (97%)	713 (97%)	19 (3%)	1 (0%)	51	36
All	All	2917/3012 (97%)	2831 (97%)	80 (3%)	6 (0%)	47	33

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	725	ASP
1	A	75	SER
1	C	75	SER
1	C	725	ASP
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%)	595 (97%)	19 (3%)	40	25
1	B	614/634 (97%)	592 (96%)	22 (4%)	35	20
1	C	611/634 (96%)	577 (94%)	34 (6%)	21	8
1	D	618/634 (98%)	592 (96%)	26 (4%)	30	15
All	All	2457/2536 (97%)	2356 (96%)	101 (4%)	30	16

All (101) 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	185	PHE
1	A	191	THR

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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	369	ARG
1	A	432	PRO
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	584	LYS
1	A	707	THR
1	A	732	LEU
1	A	749	ASP
1	A	751	ILE
1	B	157	ASN
1	B	158	LYS
1	B	185	PHE
1	B	205	ILE
1	B	227	TRP
1	B	252	ASN
1	B	274	CYS
1	B	432	PRO
1	B	440	TYR
1	B	459	ASN
1	B	552	LEU
1	B	562	LEU
1	B	565	GLU
1	B	566	LEU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
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

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Mol	Chain	Res	Type
1	C	227	TRP
1	C	237	ASP
1	C	247	PRO
1	C	252	ASN
1	C	274	CYS
1	C	285	LYS
1	C	377	ARG
1	C	440	TYR
1	C	459	ASN
1	C	488	ARG
1	C	521	ARG
1	C	552	LEU
1	C	571	LEU
1	C	578	ASP
1	C	583	LYS
1	C	584	LYS
1	C	606	LEU
1	C	616	LEU
1	C	626	LYS
1	C	633	LEU
1	C	636	ARG
1	C	639	GLU
1	C	648	LEU
1	C	713	GLN
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	73[A]	LYS
1	D	73[B]	LYS
1	D	185	PHE
1	D	191	THR
1	D	205	ILE
1	D	227	TRP
1	D	237	ASP
1	D	252	ASN
1	D	344	GLU
1	D	416[A]	THR
1	D	416[B]	THR
1	D	440	TYR

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Mol	Chain	Res	Type
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	732	LEU
1	D	747	LYS
1	D	750	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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]	1,5	38,52,52	2.45	13 (34%)	28,89,89	2.67	11 (39%)
2	HDD	C	760[A]	1,5	38,52,52	2.20	15 (39%)	28,89,89	2.97	15 (53%)
3	HDE	A	761[B]	1,5	41,52,52	2.79	15 (36%)	38,89,89	2.82	18 (47%)
2	HDD	A	760[A]	1,5	38,52,52	2.30	9 (23%)	28,89,89	2.28	9 (32%)
3	HDE	C	761[B]	1,5	41,52,52	2.68	17 (41%)	38,89,89	2.95	19 (50%)
3	HDE	D	761[B]	1,5	41,52,52	2.47	13 (31%)	38,89,89	3.04	21 (55%)
3	HDE	B	761[B]	1,5	41,52,52	2.74	15 (36%)	38,89,89	2.90	16 (42%)
2	HDD	B	760[A]	1,5	38,52,52	2.01	14 (36%)	28,89,89	3.07	11 (39%)

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]	1,5	-	0/3/89/89	0/1/9/9
2	HDD	C	760[A]	1,5	-	0/3/89/89	0/1/9/9
3	HDE	A	761[B]	1,5	-	4/7/89/89	0/1/9/9
2	HDD	A	760[A]	1,5	-	0/3/89/89	0/1/9/9
3	HDE	C	761[B]	1,5	-	4/7/89/89	0/1/9/9
3	HDE	D	761[B]	1,5	-	4/7/89/89	0/1/9/9
3	HDE	B	761[B]	1,5	-	4/7/89/89	0/1/9/9
2	HDD	B	760[A]	1,5	-	0/3/89/89	0/1/9/9

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	761[B]	HDE	C4C-C3C	8.09	1.49	1.38
3	B	761[B]	HDE	CHC-C4B	-7.80	1.43	1.51
3	C	761[B]	HDE	C4C-C3C	7.70	1.48	1.38
3	C	761[B]	HDE	CHC-C4B	-7.19	1.43	1.51
2	D	760[A]	HDD	FE-ND	6.92	2.22	1.95
3	B	761[B]	HDE	C4C-C3C	6.64	1.47	1.38
3	D	761[B]	HDE	C4C-C3C	6.54	1.47	1.38
2	C	760[A]	HDD	FE-ND	6.18	2.19	1.95
2	A	760[A]	HDD	O1D-C3D	-5.99	1.37	1.46
3	B	761[B]	HDE	CHD-C4C	-5.78	1.45	1.51
3	A	761[B]	HDE	CHC-C4B	-5.66	1.45	1.51
2	D	760[A]	HDD	C3B-C2B	-5.66	1.32	1.40
3	A	761[B]	HDE	CHD-C1D	-5.65	1.45	1.51
3	A	761[B]	HDE	CHC-C1C	-5.65	1.45	1.51
3	A	761[B]	HDE	O1A-CGA	5.35	1.44	1.35
2	A	760[A]	HDD	C3B-C2B	-5.24	1.33	1.40
3	B	761[B]	HDE	O1A-CGA	5.24	1.44	1.35
3	D	761[B]	HDE	CHC-C1C	-5.13	1.45	1.51
3	C	761[B]	HDE	O1A-CGA	5.11	1.44	1.35
3	D	761[B]	HDE	CHD-C4C	-5.02	1.46	1.51
3	D	761[B]	HDE	CHC-C4B	-5.01	1.46	1.51
2	C	760[A]	HDD	C3B-C2B	-5.00	1.33	1.40
2	A	760[A]	HDD	FE-ND	4.90	2.14	1.95
2	A	760[A]	HDD	C3C-C2C	-4.82	1.33	1.40
3	C	761[B]	HDE	CHD-C4C	-4.62	1.46	1.51
3	A	761[B]	HDE	CHD-C4C	-4.62	1.46	1.51
2	B	760[A]	HDD	FE-ND	4.59	2.13	1.95
2	D	760[A]	HDD	C3C-C2C	-4.59	1.34	1.40
3	D	761[B]	HDE	O1A-CGA	4.47	1.43	1.35
3	B	761[B]	HDE	CHD-C1D	-4.37	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	760[A]	HDD	C3C-C2C	-4.23	1.34	1.40
2	D	760[A]	HDD	CHD-C1D	4.23	1.42	1.36
2	C	760[A]	HDD	O1D-C3D	-4.20	1.40	1.46
3	D	761[B]	HDE	CHD-C1D	-4.15	1.46	1.51
3	D	761[B]	HDE	C1A-NA	4.03	1.44	1.37
2	B	760[A]	HDD	C3B-C2B	-3.99	1.34	1.40
3	D	761[B]	HDE	C3B-C2B	3.92	1.49	1.37
3	B	761[B]	HDE	CHC-C1C	-3.91	1.47	1.51
2	B	760[A]	HDD	C3C-CAC	3.83	1.55	1.47
3	C	761[B]	HDE	CHC-C1C	-3.83	1.47	1.51
2	A	760[A]	HDD	OND-C2D	3.77	1.50	1.42
3	A	761[B]	HDE	C3B-C2B	3.76	1.48	1.37
2	D	760[A]	HDD	C3B-CAB	3.74	1.55	1.47
3	C	761[B]	HDE	C3B-C2B	3.69	1.48	1.37
3	B	761[B]	HDE	C3C-C2C	3.66	1.48	1.37
3	B	761[B]	HDE	C1A-NA	3.64	1.44	1.37
3	C	761[B]	HDE	C4A-NA	3.64	1.44	1.37
3	B	761[B]	HDE	C3B-C2B	3.57	1.48	1.37
2	A	760[A]	HDD	C3C-CAC	3.55	1.55	1.47
2	A	760[A]	HDD	C3B-CAB	3.53	1.55	1.47
3	A	761[B]	HDE	C3D-C2D	3.52	1.48	1.37
2	D	760[A]	HDD	O1D-C3D	-3.45	1.41	1.46
3	D	761[B]	HDE	C4A-NA	3.44	1.43	1.37
3	A	761[B]	HDE	C3C-C2C	3.42	1.47	1.37
3	C	761[B]	HDE	CHD-C1D	-3.39	1.47	1.51
3	B	761[B]	HDE	C1C-C2C	3.38	1.42	1.38
3	A	761[B]	HDE	C1C-C2C	3.37	1.42	1.38
3	A	761[B]	HDE	C1A-NA	3.30	1.43	1.37
3	C	761[B]	HDE	C3D-C2D	3.24	1.47	1.37
3	C	761[B]	HDE	C3C-C2C	3.24	1.47	1.37
3	D	761[B]	HDE	C3D-C2D	3.17	1.47	1.37
3	C	761[B]	HDE	C1C-C2C	3.13	1.42	1.38
2	D	760[A]	HDD	CMD-C2D	3.11	1.57	1.53
2	D	760[A]	HDD	C3C-CAC	3.11	1.54	1.47
2	B	760[A]	HDD	CMD-C2D	3.08	1.57	1.53
3	B	761[B]	HDE	C3D-C2D	3.08	1.46	1.37
2	C	760[A]	HDD	C3B-CAB	3.03	1.54	1.47
3	C	761[B]	HDE	C1A-NA	2.93	1.42	1.37
2	D	760[A]	HDD	CMC-C2C	2.92	1.57	1.51
3	A	761[B]	HDE	C1B-NB	2.91	1.42	1.36
2	C	760[A]	HDD	CHD-C1D	2.91	1.40	1.36
3	B	761[B]	HDE	C1B-NB	2.89	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	761[B]	HDE	C1B-NB	2.87	1.42	1.36
3	D	761[B]	HDE	C3C-C2C	2.85	1.46	1.37
3	A	761[B]	HDE	C1B-CHB	2.85	1.48	1.41
2	A	760[A]	HDD	CMC-C2C	2.83	1.57	1.51
2	B	760[A]	HDD	CAA-C2A	2.81	1.56	1.52
2	C	760[A]	HDD	C1C-NC	2.77	1.41	1.36
3	B	761[B]	HDE	C4A-NA	2.75	1.42	1.37
2	B	760[A]	HDD	C3B-CAB	2.74	1.53	1.47
3	C	761[B]	HDE	C4D-CHA	2.74	1.48	1.41
2	C	760[A]	HDD	C1A-NA	2.73	1.41	1.36
2	C	760[A]	HDD	C1D-ND	2.72	1.42	1.37
3	B	761[B]	HDE	C4D-CHA	2.71	1.48	1.41
3	C	761[B]	HDE	C1B-NB	2.66	1.41	1.36
2	C	760[A]	HDD	C3C-CAC	2.66	1.53	1.47
3	B	761[B]	HDE	CHB-C4A	-2.64	1.31	1.36
3	D	761[B]	HDE	C4D-CHA	2.62	1.48	1.41
2	C	760[A]	HDD	C3C-C2C	-2.60	1.36	1.40
3	A	761[B]	HDE	C4A-NA	2.59	1.42	1.37
2	C	760[A]	HDD	CHA-C4D	2.44	1.40	1.36
2	B	760[A]	HDD	O1D-C3D	-2.41	1.42	1.46
2	C	760[A]	HDD	CMD-C2D	2.38	1.56	1.53
2	B	760[A]	HDD	CMC-C2C	2.37	1.56	1.51
2	A	760[A]	HDD	CAA-C2A	2.37	1.55	1.52
2	B	760[A]	HDD	C4A-NA	2.36	1.41	1.36
2	D	760[A]	HDD	CHA-C4D	2.35	1.39	1.36
2	C	760[A]	HDD	C4D-ND	2.32	1.41	1.37
3	A	761[B]	HDE	C4D-CHA	2.30	1.47	1.41
2	D	760[A]	HDD	OND-C2D	2.19	1.47	1.42
2	B	760[A]	HDD	CHA-C4D	2.18	1.39	1.36
2	C	760[A]	HDD	OND-C2D	2.17	1.47	1.42
2	D	760[A]	HDD	C1C-NC	2.15	1.40	1.36
3	C	761[B]	HDE	O1A-C2A	-2.15	1.43	1.46
2	D	760[A]	HDD	C4C-NC	2.12	1.40	1.36
2	B	760[A]	HDD	CHD-C1D	2.11	1.39	1.36
2	C	760[A]	HDD	CMC-C2C	2.10	1.56	1.51
2	B	760[A]	HDD	C4D-ND	2.08	1.41	1.37
2	B	760[A]	HDD	CMA-C3A	2.04	1.55	1.51
3	C	761[B]	HDE	C1B-CHB	2.03	1.46	1.41
3	C	761[B]	HDE	CHB-C4A	-2.01	1.32	1.36

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	760[A]	HDD	O1D-CGD-O2D	8.53	128.42	120.80
2	C	760[A]	HDD	O1D-CGD-O2D	8.29	128.20	120.80
3	A	761[B]	HDE	CHC-C4B-C3B	-6.94	121.31	129.68
2	D	760[A]	HDD	O1D-CGD-O2D	6.91	126.97	120.80
2	D	760[A]	HDD	O1D-CGD-CBD	-6.88	103.25	110.19
3	B	761[B]	HDE	CAD-CBD-CGD	-6.78	101.30	112.67
2	B	760[A]	HDD	O1D-CGD-CBD	-6.62	103.51	110.19
3	D	761[B]	HDE	CAD-CBD-CGD	-6.48	101.80	112.67
3	A	761[B]	HDE	CHD-C1D-C2D	-5.95	119.58	129.53
3	A	761[B]	HDE	CAD-CBD-CGD	-5.80	102.94	112.67
3	B	761[B]	HDE	CBC-CAC-C3C	-5.72	97.69	112.27
3	C	761[B]	HDE	CBC-CAC-C3C	-5.66	97.85	112.27
2	C	760[A]	HDD	OND-C2D-CMD	-5.57	99.33	109.59
3	C	761[B]	HDE	CHC-C4B-C3B	-5.44	123.11	129.68
3	C	761[B]	HDE	C1B-CHB-C4A	-5.43	119.36	130.12
2	A	760[A]	HDD	O1D-CGD-CBD	-5.42	104.73	110.19
3	D	761[B]	HDE	CHD-C1D-C2D	-5.34	120.60	129.53
3	C	761[B]	HDE	CAD-CBD-CGD	-5.34	103.72	112.67
2	D	760[A]	HDD	CAA-CBA-CGA	-5.32	103.74	112.67
2	A	760[A]	HDD	CAA-CBA-CGA	-5.29	103.80	112.67
3	B	761[B]	HDE	C1C-C2C-C3C	-5.26	100.21	105.81
3	A	761[B]	HDE	CHD-C4C-C3C	-5.24	123.36	129.68
2	B	760[A]	HDD	CAA-CBA-CGA	-5.15	104.03	112.67
3	D	761[B]	HDE	CHD-C4C-C3C	-5.14	123.48	129.68
3	D	761[B]	HDE	CHC-C4B-C3B	-5.11	123.51	129.68
2	B	760[A]	HDD	CMC-C2C-C1C	-5.08	120.65	128.46
2	C	760[A]	HDD	O1D-CGD-CBD	-5.06	105.08	110.19
3	B	761[B]	HDE	CHC-C4B-C3B	-5.02	123.62	129.68
3	B	761[B]	HDE	CHD-C1D-C2D	-4.88	121.37	129.53
2	C	760[A]	HDD	C4B-C3B-C2B	4.87	110.30	106.90
3	D	761[B]	HDE	C1B-CHB-C4A	-4.75	120.71	130.12
3	C	761[B]	HDE	CHD-C1D-C2D	-4.75	121.59	129.53
3	B	761[B]	HDE	C4C-CHD-C1D	4.69	124.32	112.87
3	C	761[B]	HDE	CMA-C3A-C4A	-4.64	104.38	112.63
3	D	761[B]	HDE	CMB-C2B-C3B	4.62	133.65	124.94
2	D	760[A]	HDD	C4B-C3B-C2B	4.58	110.09	106.90
3	D	761[B]	HDE	C1B-C2B-C3B	-4.52	103.85	107.00
2	C	760[A]	HDD	CMC-C2C-C1C	-4.40	121.70	128.46
2	B	760[A]	HDD	OND-C2D-CMD	-4.36	101.56	109.59
3	D	761[B]	HDE	CBC-CAC-C3C	-4.36	101.17	112.27
3	C	761[B]	HDE	CHC-C1C-C2C	-4.30	122.34	129.53
3	B	761[B]	HDE	C1B-C2B-C3B	-4.29	104.01	107.00
3	C	761[B]	HDE	C4C-CHD-C1D	4.29	123.34	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	761[B]	HDE	CHC-C1C-C2C	-4.17	122.55	129.53
3	C	761[B]	HDE	C1C-C2C-C3C	-4.14	101.40	105.81
3	D	761[B]	HDE	C1C-C2C-C3C	-3.93	101.63	105.81
3	C	761[B]	HDE	C3A-C4A-CHB	-3.88	117.87	124.28
3	D	761[B]	HDE	CMB-C2B-C1B	-3.88	122.50	128.46
3	A	761[B]	HDE	C4C-CHD-C1D	3.88	122.33	112.87
3	A	761[B]	HDE	C1B-CHB-C4A	-3.80	122.59	130.12
2	A	760[A]	HDD	C4B-C3B-C2B	3.80	109.55	106.90
3	C	761[B]	HDE	CHD-C4C-C3C	-3.73	125.17	129.68
2	A	760[A]	HDD	O1D-CGD-O2D	3.68	124.08	120.80
3	A	761[B]	HDE	CAB-C3B-C4B	-3.62	122.83	127.19
3	A	761[B]	HDE	CMD-C2D-C3D	3.58	131.69	124.94
3	B	761[B]	HDE	C1B-CHB-C4A	-3.58	123.03	130.12
3	A	761[B]	HDE	CHC-C1C-C2C	-3.58	123.55	129.53
3	D	761[B]	HDE	C4C-CHD-C1D	3.54	121.50	112.87
2	B	760[A]	HDD	CMB-C2B-C3B	3.53	131.28	124.68
3	B	761[B]	HDE	C3A-C4A-CHB	-3.53	118.45	124.28
3	C	761[B]	HDE	C4D-CHA-C1A	-3.50	123.18	130.12
3	D	761[B]	HDE	O1A-CGA-O2A	3.49	123.91	120.80
3	D	761[B]	HDE	CHC-C1C-C2C	-3.46	123.75	129.53
3	B	761[B]	HDE	CHD-C4C-C3C	-3.27	125.74	129.68
3	D	761[B]	HDE	C4D-CHA-C1A	-3.26	123.66	130.12
3	D	761[B]	HDE	CAB-C3B-C4B	-3.26	123.27	127.19
2	A	760[A]	HDD	OND-C2D-CMD	-3.23	103.65	109.59
2	B	760[A]	HDD	C1A-CHA-C4D	-3.21	123.75	130.12
3	A	761[B]	HDE	C4B-CHC-C1C	3.21	120.71	112.87
2	C	760[A]	HDD	CAA-CBA-CGA	-3.21	107.29	112.67
3	A	761[B]	HDE	C1C-C2C-C3C	-3.16	102.44	105.81
3	B	761[B]	HDE	C4D-CHA-C1A	-3.16	123.87	130.12
2	D	760[A]	HDD	OND-C2D-C3D	-3.15	102.62	110.45
2	A	760[A]	HDD	CMA-C3A-C4A	-3.12	123.67	128.46
2	B	760[A]	HDD	C4B-C3B-C2B	3.10	109.06	106.90
3	B	761[B]	HDE	C4C-C3C-C2C	3.06	110.49	105.93
2	C	760[A]	HDD	CAD-CBD-CGD	-3.05	99.85	104.56
3	A	761[B]	HDE	O1A-CGA-O2A	3.03	123.50	120.80
3	A	761[B]	HDE	C1B-C2B-C3B	-2.96	104.94	107.00
3	D	761[B]	HDE	C3A-C4A-CHB	-2.92	119.46	124.28
2	B	760[A]	HDD	CMC-C2C-C3C	2.91	130.11	124.68
2	C	760[A]	HDD	C4A-C3A-C2A	2.87	109.00	107.00
2	A	760[A]	HDD	C4A-C3A-C2A	2.85	108.98	107.00
3	C	761[B]	HDE	O1A-CGA-O2A	2.81	123.31	120.80
2	C	760[A]	HDD	C4C-CHD-C1D	-2.78	124.61	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	761[B]	HDE	C4B-CHC-C1C	2.77	119.63	112.87
3	D	761[B]	HDE	CAC-C3C-C4C	-2.73	123.90	127.19
3	A	761[B]	HDE	C1D-C2D-C3D	-2.70	102.94	105.81
3	C	761[B]	HDE	C4B-CHC-C1C	2.68	119.40	112.87
3	C	761[B]	HDE	CMD-C2D-C3D	2.67	129.97	124.94
2	C	760[A]	HDD	C3B-C4B-NB	-2.56	106.10	110.94
2	D	760[A]	HDD	C1A-CHA-C4D	-2.56	125.05	130.12
3	B	761[B]	HDE	C4B-CHC-C1C	2.54	119.06	112.87
3	C	761[B]	HDE	C1B-C2B-C3B	-2.50	105.25	107.00
2	D	760[A]	HDD	C3C-C4C-NC	-2.49	105.99	109.21
3	C	761[B]	HDE	CMC-C2C-C3C	2.47	129.59	124.94
3	D	761[B]	HDE	CMA-C3A-C4A	-2.41	108.34	112.63
2	A	760[A]	HDD	CAD-CBD-CGD	-2.40	100.85	104.56
2	D	760[A]	HDD	C4A-C3A-C2A	2.38	108.65	107.00
2	A	760[A]	HDD	C3B-C4B-NB	-2.38	106.46	110.94
2	C	760[A]	HDD	C3C-C4C-NC	-2.38	106.14	109.21
3	B	761[B]	HDE	CMC-C2C-C3C	2.37	129.42	124.94
3	B	761[B]	HDE	O1A-CGA-O2A	2.37	122.91	120.80
2	C	760[A]	HDD	OND-C2D-C3D	-2.30	104.73	110.45
3	A	761[B]	HDE	C4D-CHA-C1A	-2.26	125.64	130.12
2	D	760[A]	HDD	OND-C2D-CMD	-2.19	105.56	109.59
3	A	761[B]	HDE	CMB-C2B-C3B	2.18	129.05	124.94
3	C	761[B]	HDE	O1A-C2A-CAA	2.17	107.10	103.01
2	D	760[A]	HDD	C3B-C4B-NB	-2.17	106.85	110.94
2	B	760[A]	HDD	C3B-C4B-NB	-2.15	106.88	110.94
2	C	760[A]	HDD	CMA-C3A-C4A	-2.13	125.19	128.46
3	A	761[B]	HDE	CBC-CAC-C3C	-2.13	106.84	112.27
3	D	761[B]	HDE	CHB-C4A-NA	2.13	127.32	124.20
2	C	760[A]	HDD	CMC-C2C-C3C	2.13	128.66	124.68
2	B	760[A]	HDD	CMD-C2D-C1D	2.11	116.38	112.63
2	C	760[A]	HDD	CMD-C2D-C1D	2.07	116.30	112.63
2	D	760[A]	HDD	C2D-C1D-CHD	2.04	127.65	124.28
3	A	761[B]	HDE	C3A-C4A-CHB	-2.01	120.96	124.28
3	D	761[B]	HDE	CMC-C2C-C3C	2.01	128.73	124.94
3	C	761[B]	HDE	C4C-C3C-C2C	2.00	108.92	105.93

There are no chirality outliers.

All (16) 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

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Mol	Chain	Res	Type	Atoms
3	A	761[B]	HDE	C2C-C3C-CAC-CBC
3	A	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	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

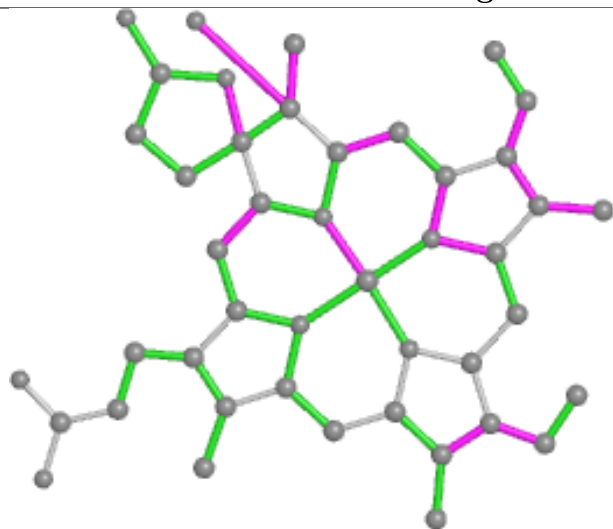
There are no ring outliers.

8 monomers are involved in 102 short contacts:

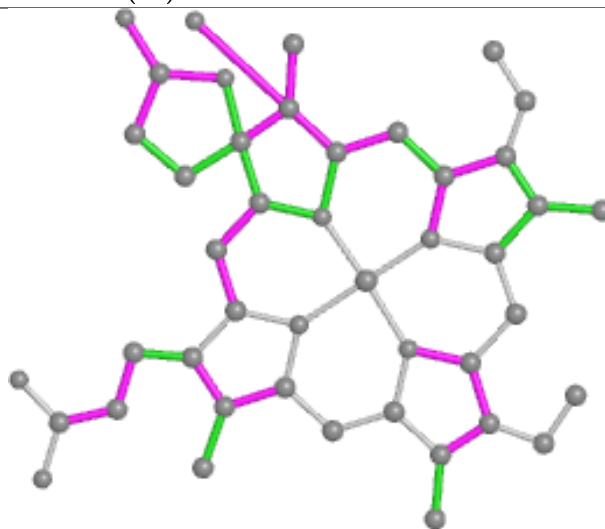
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	760[A]	HDD	10	0
2	C	760[A]	HDD	15	0
3	A	761[B]	HDE	11	0
2	A	760[A]	HDD	12	0
3	C	761[B]	HDE	14	0
3	D	761[B]	HDE	11	0
3	B	761[B]	HDE	14	0
2	B	760[A]	HDD	15	0

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.

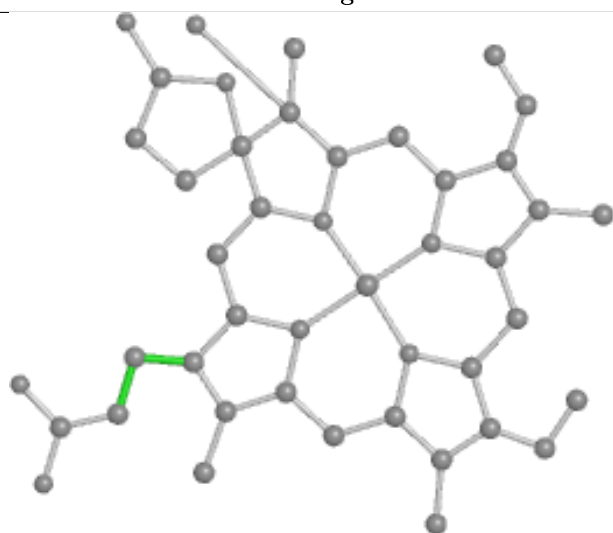
Ligand HDD D 760 (A)



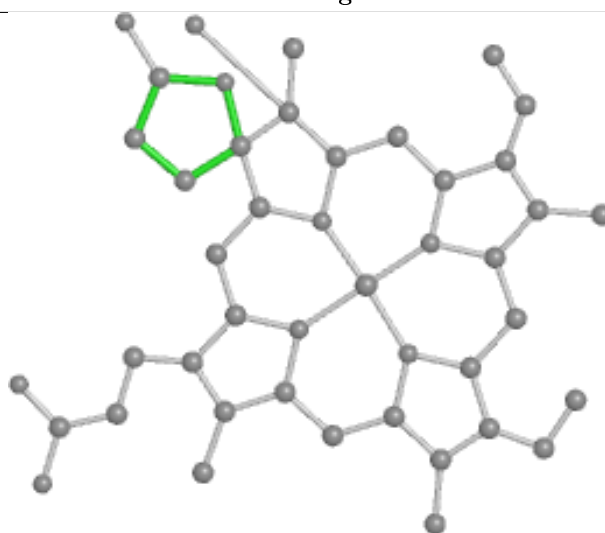
Bond lengths



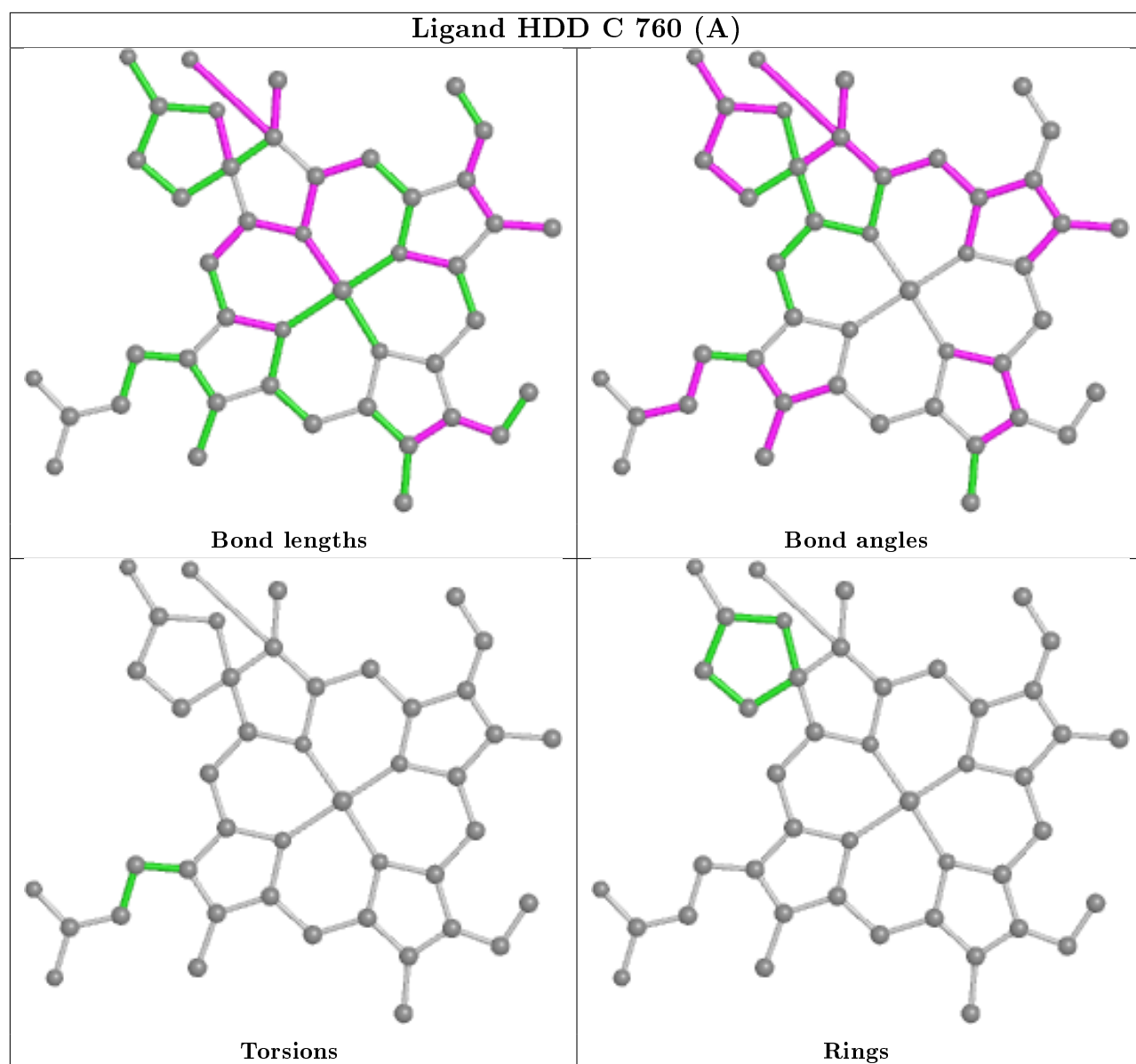
Bond angles



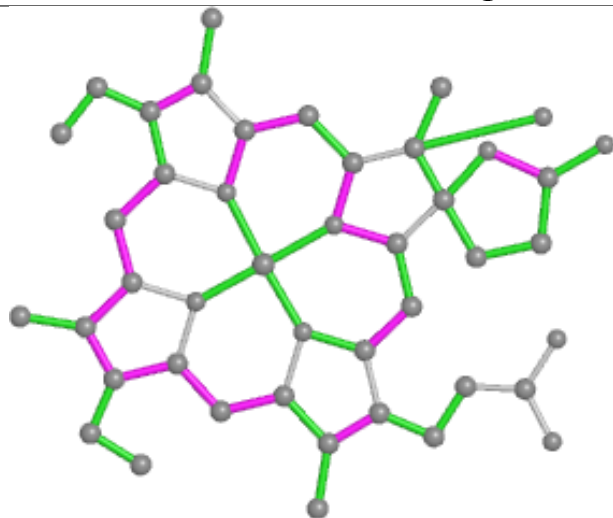
Torsions



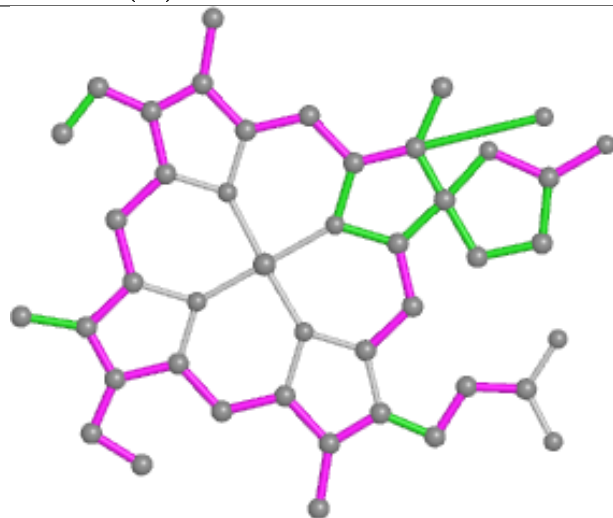
Rings



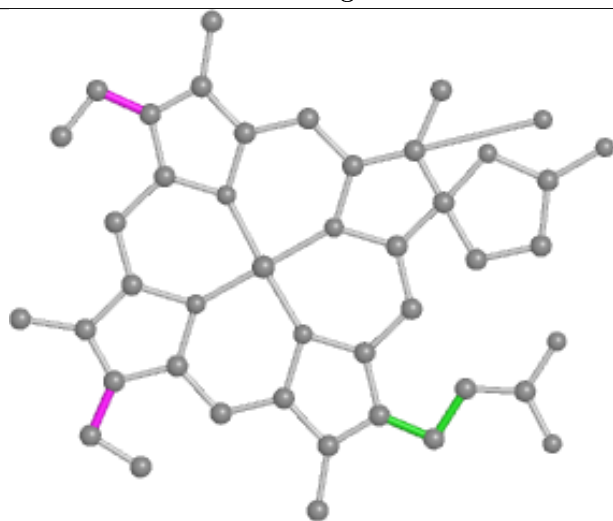
Ligand HDE A 761 (B)



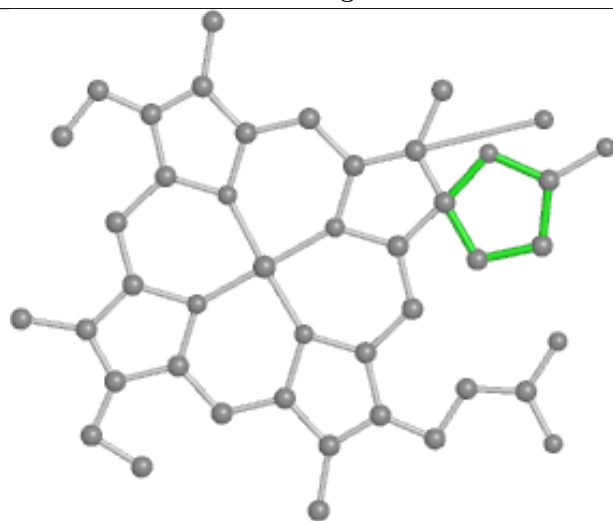
Bond lengths



Bond angles

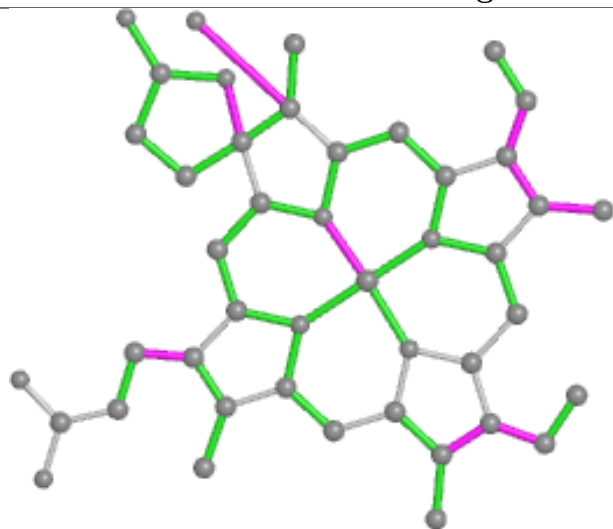


Torsions

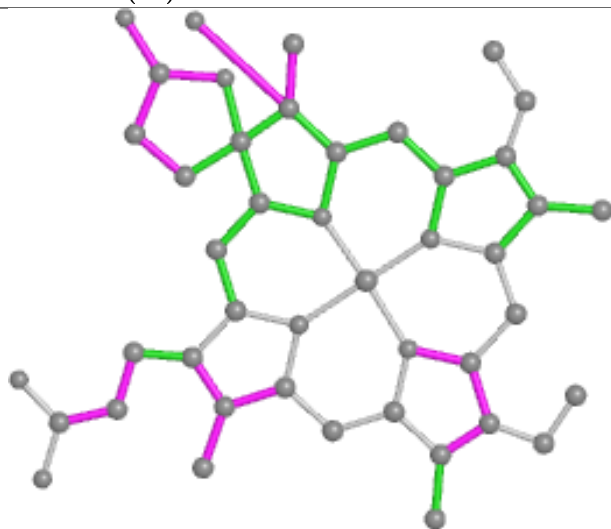


Rings

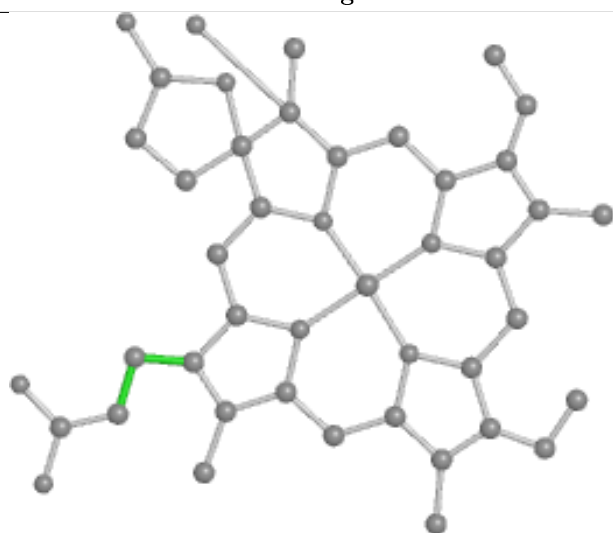
Ligand HDD A 760 (A)



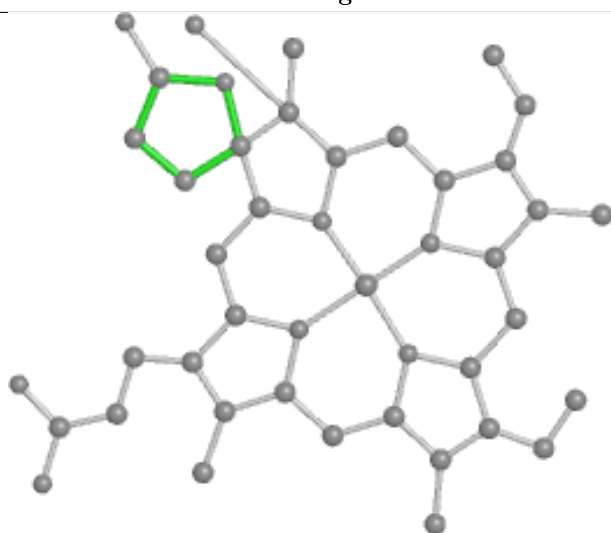
Bond lengths



Bond angles

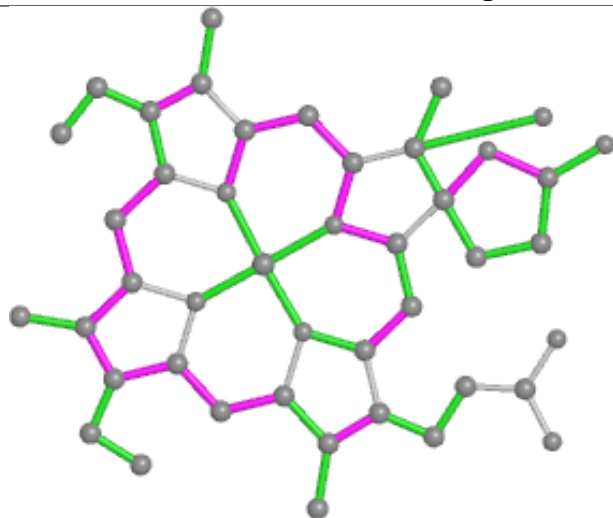


Torsions

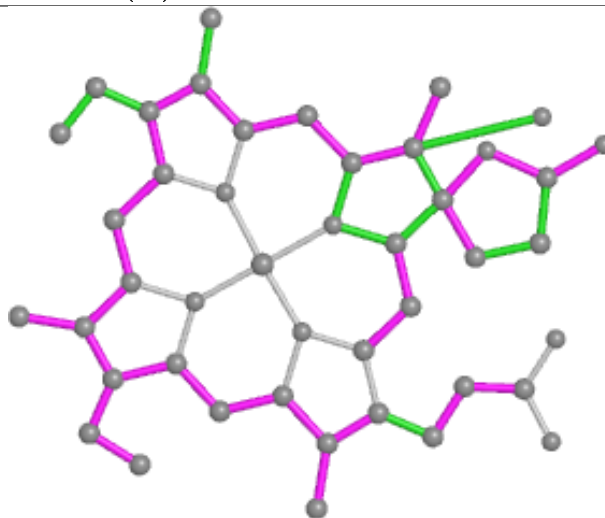


Rings

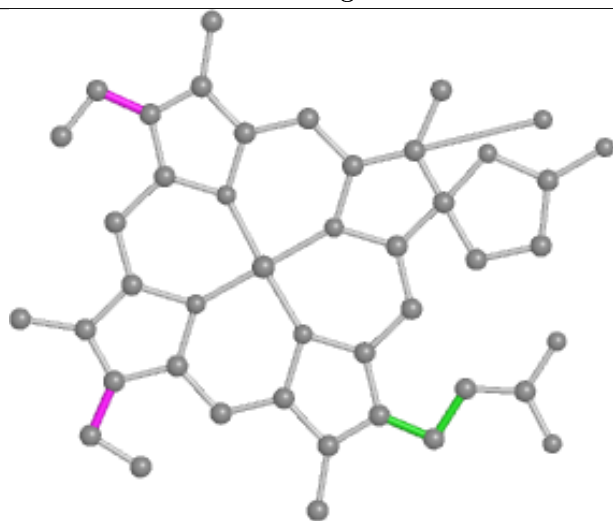
Ligand HDE C 761 (B)



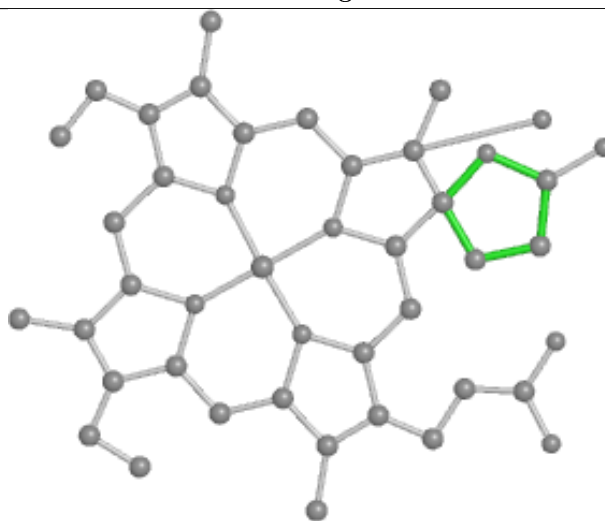
Bond lengths



Bond angles

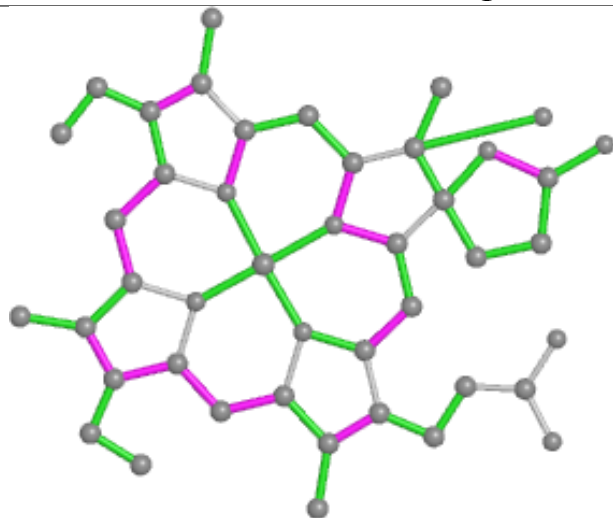


Torsions

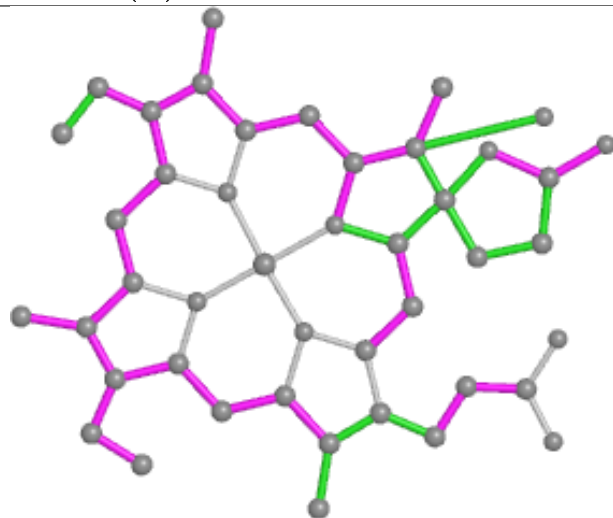


Rings

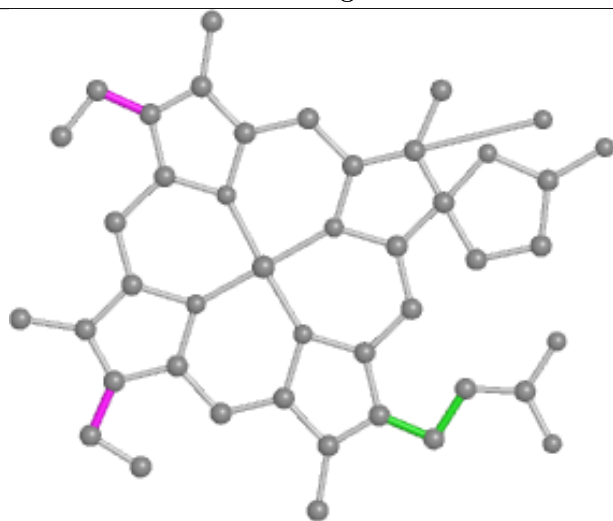
Ligand HDE D 761 (B)



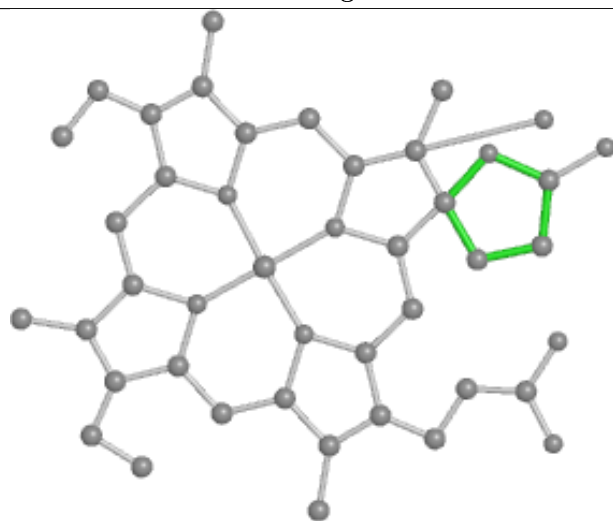
Bond lengths



Bond angles

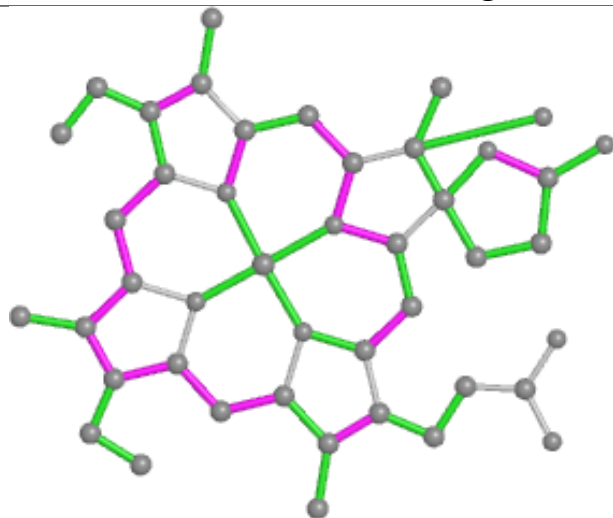


Torsions

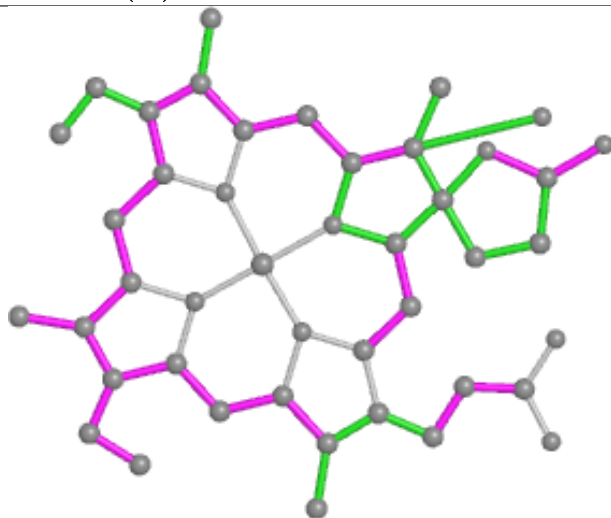


Rings

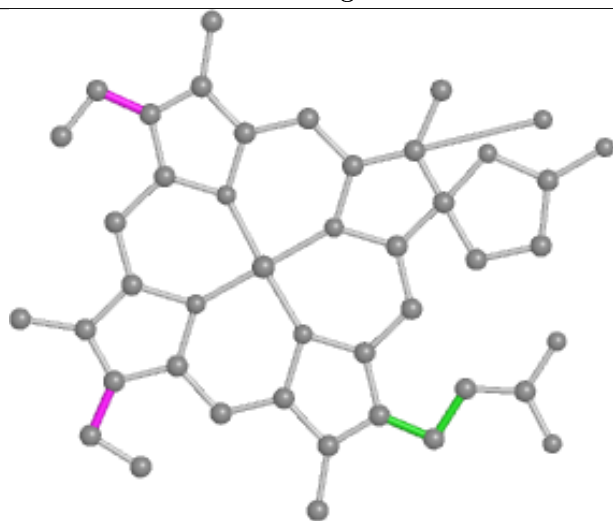
Ligand HDE B 761 (B)



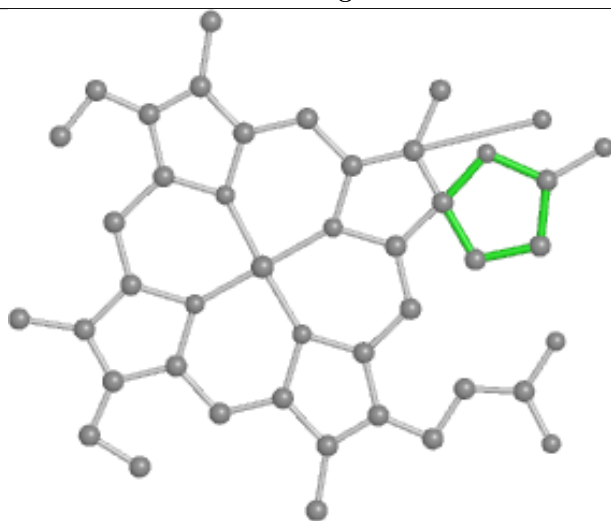
Bond lengths



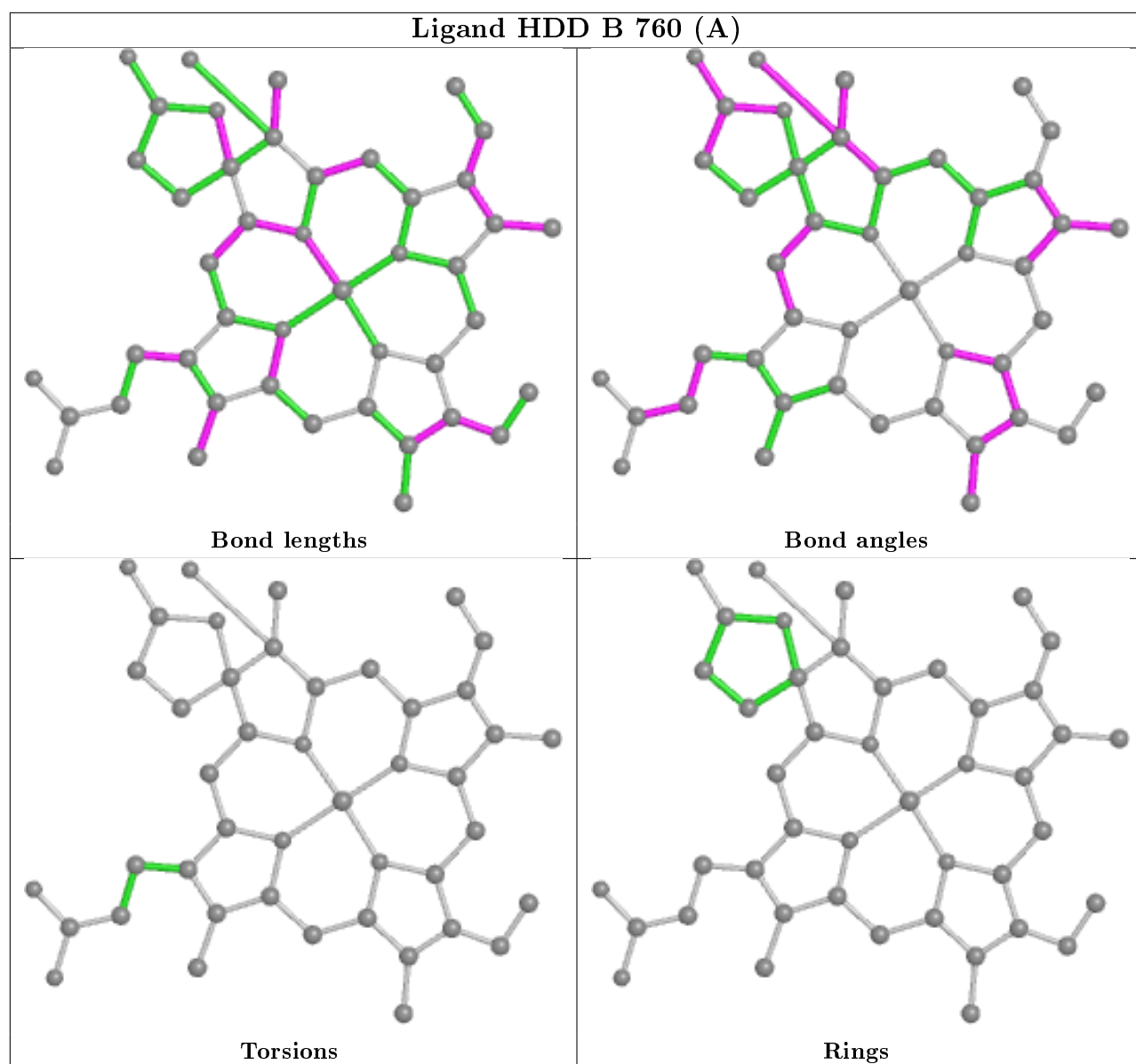
Bond angles



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, 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%)	-0.60	3 (0%) 92 90	3, 10, 27, 45	2 (0%)
1	B	726/753 (96%)	-0.45	16 (2%) 62 57	4, 12, 32, 48	2 (0%)
1	C	726/753 (96%)	-0.50	7 (0%) 82 80	4, 12, 32, 47	2 (0%)
1	D	726/753 (96%)	-0.60	4 (0%) 89 87	3, 10, 28, 45	1 (0%)
All	All	2904/3012 (96%)	-0.54	30 (1%) 82 80	3, 11, 30, 48	7 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	726	GLY	5.1
1	B	28	SER	4.0
1	D	28	SER	3.7
1	B	713	GLN	3.3
1	A	713	GLN	3.3
1	A	28	SER	3.2
1	D	713	GLN	3.1
1	B	568	ASP	3.1
1	D	749	ASP	3.1
1	B	32	GLU	3.0
1	C	594	PRO	2.9
1	B	647	VAL	2.8
1	C	583	LYS	2.8
1	B	645	GLY	2.7
1	B	572	ASN	2.7
1	B	712	ASP	2.6
1	D	750	LYS	2.5
1	B	725	ASP	2.5
1	B	583	LYS	2.5
1	B	569	ASP	2.5
1	C	672	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	727	SER	2.3
1	A	32	GLU	2.2
1	C	596	GLY	2.2
1	C	726	GLY	2.2
1	B	673	ALA	2.1
1	C	711	ALA	2.1
1	B	646	THR	2.1
1	C	714	GLY	2.0
1	B	677	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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

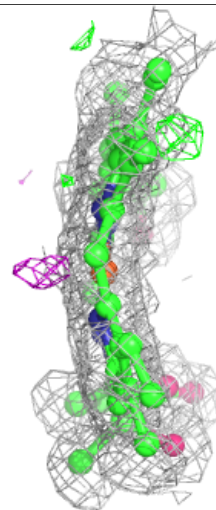
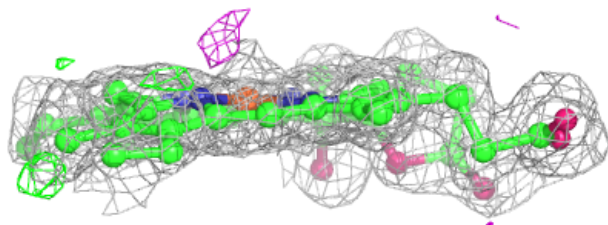
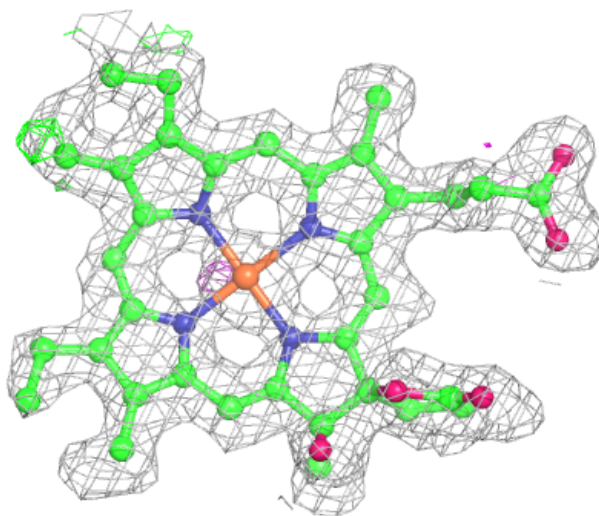
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	H2S	C	754	1/1	0.95	0.23	24,24,24,24	1
4	H2S	A	754	1/1	0.97	0.22	22,22,22,22	1
4	H2S	D	754	1/1	0.97	0.25	19,19,19,19	1
4	H2S	B	754	1/1	0.97	0.21	25,25,25,25	1
3	HDE	B	761[B]	44/44	0.98	0.08	3,11,14,15	44
2	HDD	B	760[A]	44/44	0.98	0.08	2,4,8,8	44
3	HDE	A	761[B]	44/44	0.99	0.08	2,8,11,15	44
3	HDE	C	761[B]	44/44	0.99	0.08	6,10,13,15	44
2	HDD	D	760[A]	44/44	0.99	0.07	2,3,6,13	44
3	HDE	D	761[B]	44/44	0.99	0.07	2,9,13,15	44
2	HDD	C	760[A]	44/44	0.99	0.08	2,4,8,9	44
2	HDD	A	760[A]	44/44	0.99	0.08	2,4,8,12	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.

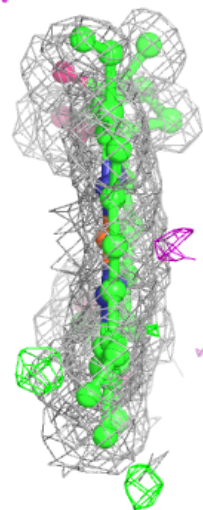
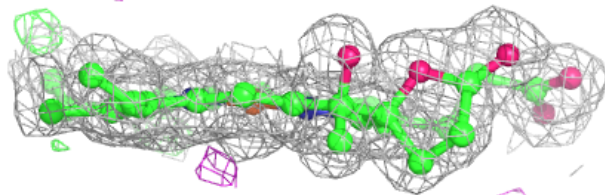
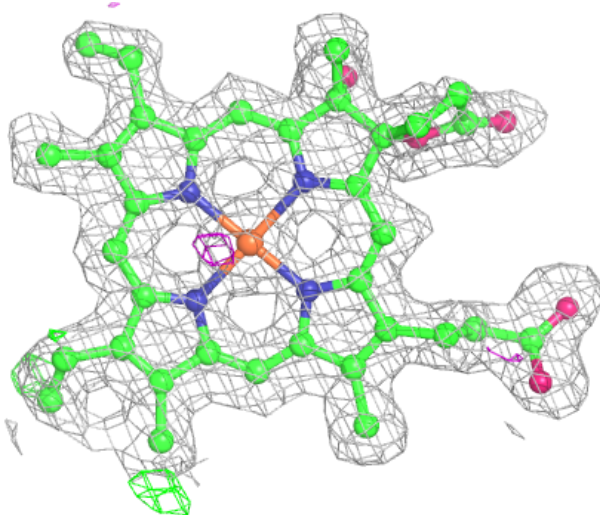
Electron density around HDE B 761 (B):

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



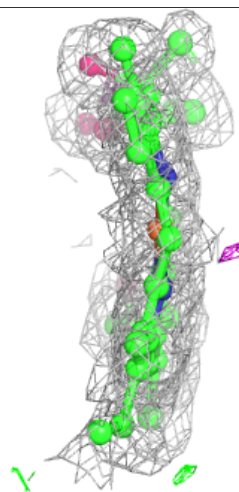
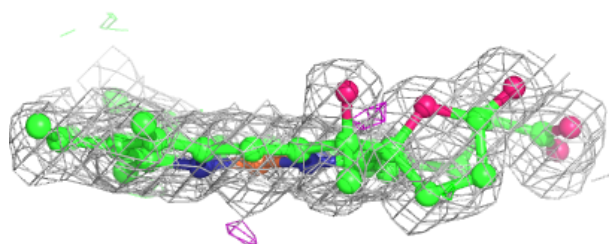
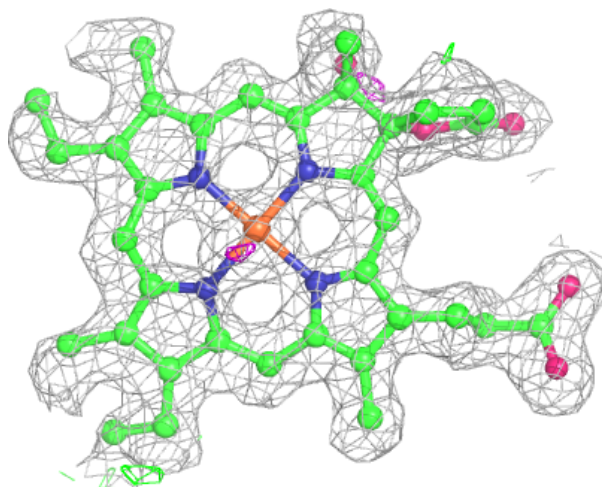
Electron density around HDD B 760 (A):

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



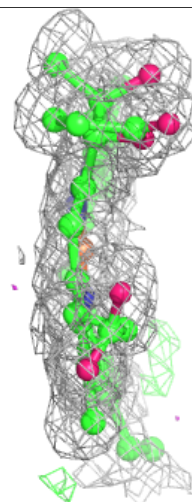
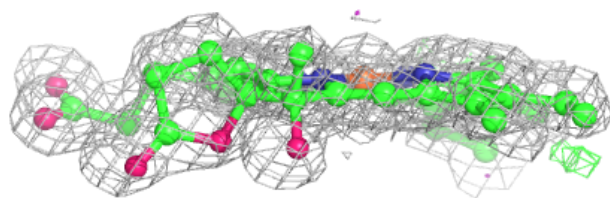
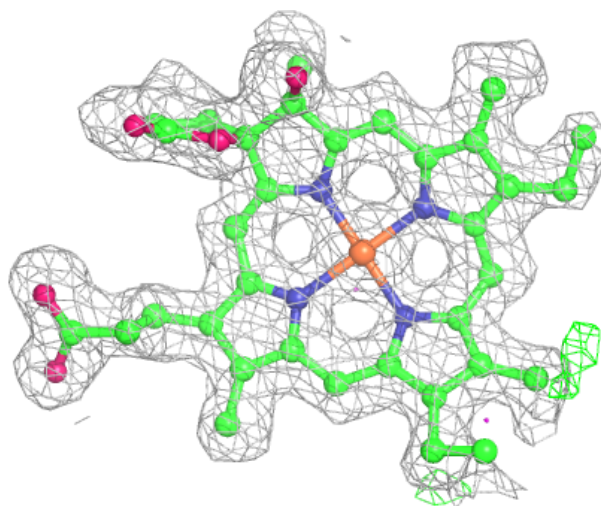
Electron density around HDE A 761 (B):

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



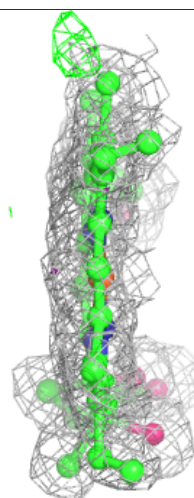
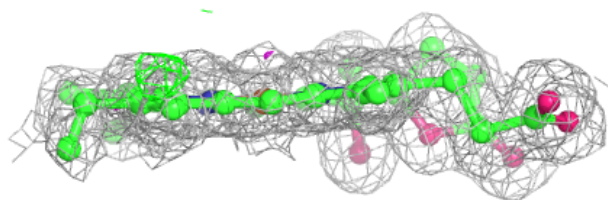
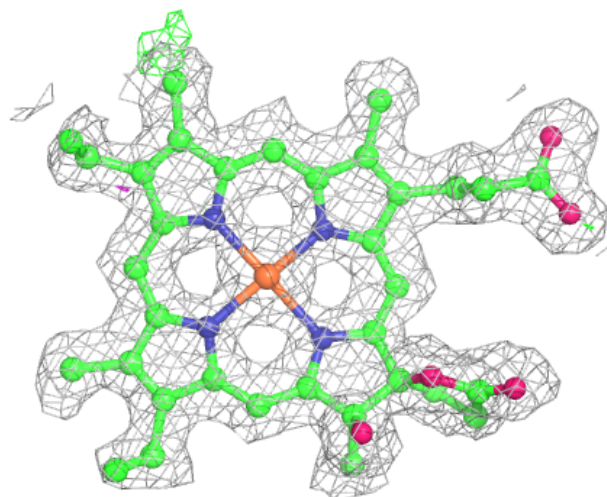
Electron density around HDE C 761 (B):

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



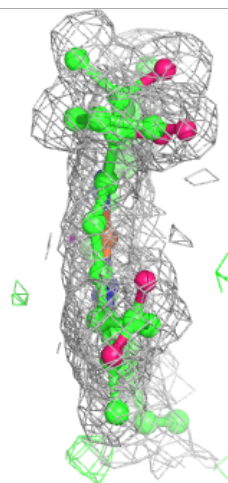
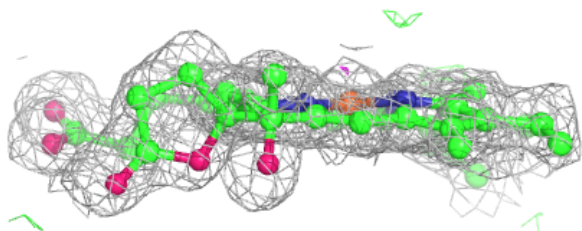
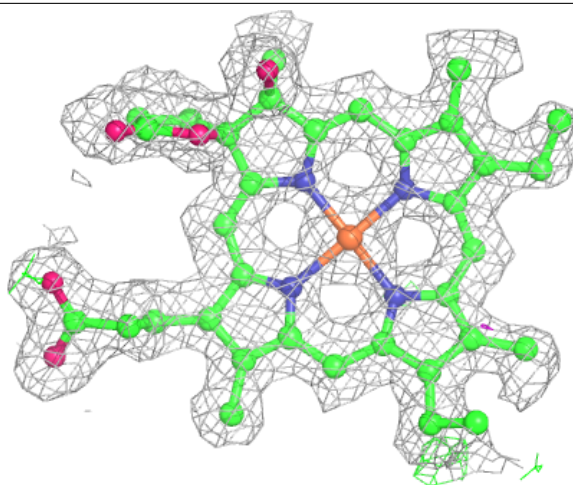
Electron density around HDD D 760 (A):

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



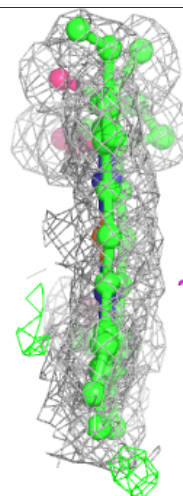
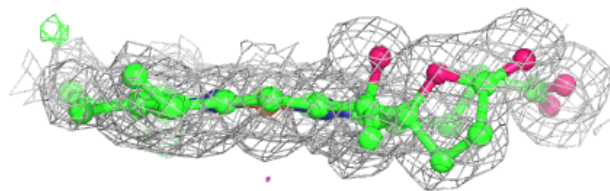
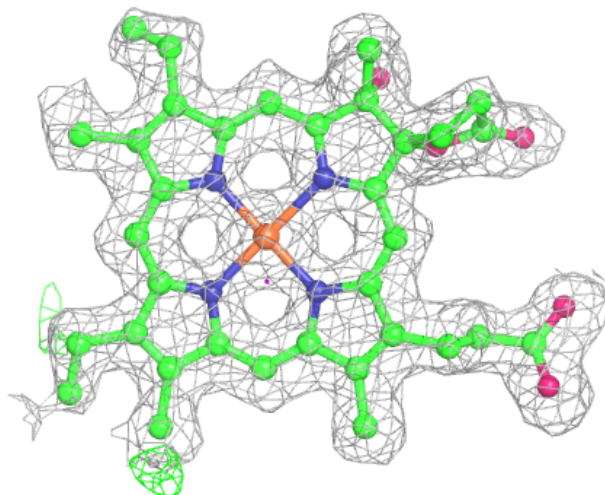
Electron density around HDE D 761 (B):

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



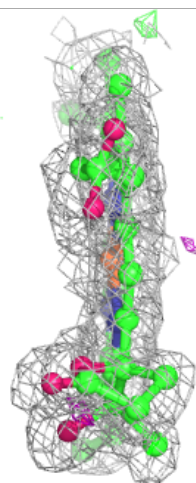
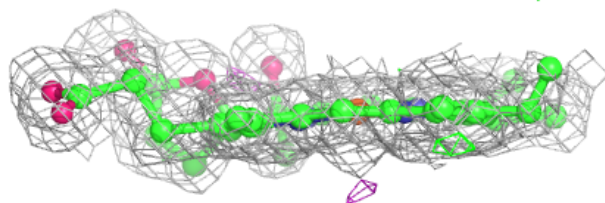
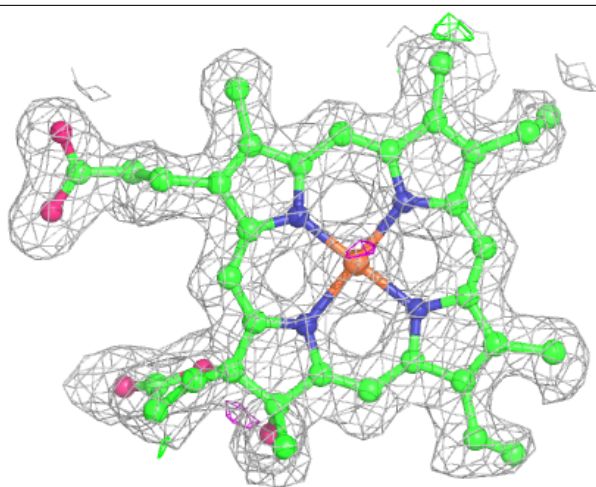
Electron density around HDD C 760 (A):

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



Electron density around HDD A 760 (A):

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



6.5 Other polymers [i](#)

There are no such residues in this entry.