Full wwPDB X-ray Structure Validation Report (i)

Mar 20, 2026 – 08:39 AM UTC

PDB ID	:	3PQ7 / pdb_00003pq7
Title	:	Structure of I274C variant of E. coli KatE[] - Images 31-36
Authors	:	Loewen, P.C.; Jha, V.; Louis, S.; Chelikani, P.; Carpena, X.; Fita, I.
Deposited on	:	2010-11-25
Resolution	:	1.80 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

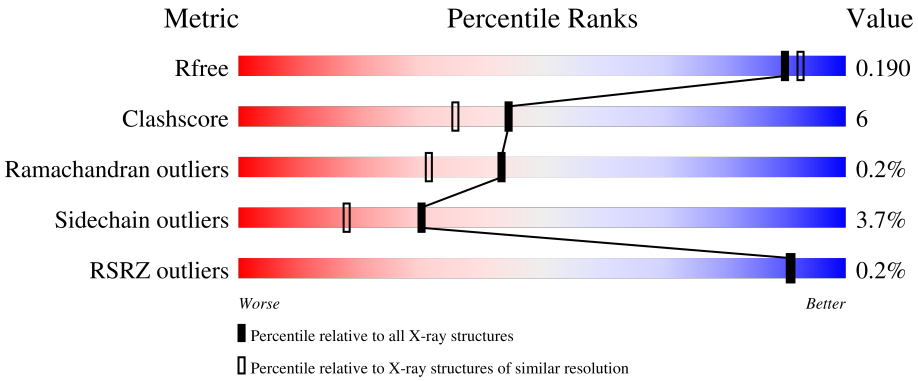
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	753	83% 12%
1	B	753	83% 11%
1	C	753	84% 11%
1	D	753	85% 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 26809 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

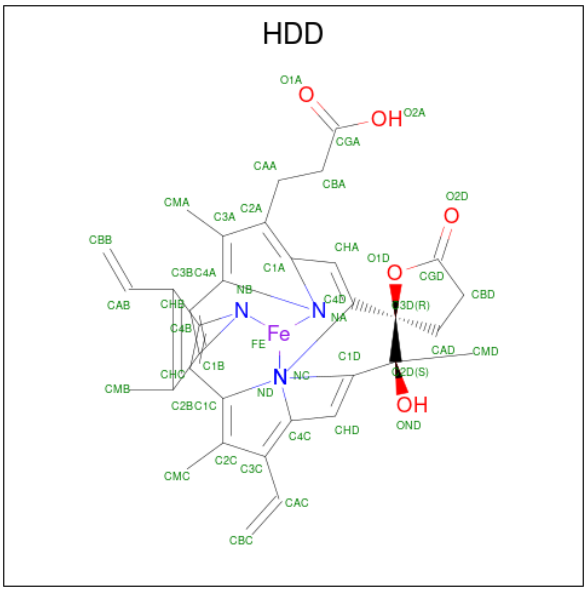
- Molecule 1 is a protein called Catalase HPII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	5	0
			5755	3652	1009	1083	11			
1	B	726	Total	C	N	O	S	0	5	0
			5757	3654	1009	1083	11			
1	C	726	Total	C	N	O	S	0	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:

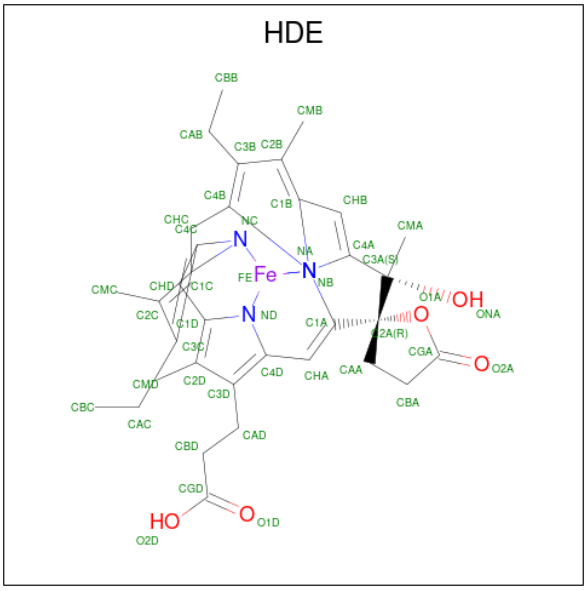
Chain	Residue	Modelled	Actual	Comment	Reference
A	274	CYS	ILE	engineered mutation	UNP P21179
A	438	ALA	CYS	engineered mutation	UNP P21179
A	669	ALA	CYS	engineered mutation	UNP P21179
B	274	CYS	ILE	engineered mutation	UNP P21179
B	438	ALA	CYS	engineered mutation	UNP P21179
B	669	ALA	CYS	engineered mutation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



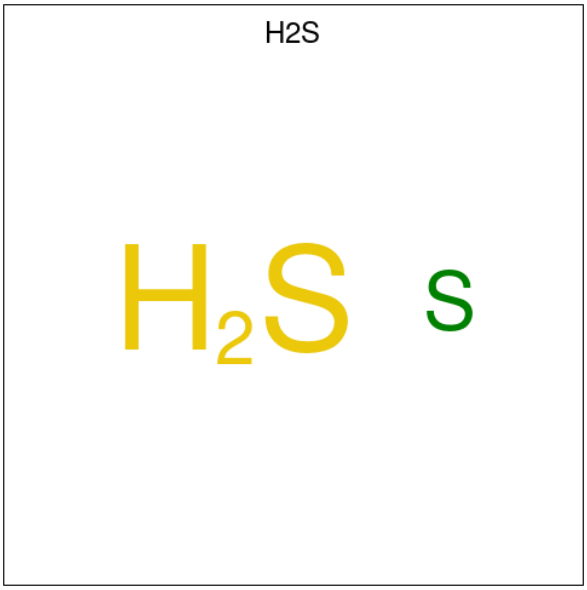
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
2	B	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
2	C	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
2	D	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		

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



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

- Molecule 4 is HYDROSULFURIC ACID (CCD ID: H2S) (formula: H_2S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	895	Total	O	0	0
			895	895		
5	B	779	Total	O	0	0
			779	779		

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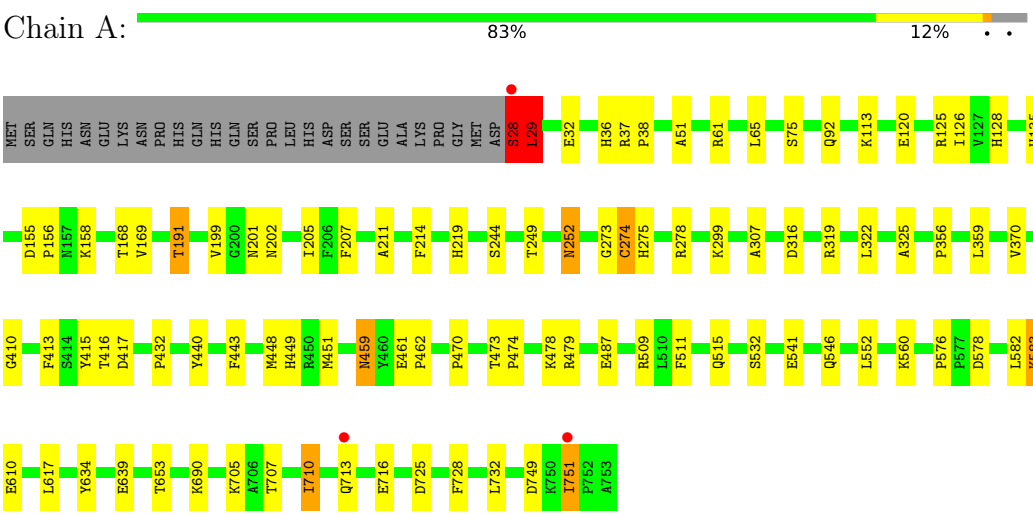
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	847	Total O 847 847	0	0
5	D	902	Total O 902 902	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

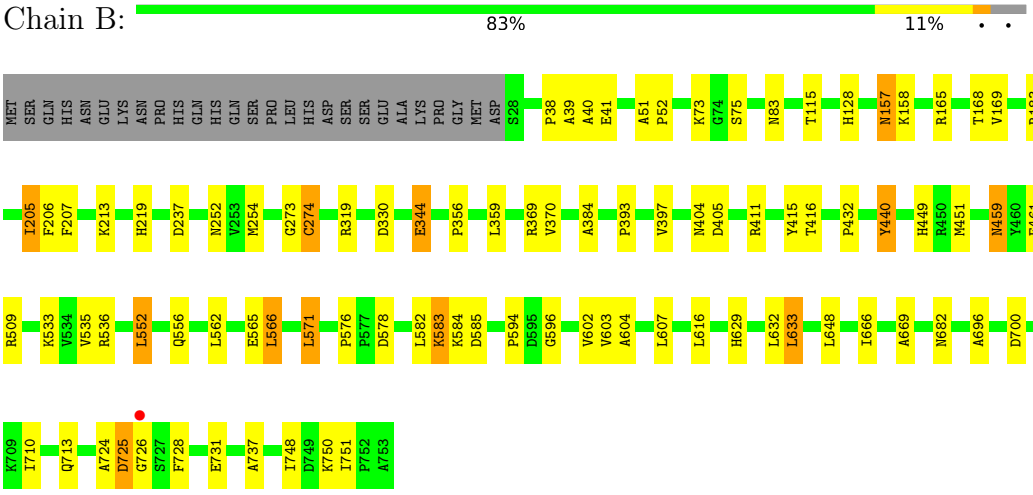
• Molecule 1: Catalase HPII

Chain A:



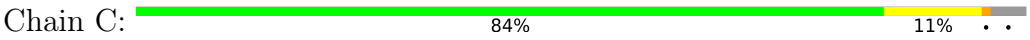
• Molecule 1: Catalase HPII

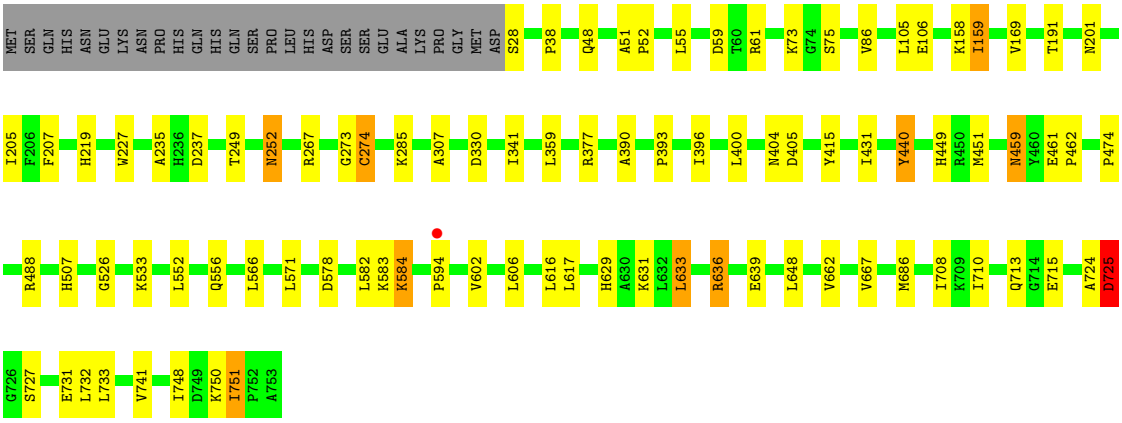
Chain B:



• Molecule 1: Catalase HPII

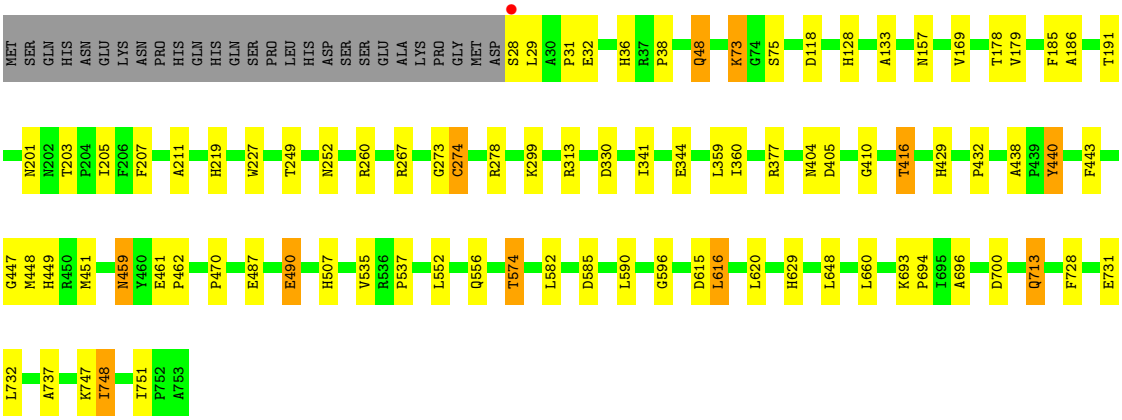
Chain C:





• Molecule 1: Catalase HPII

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.50Å 133.02Å 122.67Å 90.00° 109.40° 90.00°	Depositor
Resolution (Å)	34.25 – 1.80 34.25 – 1.80	Depositor EDS
% Data completeness (in resolution range)	92.5 (34.25-1.80) 93.0 (34.25-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 1.79Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.142 , 0.190 0.142 , 0.190	Depositor DCC
R_{free} test set	12185 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	11.8	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	26809	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 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HDD, HDE, 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	1.33	13/5932 (0.2%)	1.14	9/8064 (0.1%)
1	B	1.31	6/5931 (0.1%)	1.12	8/8062 (0.1%)
1	C	1.32	10/5908 (0.2%)	1.14	14/8033 (0.2%)
1	D	1.37	9/5966 (0.2%)	1.11	6/8109 (0.1%)
All	All	1.33	38/23737 (0.2%)	1.13	37/32268 (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 (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	LEU	N-CA	-7.93	1.34	1.46
1	C	474	PRO	CA-C	7.50	1.56	1.51
1	C	235	ALA	CA-CB	6.86	1.61	1.52
1	D	203	THR	N-CA	6.73	1.51	1.45
1	B	384	ALA	N-CA	6.43	1.54	1.46
1	B	535	VAL	CA-CB	6.34	1.63	1.54
1	D	447	GLY	N-CA	6.21	1.51	1.45
1	D	179	VAL	CA-CB	6.13	1.62	1.54
1	C	396	ILE	CA-CB	6.03	1.62	1.54
1	C	526	GLY	N-CA	5.97	1.53	1.45
1	D	299	LYS	C-O	5.80	1.31	1.24
1	B	356	PRO	C-O	-5.77	1.18	1.23
1	D	438	ALA	CA-CB	5.72	1.61	1.53
1	A	307	ALA	CA-CB	5.67	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	341	ILE	CA-CB	5.53	1.58	1.54
1	A	322	LEU	C-O	5.49	1.30	1.24
1	D	186	ALA	CA-C	-5.49	1.46	1.52
1	B	40	ALA	CA-CB	-5.47	1.45	1.52
1	A	169	VAL	N-CA	5.46	1.51	1.46
1	D	133	ALA	N-CA	5.44	1.52	1.45
1	A	473	THR	C-N	5.42	1.38	1.33
1	B	397	VAL	N-CA	5.37	1.51	1.46
1	C	400	LEU	C-O	5.37	1.30	1.23
1	C	390	ALA	CA-CB	5.36	1.61	1.53
1	D	178	THR	CA-CB	5.35	1.60	1.52
1	A	92	GLN	N-CA	5.33	1.53	1.45
1	A	710	ILE	CA-CB	5.30	1.60	1.54
1	A	191	THR	CA-CB	5.28	1.62	1.53
1	A	592	ALA	N-CA	5.26	1.52	1.46
1	C	86	VAL	N-CA	5.19	1.52	1.46
1	D	377	ARG	CZ-NH2	5.19	1.40	1.33
1	A	316	ASP	N-CA	5.14	1.52	1.46
1	A	126	ILE	N-CA	5.10	1.52	1.46
1	C	741	VAL	N-CA	5.09	1.52	1.46
1	A	202	ASN	N-CA	5.05	1.52	1.46
1	C	159	ILE	CB-CG1	-5.03	1.43	1.53
1	A	113	LYS	C-O	5.02	1.29	1.24
1	B	205	ILE	CA-CB	5.02	1.61	1.54

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	159	ILE	CB-CG1-CD1	-7.54	97.97	113.80
1	C	48	GLN	CA-C-N	-7.47	112.30	119.85
1	C	48	GLN	C-N-CA	-7.47	112.30	119.85
1	A	28	SER	CA-C-N	-6.84	111.52	122.53
1	A	28	SER	C-N-CA	-6.84	111.52	122.53
1	C	725	ASP	N-CA-C	6.55	124.75	110.80
1	D	574	THR	CB-CA-C	6.46	118.76	109.26
1	C	431	ILE	N-CA-C	-6.27	102.80	108.95
1	C	169	VAL	CB-CA-C	-6.27	105.47	111.05
1	D	615	ASP	N-CA-C	-6.17	104.47	111.14
1	C	307	ALA	N-CA-C	-5.81	105.03	111.36
1	C	667	VAL	CA-C-N	-5.79	114.78	120.52
1	C	667	VAL	C-N-CA	-5.79	114.78	120.52
1	B	731	GLU	N-CA-C	-5.75	104.93	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	237	ASP	N-CA-C	5.75	118.01	111.11
1	C	158	LYS	CA-C-N	-5.73	116.09	123.19
1	C	158	LYS	C-N-CA	-5.73	116.09	123.19
1	A	359	LEU	CA-C-N	-5.70	117.10	123.02
1	A	359	LEU	C-N-CA	-5.70	117.10	123.02
1	B	648	LEU	CA-C-N	5.61	125.79	119.90
1	B	648	LEU	C-N-CA	5.61	125.79	119.90
1	B	536	ARG	CA-C-N	-5.47	113.40	119.19
1	B	536	ARG	C-N-CA	-5.47	113.40	119.19
1	A	325	ALA	N-CA-C	-5.45	105.42	111.36
1	A	560	LYS	N-CA-C	-5.34	105.46	111.28
1	D	585	ASP	CA-C-N	-5.31	114.35	119.87
1	D	585	ASP	C-N-CA	-5.31	114.35	119.87
1	B	585	ASP	CA-C-N	-5.31	114.35	119.87
1	B	585	ASP	C-N-CA	-5.31	114.35	119.87
1	A	474	PRO	O-C-N	5.28	123.74	121.31
1	C	106	GLU	N-CA-C	5.20	119.37	113.19
1	A	583	LYS	N-CA-C	-5.17	107.02	113.38
1	B	237	ASP	N-CA-C	5.15	117.29	111.11
1	A	120	GLU	N-CA-C	5.10	116.92	111.36
1	D	377	ARG	CG-CD-NE	-5.05	100.90	112.00
1	D	377	ARG	NE-CZ-NH1	-5.02	116.48	121.50
1	C	636	ARG	CG-CD-NE	-5.02	100.97	112.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5755	0	5582	79	0
1	B	5757	0	5587	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5747	0	5577	55	2
1	D	5771	0	5598	48	0
2	A	44	0	31	7	0
2	B	44	0	31	8	0
2	C	44	0	31	9	0
2	D	44	0	31	2	0
3	A	44	0	36	8	0
3	B	44	0	36	10	0
3	C	44	0	36	10	0
3	D	44	0	36	6	0
4	A	1	0	0	1	0
4	B	1	0	0	0	0
4	C	1	0	0	1	0
4	D	1	0	0	0	0
5	A	895	0	0	20	3
5	B	779	0	0	9	2
5	C	847	0	0	19	0
5	D	902	0	0	21	2
All	All	26809	0	22612	275	5

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:578:ASP:HB3	5:C:2919:HOH:O	1.30	1.27
1:A:716:GLU:HG2	5:A:3090:HOH:O	1.39	1.21
1:D:451:MET:SD	5:D:3617:HOH:O	1.95	1.21
1:A:29:LEU:HD22	5:C:2405:HOH:O	1.46	1.11
1:B:416:THR:HG21	5:D:2464:HOH:O	1.51	1.11
3:B:761[B]:HDE:HMCB	3:B:761[B]:HDE:HBCA	1.11	1.10
3:D:761[B]:HDE:HBCB	3:D:761[B]:HDE:HMC	1.37	1.07
1:B:451:MET:HE2	1:D:451:MET:HE2	1.10	1.07
3:B:761[B]:HDE:HMCB	3:B:761[B]:HDE:CBC	1.86	1.06
1:C:451:MET:SD	5:C:3612:HOH:O	2.13	1.04
1:A:451:MET:HE2	1:C:451:MET:HE2	1.05	1.01
3:B:761[B]:HDE:HBCA	3:B:761[B]:HDE:CMC	1.87	1.00
3:B:761[B]:HDE:CBC	3:B:761[B]:HDE:CMC	2.40	0.97
1:A:610:GLU:HG2	5:A:3555:HOH:O	1.65	0.95
1:A:416[A]:THR:HG21	5:A:3313:HOH:O	1.65	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:ARG:HG3	5:C:2916:HOH:O	1.64	0.94
1:A:201:ASN:CG	2:A:760[A]:HDD:HMB1	1.95	0.91
1:C:440:TYR:HD1	5:C:3454:HOH:O	1.53	0.91
3:C:761[B]:HDE:CBC	3:C:761[B]:HDE:HMCB	2.00	0.90
1:D:201:ASN:CG	2:D:760[A]:HDD:HMB1	1.95	0.90
1:B:451:MET:SD	5:B:3614:HOH:O	2.32	0.87
2:C:760[A]:HDD:HMB3	2:C:760[A]:HDD:HBB1	1.56	0.86
1:C:751:ILE:HB	5:C:2367:HOH:O	1.74	0.86
3:D:761[B]:HDE:HBCB	3:D:761[B]:HDE:CMC	2.01	0.86
2:C:760[A]:HDD:HBB1	2:C:760[A]:HDD:CMB	2.05	0.85
1:B:201:ASN:CG	2:B:760[A]:HDD:HMB1	2.02	0.85
3:C:761[B]:HDE:HMCB	3:C:761[B]:HDE:HBCA	1.59	0.83
1:A:751:ILE:HD12	1:A:751:ILE:O	1.80	0.82
1:C:201:ASN:CG	2:C:760[A]:HDD:HMB1	2.05	0.81
1:A:28:SER:O	1:A:28:SER:OG	1.93	0.81
1:A:29:LEU:HD23	5:C:3144:HOH:O	1.80	0.81
1:A:541:GLU:OE2	5:A:2550:HOH:O	1.99	0.80
1:B:440:TYR:O	1:D:73[B]:LYS:HE3	1.81	0.80
1:C:725:ASP:O	5:C:2403:HOH:O	2.00	0.78
1:C:636:ARG:HD3	5:C:2717:HOH:O	1.84	0.78
3:C:761[B]:HDE:HMB	3:C:761[B]:HDE:CBB	2.14	0.78
1:A:610:GLU:CG	5:A:3555:HOH:O	2.27	0.77
1:B:73:LYS:HE3	5:D:3517:HOH:O	1.85	0.77
3:B:761[B]:HDE:HMB	3:B:761[B]:HDE:HBBB	1.67	0.76
1:D:556:GLN:NE2	5:D:2773:HOH:O	2.17	0.76
3:C:761[B]:HDE:CMC	3:C:761[B]:HDE:HBCB	2.15	0.76
3:C:761[B]:HDE:CBC	3:C:761[B]:HDE:CMC	2.63	0.75
3:C:761[B]:HDE:HMB	3:C:761[B]:HDE:HBBA	1.69	0.74
3:C:761[B]:HDE:HMCB	3:C:761[B]:HDE:HBCB	1.70	0.74
1:B:451:MET:HE2	1:D:451:MET:CE	2.05	0.73
1:B:533[A]:LYS:HE2	5:B:3100:HOH:O	1.87	0.73
3:B:761[B]:HDE:CMC	3:B:761[B]:HDE:HBCB	2.18	0.73
1:B:748:ILE:O	1:B:751:ILE:HG22	1.87	0.73
3:D:761[B]:HDE:CMC	3:D:761[B]:HDE:CBC	2.67	0.73
1:D:731:GLU:OE2	5:D:3028:HOH:O	2.04	0.73
3:A:761[B]:HDE:HBCB	3:A:761[B]:HDE:HMC	1.71	0.72
3:D:761[B]:HDE:HMB	3:D:761[B]:HDE:HBBB	1.72	0.72
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.73	0.71
1:D:28:SER:HA	5:D:2467:HOH:O	1.90	0.70
1:B:700:ASP:HB2	5:B:3595:HOH:O	1.92	0.68
1:A:451:MET:CE	1:C:451:MET:HE2	2.01	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:583:LYS:NZ	1:B:583:LYS:H	1.92	0.67
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.77	0.67
1:A:451:MET:HE2	1:C:451:MET:CE	2.01	0.66
3:B:761[B]:HDE:HMB	3:B:761[B]:HDE:CBB	2.26	0.66
1:C:578:ASP:HB2	1:C:582:LEU:O	1.96	0.65
1:B:201:ASN:CG	2:B:760[A]:HDD:CMB	2.69	0.65
1:A:451:MET:SD	5:A:3609:HOH:O	2.53	0.65
3:A:761[B]:HDE:HBCB	3:A:761[B]:HDE:CMC	2.27	0.64
1:A:532:SER:OG	5:A:2410:HOH:O	2.10	0.64
1:A:582:LEU:O	5:A:3093:HOH:O	2.15	0.63
1:B:724:ALA:O	1:B:725:ASP:O	2.17	0.62
1:C:59:ASP:OD2	5:C:2529:HOH:O	2.16	0.62
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.07	0.62
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.81	0.62
1:D:490:GLU:OE1	5:D:2308:HOH:O	2.16	0.61
1:B:115:THR:HG21	5:D:3420:HOH:O	1.99	0.61
1:C:556:GLN:HG3	1:C:566:LEU:HD12	1.83	0.61
1:B:449[B]:HIS:HE1	5:D:1789:HOH:O	1.82	0.60
1:C:28:SER:N	5:C:2523:HOH:O	2.34	0.60
1:A:610:GLU:CD	5:A:3555:HOH:O	2.41	0.60
1:A:201:ASN:CG	2:A:760[A]:HDD:CMB	2.74	0.60
1:D:416[B]:THR:HG22	5:D:1415:HOH:O	2.03	0.59
1:A:36:HIS:HE1	5:A:1872:HOH:O	1.86	0.59
1:C:273:GLY:C	1:C:274:CYS:SG	2.86	0.58
1:D:748:ILE:O	1:D:751:ILE:HG22	2.02	0.58
1:A:639:GLU:HG3	5:A:2414:HOH:O	2.02	0.58
1:A:416[B]:THR:HG22	5:A:908:HOH:O	2.04	0.58
1:C:533:LYS:NZ	5:C:2231:HOH:O	2.37	0.58
1:A:244:SER:HA	1:A:546[B]:GLN:NE2	2.18	0.57
1:A:199:VAL:HG12	3:A:761[B]:HDE:HHDA	1.86	0.57
1:C:201:ASN:CG	2:C:760[A]:HDD:CMB	2.77	0.57
1:D:201:ASN:CG	2:D:760[A]:HDD:CMB	2.74	0.57
1:D:449[A]:HIS:HE1	5:D:1789:HOH:O	1.88	0.57
3:A:761[B]:HDE:HMB	3:A:761[B]:HDE:HBBB	1.86	0.57
1:D:267:ARG:HG3	5:D:1920:HOH:O	2.04	0.56
1:A:690:LYS:HG3	1:A:751:ILE:HD11	1.86	0.56
1:B:726:GLY:HA2	5:B:3590:HOH:O	2.05	0.56
2:C:760[A]:HDD:HMB3	2:C:760[A]:HDD:CBB	2.33	0.56
1:C:274:CYS:CA	4:C:754:H2S:S	2.94	0.56
1:B:602:VAL:HG22	1:B:629:HIS:HB2	1.87	0.56
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:LEU:H	1:C:507:HIS:HD2	1.54	0.56
1:C:440:TYR:CD1	5:C:3454:HOH:O	2.38	0.55
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.22	0.55
1:D:616:LEU:HD22	1:D:620:LEU:HG	1.88	0.55
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.37	0.55
1:C:359:LEU:C	1:C:359:LEU:HD12	2.32	0.55
1:D:440:TYR:CZ	5:D:3517:HOH:O	2.53	0.55
1:C:727:SER:O	1:C:731:GLU:HG3	2.07	0.55
1:B:411:ARG:HG2	3:B:761[B]:HDE:C3B	2.37	0.54
2:C:760[A]:HDD:HBC1	2:C:760[A]:HDD:CMC	2.37	0.54
1:B:157:ASN:C	1:B:157:ASN:HD22	2.15	0.54
1:B:440:TYR:CE1	1:D:73[B]:LYS:HE2	2.44	0.53
1:D:629:HIS:HD2	5:D:1554:HOH:O	1.90	0.53
1:B:359:LEU:H	1:B:507:HIS:HD2	1.56	0.53
2:B:760[A]:HDD:HBC1	2:B:760[A]:HDD:CMC	2.39	0.53
1:C:583:LYS:O	1:C:584:LYS:HB3	2.07	0.52
3:C:761[B]:HDE:HMB	3:C:761[B]:HDE:HBBB	1.89	0.52
1:C:629:HIS:HD2	5:C:1129:HOH:O	1.92	0.52
1:B:603:VAL:HG11	1:B:666:ILE:CD1	2.40	0.51
1:B:578:ASP:HB3	1:B:582:LEU:O	2.10	0.51
1:B:583:LYS:H	1:B:583:LYS:HZ3	1.57	0.51
1:B:273:GLY:C	1:B:274:CYS:SG	2.93	0.51
1:C:359:LEU:H	1:C:507:HIS:CD2	2.29	0.51
1:D:359:LEU:HD21	5:D:2971:HOH:O	2.10	0.51
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.27	0.50
1:A:583:LYS:O	1:A:584:LYS:HB3	2.11	0.50
1:B:583:LYS:O	1:B:584:LYS:HB3	2.12	0.50
1:A:413:PHE:HB2	1:C:105:LEU:HD11	1.93	0.50
1:A:273:GLY:C	1:A:274:CYS:SG	2.94	0.50
1:A:705:LYS:HE3	1:A:710:ILE:CG2	2.42	0.50
1:A:393:PRO:HD2	1:A:415:TYR:CG	2.47	0.49
1:A:725:ASP:H	1:A:728:PHE:HB3	1.77	0.49
1:D:713:GLN:HG2	1:D:713:GLN:O	2.11	0.49
1:B:73:LYS:CD	5:D:3517:HOH:O	2.60	0.49
1:C:440:TYR:HB3	5:C:3454:HOH:O	2.13	0.49
1:A:749:ASP:HB2	5:A:3511:HOH:O	2.11	0.49
1:B:165:ARG:HD3	3:B:761[B]:HDE:O2D	2.12	0.49
1:B:38:PRO:HG2	1:B:51:ALA:HB2	1.95	0.48
1:B:201:ASN:ND2	2:B:760[A]:HDD:CMB	2.75	0.48
1:B:183:ARG:HG2	5:B:3407:HOH:O	2.13	0.48
1:D:278:ARG:HH12	1:D:487:GLU:CD	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.29	0.48
1:D:157:ASN:ND2	5:D:2055:HOH:O	2.47	0.48
1:B:556:GLN:HG2	1:B:566:LEU:HD22	1.96	0.48
1:C:201:ASN:ND2	2:C:760[A]:HDD:CMB	2.77	0.48
1:B:393:PRO:HD2	1:B:415:TYR:CG	2.49	0.47
1:D:535:VAL:O	1:D:537:PRO:HD3	2.14	0.47
3:D:761[B]:HDE:CMB	3:D:761[B]:HDE:CBB	2.91	0.47
1:B:604:ALA:HB1	1:B:633:LEU:HD22	1.96	0.47
1:B:629:HIS:HD2	5:B:1046:HOH:O	1.97	0.47
1:C:38:PRO:HG2	1:C:51:ALA:HB2	1.97	0.47
3:D:761[B]:HDE:HMB	3:D:761[B]:HDE:CBB	2.43	0.47
1:A:125:ARG:HB3	3:A:761[B]:HDE:HBA	1.97	0.47
1:A:275:HIS:NE2	2:A:760[A]:HDD:HBB1	2.30	0.47
1:B:201:ASN:OD1	2:B:760[A]:HDD:HMB1	2.12	0.47
2:C:760[A]:HDD:CMC	2:C:760[A]:HDD:CBC	2.93	0.47
1:A:751:ILE:O	1:A:751:ILE:CD1	2.58	0.47
1:D:31:PRO:HD2	1:D:36:HIS:HB3	1.98	0.46
1:A:610:GLU:HG2	5:A:2551:HOH:O	2.15	0.46
3:A:761[B]:HDE:HMA	3:A:761[B]:HDE:HAAA	1.64	0.46
1:A:201:ASN:ND2	2:A:760[A]:HDD:CMB	2.78	0.46
1:D:341:ILE:HD11	1:D:360:ILE:HD13	1.96	0.46
1:B:52:PRO:HG3	5:D:1451:HOH:O	2.16	0.46
1:B:344:GLU:CD	1:B:344:GLU:H	2.23	0.46
2:B:760[A]:HDD:HMD2	2:B:760[A]:HDD:HAD2	1.67	0.46
1:C:583:LYS:HE2	1:C:583:LYS:HB2	1.72	0.46
1:C:602[B]:VAL:HG13	1:C:662:VAL:HA	1.97	0.46
1:A:29:LEU:HB2	5:C:2405:HOH:O	2.15	0.46
1:B:319:ARG:HD3	1:C:227:TRP:O	2.16	0.46
1:C:594:PRO:HA	5:C:3460:HOH:O	2.16	0.46
1:A:356:PRO:HG3	1:A:407:LEU:HB2	1.97	0.45
1:B:725:ASP:OD2	1:B:725:ASP:C	2.59	0.45
1:C:631:LYS:HG3	1:C:633:LEU:HD13	1.98	0.45
1:C:748:ILE:O	1:C:751:ILE:HG22	2.16	0.45
1:D:404:ASN:O	1:D:405:ASP:C	2.59	0.45
1:A:36:HIS:CD2	1:A:36:HIS:H	2.34	0.45
1:A:201:ASN:CG	3:A:761[B]:HDE:HAC	2.41	0.45
1:A:751:ILE:HD12	1:A:751:ILE:C	2.40	0.45
1:A:65:LEU:HD21	1:A:135:HIS:CG	2.51	0.45
1:A:275:HIS:CE1	2:A:760[A]:HDD:CBB	2.99	0.45
1:B:583:LYS:H	1:B:583:LYS:HZ2	1.62	0.45
1:D:696:ALA:HB1	1:D:728:PHE:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LEU:HD11	1:A:370:VAL:HG13	1.99	0.45
1:A:155:ASP:CG	5:A:3378:HOH:O	2.60	0.45
1:B:596:GLY:HA3	1:B:737:ALA:O	2.17	0.45
1:C:52:PRO:HG2	1:C:55:LEU:HD12	1.99	0.45
1:A:448:MET:HG3	1:A:449[B]:HIS:CD2	2.51	0.45
1:B:73:LYS:CE	5:D:3517:HOH:O	2.52	0.45
1:A:511:PHE:O	1:A:515:GLN:HG2	2.18	0.44
1:B:603:VAL:HG11	1:B:666:ILE:HD12	1.99	0.44
1:B:157:ASN:C	1:B:157:ASN:ND2	2.75	0.44
1:A:610:GLU:OE1	5:A:2394:HOH:O	2.21	0.44
1:C:207:PHE:O	1:C:249:THR:HA	2.17	0.44
1:B:669:ALA:HB1	5:B:3595:HOH:O	2.16	0.44
1:A:128:HIS:HA	1:A:168:THR:O	2.18	0.44
1:A:207:PHE:O	1:A:249:THR:HA	2.18	0.44
1:A:479:ARG:NH2	5:A:2607:HOH:O	2.45	0.44
1:B:369:ARG:HG2	5:B:1639:HOH:O	2.17	0.44
1:A:37:ARG:HA	1:A:38:PRO:HD3	1.91	0.44
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.99	0.43
1:B:607:LEU:HD11	1:B:632:LEU:HB3	2.00	0.43
3:B:761[B]:HDE:HMAB	3:B:761[B]:HDE:HAAA	1.63	0.43
3:C:761[B]:HDE:HMAA	3:C:761[B]:HDE:HAAA	1.73	0.43
1:A:443:PHE:CZ	1:A:470:PRO:HD2	2.54	0.43
1:B:213:LYS:HB3	1:B:213:LYS:HE3	1.86	0.43
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.99	0.43
1:C:73:LYS:HB3	1:C:73:LYS:HE3	1.86	0.43
1:C:201:ASN:OD1	2:C:760[A]:HDD:HMB1	2.19	0.43
1:D:38:PRO:HA	1:D:48:GLN:HE21	1.84	0.43
1:D:448:MET:O	1:D:449[A]:HIS:HB2	2.18	0.43
1:D:273:GLY:C	1:D:274:CYS:SG	3.02	0.43
1:B:708:ILE:HG13	1:B:710:ILE:HG12	2.00	0.43
1:D:461:GLU:HA	1:D:462:PRO:C	2.44	0.43
1:A:274:CYS:CA	4:A:754:H2S:S	3.06	0.42
1:C:393:PRO:HD2	1:C:415:TYR:CG	2.53	0.42
1:D:29:LEU:N	5:D:2467:HOH:O	2.38	0.42
1:A:146:ASP:HB2	5:A:2592:HOH:O	2.19	0.42
1:B:359:LEU:H	1:B:507:HIS:CD2	2.35	0.42
1:B:552:LEU:HD22	1:B:556:GLN:HG3	2.00	0.42
1:C:461:GLU:HA	1:C:462:PRO:C	2.44	0.42
1:A:61:ARG:HG2	1:A:61:ARG:HH11	1.83	0.42
1:A:393:PRO:HD2	1:A:415:TYR:CD2	2.54	0.42
1:B:449[B]:HIS:CE1	5:D:1789:HOH:O	2.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:359:LEU:H	1:D:507:HIS:HD2	1.66	0.42
1:C:61:ARG:HG3	5:C:2648:HOH:O	2.20	0.42
1:A:156:PRO:HD2	5:A:3378:HOH:O	2.20	0.42
1:B:39:ALA:HB1	1:B:41:GLU:HG2	2.01	0.42
3:A:761[B]:HDE:CMC	3:A:761[B]:HDE:CBC	2.97	0.42
1:B:461:GLU:HA	1:B:462:PRO:C	2.44	0.42
1:A:38:PRO:HG2	1:A:51:ALA:HB2	2.01	0.42
1:A:751:ILE:CD1	1:A:751:ILE:C	2.92	0.42
1:C:404:ASN:O	1:C:405:ASP:C	2.61	0.42
1:B:201:ASN:ND2	2:B:760[A]:HDD:HMB3	2.35	0.41
1:B:254:MET:HE3	1:B:254:MET:HB3	1.94	0.41
1:D:443:PHE:CZ	1:D:470:PRO:HD2	2.55	0.41
1:D:693:LYS:HA	1:D:694:PRO:HD3	1.96	0.41
1:A:459:ASN:HD22	1:A:459:ASN:C	2.26	0.41
1:B:128:HIS:HA	1:B:168:THR:O	2.20	0.41
1:B:507:HIS:HE1	5:B:888:HOH:O	2.02	0.41
1:B:696:ALA:HB1	1:B:728:PHE:CZ	2.55	0.41
1:C:461:GLU:HB2	1:C:462:PRO:HA	2.02	0.41
1:B:128:HIS:CE1	1:B:169:VAL:HG22	2.55	0.41
1:A:634:TYR:O	1:A:653:THR:HA	2.20	0.41
1:D:596:GLY:HA3	1:D:737:ALA:O	2.20	0.41
1:A:578:ASP:OD1	1:A:583:LYS:NZ	2.53	0.41
1:B:509:ARG:HD2	1:B:576:PRO:HD2	2.03	0.41
1:A:319:ARG:HD3	1:D:227:TRP:O	2.20	0.41
1:B:751:ILE:O	1:B:751:ILE:HG23	2.21	0.41
1:A:299:LYS:HB2	1:A:299:LYS:HE3	1.90	0.41
1:A:461:GLU:HA	1:A:462:PRO:C	2.45	0.41
1:D:260:ARG:HD3	1:D:590:LEU:HD21	2.03	0.41
1:A:211:ALA:HB3	1:A:410:GLY:HA3	2.03	0.41
1:A:275:HIS:CE1	2:A:760[A]:HDD:HBB2	2.56	0.41
1:A:509:ARG:HD2	1:A:576:PRO:HD2	2.03	0.41
1:B:83:ASN:HB3	1:D:429:HIS:CG	2.56	0.41
1:C:710:ILE:HG23	1:C:715:GLU:HG2	2.02	0.41
1:C:748:ILE:O	1:C:751:ILE:CG2	2.69	0.41
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.50	0.41
1:D:313:ARG:HG3	1:D:660:LEU:HD12	2.03	0.41
1:A:214:PHE:CD1	2:A:760[A]:HDD:HAC	2.56	0.41
1:A:252:ASN:HD22	1:A:252:ASN:HA	1.71	0.41
5:A:1788:HOH:O	1:C:449[A]:HIS:HE1	2.02	0.41
1:C:252:ASN:HD22	1:C:252:ASN:HA	1.68	0.41
1:C:602[A]:VAL:HG21	5:C:2034:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:HIS:CE1	1:D:169:VAL:HG22	2.56	0.41
1:B:393:PRO:HD2	1:B:415:TYR:CD2	2.56	0.40
2:B:760[A]:HDD:CMC	2:B:760[A]:HDD:CBC	2.99	0.40
1:D:48:GLN:HE21	1:D:48:GLN:HB3	1.72	0.40
1:A:417:ASP:OD2	1:D:118:ASP:OD1	2.39	0.40
1:B:404:ASN:O	1:B:405:ASP:C	2.65	0.40
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.36	0.40
3:C:761[B]:HDE:HBBA	3:C:761[B]:HDE:CMB	2.46	0.40
1:D:207:PHE:O	1:D:249:THR:HA	2.21	0.40
1:C:686:MET:HB3	1:C:751:ILE:HD11	2.03	0.40
1:B:206:PHE:CG	1:B:207:PHE:N	2.90	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:ASP:CB	5:B:3206:HOH:O[2_545]	1.99	0.21
1:C:584:LYS:NZ	5:A:1624:HOH:O[1_554]	2.06	0.14
5:D:2178:HOH:O	5:D:2976:HOH:O[1_655]	2.06	0.14
5:A:3348:HOH:O	5:B:2822:HOH:O[2_545]	2.10	0.10
5:A:3241:HOH:O	5:D:2457:HOH:O[2_646]	2.12	0.08

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	729/753 (97%)	708 (97%)	20 (3%)	1 (0%)	48	34
1	B	729/753 (97%)	709 (97%)	18 (2%)	2 (0%)	36	25
1	C	726/753 (96%)	703 (97%)	22 (3%)	1 (0%)	48	34
1	D	733/753 (97%)	712 (97%)	20 (3%)	1 (0%)	48	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2917/3012 (97%)	2832 (97%)	80 (3%)	5 (0%)	43 31

All (5) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	614/634 (97%)	596 (97%)	18 (3%)	37 25
1	B	614/634 (97%)	591 (96%)	23 (4%)	30 18
1	C	611/634 (96%)	586 (96%)	25 (4%)	27 15
1	D	618/634 (98%)	592 (96%)	26 (4%)	26 14
All	All	2457/2536 (97%)	2365 (96%)	92 (4%)	30 18

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	29	LEU
1	A	32	GLU
1	A	191	THR
1	A	205	ILE
1	A	252	ASN
1	A	274	CYS
1	A	432	PRO
1	A	440	TYR
1	A	459	ASN

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Mol	Chain	Res	Type
1	A	478	LYS
1	A	552	LEU
1	A	584	LYS
1	A	617	LEU
1	A	707	THR
1	A	713	GLN
1	A	732	LEU
1	A	751	ILE
1	B	157	ASN
1	B	158	LYS
1	B	185	PHE
1	B	205	ILE
1	B	252	ASN
1	B	274	CYS
1	B	344	GLU
1	B	370	VAL
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	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	285	LYS
1	C	377	ARG
1	C	440	TYR
1	C	459	ASN
1	C	488	ARG
1	C	552	LEU

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Mol	Chain	Res	Type
1	C	571	LEU
1	C	584	LYS
1	C	606	LEU
1	C	616	LEU
1	C	617	LEU
1	C	633	LEU
1	C	639	GLU
1	C	648	LEU
1	C	713	GLN
1	C	725	ASP
1	C	732	LEU
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	252	ASN
1	D	274	CYS
1	D	344	GLU
1	D	416[A]	THR
1	D	416[B]	THR
1	D	432	PRO
1	D	440	TYR
1	D	459	ASN
1	D	490	GLU
1	D	552	LEU
1	D	574	THR
1	D	582	LEU
1	D	616	LEU
1	D	648	LEU
1	D	700	ASP
1	D	713	GLN
1	D	732	LEU
1	D	747	LYS
1	D	748	ILE

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	84	GLN
1	A	201	ASN
1	A	252	ASN
1	A	459	ASN
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
1	D	48	GLN
1	D	157	ASN
1	D	252	ASN
1	D	459	ASN
1	D	507	HIS
1	D	549	HIS
1	D	556	GLN
1	D	629	HIS
1	D	671	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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	A	760[A]	5,1	46,52,52	1.64	10 (21%)	62,89,89	2.14	20 (32%)
2	HDD	C	760[A]	5,1	46,52,52	1.25	6 (13%)	62,89,89	2.34	16 (25%)
3	HDE	D	761[B]	5,1	42,52,52	1.84	10 (23%)	49,89,89	2.04	19 (38%)
2	HDD	B	760[A]	5,1	46,52,52	1.58	10 (21%)	62,89,89	2.00	12 (19%)
3	HDE	B	761[B]	5,1	42,52,52	1.92	12 (28%)	49,89,89	1.97	16 (32%)
3	HDE	C	761[B]	5,1	42,52,52	1.91	12 (28%)	49,89,89	2.28	17 (34%)
3	HDE	A	761[B]	5,1	42,52,52	1.95	12 (28%)	49,89,89	2.00	12 (24%)
2	HDD	D	760[A]	5,1	46,52,52	1.50	9 (19%)	62,89,89	2.13	19 (30%)

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	A	760[A]	5,1	-	6/9/89/89	0/1/9/9
2	HDD	C	760[A]	5,1	-	2/9/89/89	0/1/9/9
3	HDE	D	761[B]	5,1	-	6/9/89/89	0/1/9/9
2	HDD	B	760[A]	5,1	-	2/9/89/89	0/1/9/9
3	HDE	B	761[B]	5,1	-	6/9/89/89	0/1/9/9
3	HDE	C	761[B]	5,1	-	6/9/89/89	0/1/9/9
3	HDE	A	761[B]	5,1	-	6/9/89/89	0/1/9/9
2	HDD	D	760[A]	5,1	-	6/9/89/89	0/1/9/9

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	760[A]	HDD	O1D-C3D	-5.53	1.37	1.46
3	B	761[B]	HDE	O1A-CGA	5.40	1.44	1.35
3	C	761[B]	HDE	O1A-CGA	5.26	1.43	1.35
3	D	761[B]	HDE	O1A-CGA	4.87	1.43	1.35
3	A	761[B]	HDE	O1A-CGA	4.81	1.43	1.35
3	D	761[B]	HDE	CHA-C4D	4.23	1.48	1.39
3	D	761[B]	HDE	C3B-C2B	4.19	1.49	1.38
3	A	761[B]	HDE	C3D-C2D	4.05	1.49	1.38
3	A	761[B]	HDE	CHB-C1B	4.04	1.48	1.39
3	A	761[B]	HDE	C3B-C2B	4.00	1.49	1.38
3	B	761[B]	HDE	CHA-C4D	3.96	1.48	1.39
2	D	760[A]	HDD	O1D-C3D	-3.95	1.40	1.46
3	C	761[B]	HDE	C3B-C2B	3.84	1.48	1.38
3	B	761[B]	HDE	C3C-C2C	3.84	1.48	1.38
3	C	761[B]	HDE	C4C-C3C	3.78	1.49	1.38
3	A	761[B]	HDE	CHA-C4D	3.68	1.47	1.39
3	C	761[B]	HDE	C3C-C2C	3.60	1.48	1.38
3	B	761[B]	HDE	C4A-NA	3.59	1.43	1.37
3	B	761[B]	HDE	C4C-C3C	3.59	1.48	1.38
2	B	760[A]	HDD	O1D-C3D	-3.47	1.41	1.46
3	B	761[B]	HDE	C3B-C2B	3.41	1.47	1.38
3	A	761[B]	HDE	C1A-NA	3.40	1.43	1.37
2	D	760[A]	HDD	CAB-C3B	3.35	1.56	1.47
3	A	761[B]	HDE	C3C-C2C	3.32	1.47	1.38
3	C	761[B]	HDE	C3D-C2D	3.32	1.47	1.38
3	C	761[B]	HDE	C4A-NA	3.31	1.43	1.37
3	D	761[B]	HDE	C4A-NA	3.29	1.43	1.37
3	A	761[B]	HDE	C4C-C3C	3.26	1.47	1.38
2	B	760[A]	HDD	CMA-C3A	3.26	1.57	1.50
2	D	760[A]	HDD	CAC-C3C	3.24	1.56	1.47
3	A	761[B]	HDE	C4D-ND	-3.23	1.33	1.39
3	B	761[B]	HDE	C1A-NA	3.23	1.43	1.37
3	C	761[B]	HDE	CHA-C4D	3.21	1.46	1.39
3	D	761[B]	HDE	C3D-C2D	3.21	1.47	1.38
3	D	761[B]	HDE	C3C-C2C	3.11	1.47	1.38
2	D	760[A]	HDD	OND-C2D	3.09	1.48	1.42
3	D	761[B]	HDE	C1A-NA	3.06	1.42	1.37
2	B	760[A]	HDD	CMC-C2C	3.05	1.57	1.50
2	A	760[A]	HDD	CMC-C2C	2.99	1.56	1.50
3	C	761[B]	HDE	C4D-ND	-2.93	1.34	1.39
3	D	761[B]	HDE	C4C-C3C	2.92	1.46	1.38
2	A	760[A]	HDD	C3B-C2B	-2.91	1.31	1.37
2	B	760[A]	HDD	CAB-C3B	2.86	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	761[B]	HDE	CHB-C1B	2.85	1.45	1.39
3	A	761[B]	HDE	C4A-NA	2.84	1.42	1.37
2	C	760[A]	HDD	O1D-C3D	-2.81	1.42	1.46
3	C	761[B]	HDE	CHB-C1B	2.74	1.45	1.39
2	B	760[A]	HDD	CMD-C2D	2.71	1.56	1.53
2	B	760[A]	HDD	C2A-C3A	-2.71	1.31	1.38
2	B	760[A]	HDD	CAC-C3C	2.62	1.54	1.47
2	A	760[A]	HDD	CAC-C3C	2.61	1.54	1.47
2	C	760[A]	HDD	CAB-C3B	2.58	1.54	1.47
2	D	760[A]	HDD	CMC-C2C	2.57	1.56	1.50
2	A	760[A]	HDD	CAB-C3B	2.56	1.54	1.47
3	B	761[B]	HDE	C3D-C2D	2.53	1.45	1.38
2	A	760[A]	HDD	C3C-C2C	-2.51	1.32	1.41
2	C	760[A]	HDD	CMA-C3A	2.47	1.55	1.50
3	B	761[B]	HDE	CHB-C1B	2.47	1.45	1.39
3	C	761[B]	HDE	C1A-NA	2.40	1.41	1.37
2	B	760[A]	HDD	C3C-C2C	-2.39	1.33	1.41
2	C	760[A]	HDD	CMD-C2D	2.36	1.56	1.53
2	D	760[A]	HDD	CMB-C2B	2.35	1.55	1.50
2	D	760[A]	HDD	C3B-C2B	-2.30	1.32	1.37
3	B	761[B]	HDE	C4D-C3D	2.19	1.49	1.44
2	B	760[A]	HDD	C4D-ND	2.16	1.41	1.37
3	A	761[B]	HDE	O2D-CGD	-2.15	1.23	1.30
2	A	760[A]	HDD	C2A-C3A	-2.15	1.33	1.38
2	D	760[A]	HDD	C2A-C3A	-2.09	1.33	1.38
2	D	760[A]	HDD	CMD-C2D	2.07	1.56	1.53
2	C	760[A]	HDD	CMC-C2C	2.06	1.55	1.50
3	B	761[B]	HDE	C1C-C2C	2.06	1.42	1.37
3	B	761[B]	HDE	CHB-C4A	-2.06	1.31	1.37
2	A	760[A]	HDD	CAA-C2A	2.04	1.56	1.51
3	C	761[B]	HDE	O1A-C2A	-2.03	1.43	1.46
3	A	761[B]	HDE	C1C-C2C	2.02	1.42	1.37
2	A	760[A]	HDD	OND-C2D	2.02	1.46	1.42
3	C	761[B]	HDE	C1C-C2C	2.02	1.42	1.37
3	D	761[B]	HDE	C1B-C2B	-2.01	1.38	1.43
2	A	760[A]	HDD	O2A-CGA	-2.01	1.24	1.30
2	C	760[A]	HDD	C3C-C2C	-2.00	1.34	1.41
2	B	760[A]	HDD	C1D-ND	2.00	1.41	1.37

All (131) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	760[A]	HDD	O1D-CGD-O2D	10.35	129.53	120.81
2	B	760[A]	HDD	O1D-CGD-O2D	8.46	127.94	120.81
2	A	760[A]	HDD	O1D-CGD-CBD	-7.40	103.42	110.17
2	B	760[A]	HDD	O1D-CGD-CBD	-6.68	104.08	110.17
3	A	761[B]	HDE	C4C-NC-C1C	-6.66	102.96	106.81
3	C	761[B]	HDE	C4C-NC-C1C	-6.65	102.96	106.81
2	D	760[A]	HDD	O1D-CGD-O2D	6.27	126.09	120.81
2	C	760[A]	HDD	OND-C2D-CMD	-5.71	98.40	109.45
2	C	760[A]	HDD	C3C-C4C-NC	-5.44	105.22	109.80
2	A	760[A]	HDD	CAD-CBD-CGD	-5.43	96.41	104.48
3	C	761[B]	HDE	CMA-C3A-C4A	-5.34	103.63	112.68
2	D	760[A]	HDD	C3D-O1D-CGD	5.33	116.11	111.14
2	A	760[A]	HDD	C3D-O1D-CGD	5.30	116.08	111.14
3	B	761[B]	HDE	CBC-CAC-C3C	-5.16	98.44	112.42
2	C	760[A]	HDD	O1D-CGD-CBD	-5.08	105.54	110.17
3	B	761[B]	HDE	C4C-NC-C1C	-5.03	103.90	106.81
2	B	760[A]	HDD	CBD-CAD-C3D	-4.93	96.95	103.98
3	A	761[B]	HDE	CAD-CBD-CGD	-4.88	100.72	113.67
2	D	760[A]	HDD	O1D-CGD-CBD	-4.86	105.74	110.17
3	D	761[B]	HDE	C4C-NC-C1C	-4.55	104.18	106.81
3	D	761[B]	HDE	CBC-CAC-C3C	-4.53	100.14	112.42
3	C	761[B]	HDE	C3A-C4A-CHB	-4.18	117.77	124.27
2	D	760[A]	HDD	C2A-C1A-NA	-4.14	105.56	110.15
3	A	761[B]	HDE	CBA-CAA-C2A	4.05	109.75	103.98
3	C	761[B]	HDE	C3D-C4D-ND	3.98	114.57	110.15
3	B	761[B]	HDE	CAD-CBD-CGD	-3.96	103.17	113.67
3	D	761[B]	HDE	CAD-CBD-CGD	-3.89	103.34	113.67
2	B	760[A]	HDD	CAA-CBA-CGA	-3.86	103.41	113.67
2	A	760[A]	HDD	CAA-CBA-CGA	-3.83	103.52	113.67
3	C	761[B]	HDE	C4B-C3B-C2B	-3.78	103.77	107.10
3	D	761[B]	HDE	C3A-C4A-CHB	-3.71	118.50	124.27
2	C	760[A]	HDD	CBC-CAC-C3C	-3.68	109.12	127.53
3	B	761[B]	HDE	C3A-C4A-CHB	-3.67	118.56	124.27
2	D	760[A]	HDD	CAA-CBA-CGA	-3.66	103.97	113.67
3	A	761[B]	HDE	C3D-C4D-ND	3.61	114.15	110.15
2	D	760[A]	HDD	CHA-C1A-NA	3.60	130.40	123.86
2	D	760[A]	HDD	C3C-C4C-NC	-3.55	106.81	109.80
2	A	760[A]	HDD	C4B-C3B-C2B	3.50	109.85	106.81
3	C	761[B]	HDE	C4D-C3D-C2D	-3.48	101.48	106.87
2	C	760[A]	HDD	CHD-C4C-NC	3.46	130.13	123.86
2	D	760[A]	HDD	C4B-C3B-C2B	3.45	109.80	106.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	761[B]	HDE	CBC-CAC-C3C	-3.45	103.08	112.42
2	B	760[A]	HDD	C3C-C4C-NC	-3.44	106.90	109.80
3	C	761[B]	HDE	C1B-CHB-C4A	-3.34	119.31	125.81
3	C	761[B]	HDE	CAD-CBD-CGD	-3.29	104.93	113.67
3	D	761[B]	HDE	C4D-C3D-C2D	-3.27	101.81	106.87
3	A	761[B]	HDE	C4D-C3D-C2D	-3.17	101.95	106.87
3	B	761[B]	HDE	CBA-CAA-C2A	3.15	108.48	103.98
3	D	761[B]	HDE	CMB-C2B-C3B	3.15	132.31	125.62
3	D	761[B]	HDE	CBA-CAA-C2A	3.14	108.45	103.98
3	A	761[B]	HDE	CAB-C3B-C2B	3.08	131.76	126.89
3	D	761[B]	HDE	CBB-CAB-C3B	-3.07	104.10	112.42
2	D	760[A]	HDD	CHB-C4A-NA	3.04	129.38	123.86
2	D	760[A]	HDD	OND-C2D-CMD	-3.03	103.60	109.45
3	D	761[B]	HDE	C4B-C3B-C2B	-3.01	104.44	107.10
2	A	760[A]	HDD	CHB-C4A-NA	2.96	129.23	123.86
2	A	760[A]	HDD	CHA-C1A-NA	2.94	129.20	123.86
2	A	760[A]	HDD	OND-C2D-CMD	-2.90	103.84	109.45
3	C	761[B]	HDE	O1A-CGA-O2A	2.84	123.20	120.81
3	C	761[B]	HDE	CHB-C4A-NA	2.81	128.16	124.28
2	A	760[A]	HDD	CAB-C3B-C2B	-2.81	119.30	128.43
3	A	761[B]	HDE	CMD-C2D-C3D	2.77	131.50	125.62
2	C	760[A]	HDD	CMD-C2D-C1D	2.77	117.38	112.68
3	B	761[B]	HDE	C4B-C3B-C2B	-2.76	104.66	107.10
3	D	761[B]	HDE	CAD-C3D-C4D	2.71	130.24	124.94
2	C	760[A]	HDD	CHA-C1A-NA	2.69	128.74	123.86
3	B	761[B]	HDE	C2B-C1B-NB	2.66	114.40	110.14
3	B	761[B]	HDE	C4C-C3C-C2C	2.65	109.45	107.10
2	C	760[A]	HDD	CHC-C1C-NC	2.65	128.66	123.86
2	D	760[A]	HDD	CHC-C4B-C3B	2.64	129.66	125.21
2	B	760[A]	HDD	CAD-CBD-CGD	-2.63	100.57	104.48
3	C	761[B]	HDE	CBA-CAA-C2A	2.63	107.73	103.98
3	D	761[B]	HDE	C3D-C4D-ND	2.63	113.07	110.15
2	A	760[A]	HDD	CHC-C4B-NB	2.62	127.31	124.45
2	C	760[A]	HDD	CBB-CAB-C3B	-2.62	114.45	127.53
2	D	760[A]	HDD	C2C-C1C-NC	-2.61	105.96	110.14
2	A	760[A]	HDD	CHD-C4C-NC	2.58	128.53	123.86
2	C	760[A]	HDD	C4C-C3C-C2C	2.57	110.50	107.30
2	A	760[A]	HDD	CBB-CAB-C3B	-2.56	114.72	127.53
3	C	761[B]	HDE	C4C-C3C-C2C	2.56	109.36	107.10
2	C	760[A]	HDD	C3D-O1D-CGD	2.56	113.53	111.14
2	D	760[A]	HDD	C4A-C3A-C2A	2.55	109.74	106.82
3	D	761[B]	HDE	C2B-C1B-NB	2.54	114.21	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	760[A]	HDD	CBB-CAB-C3B	-2.53	114.87	127.53
2	A	760[A]	HDD	CAB-C3B-C4B	2.52	130.85	124.82
2	C	760[A]	HDD	C4C-NC-C1C	2.52	109.92	105.82
2	D	760[A]	HDD	C4C-NC-C1C	2.47	109.85	105.82
2	B	760[A]	HDD	CBC-CAC-C3C	-2.47	115.20	127.53
3	A	761[B]	HDE	CBC-CAC-C3C	-2.47	105.73	112.42
2	A	760[A]	HDD	C2A-C1A-NA	-2.43	107.45	110.15
2	B	760[A]	HDD	CHA-C1A-NA	2.43	128.27	123.86
2	B	760[A]	HDD	C2A-C1A-NA	-2.43	107.46	110.15
3	A	761[B]	HDE	O1A-CGA-O2A	2.41	122.84	120.81
2	D	760[A]	HDD	C3A-C4A-NA	-2.36	106.35	110.14
2	D	760[A]	HDD	C4A-NA-C1A	2.36	109.66	105.82
3	B	761[B]	HDE	CHB-C1B-C2B	-2.34	120.63	127.43
3	C	761[B]	HDE	C2B-C1B-NB	2.34	113.89	110.14
3	B	761[B]	HDE	CAC-C3C-C2C	-2.34	123.19	126.89
2	A	760[A]	HDD	C4A-C3A-C2A	2.33	109.49	106.82
3	B	761[B]	HDE	C3D-C4D-ND	2.32	112.73	110.15
3	D	761[B]	HDE	CHB-C4A-NA	2.32	127.48	124.28
3	B	761[B]	HDE	CAD-C3D-C4D	2.30	129.43	124.94
3	C	761[B]	HDE	CAD-C3D-C2D	2.30	132.23	127.07
3	D	761[B]	HDE	C1B-C2B-C3B	-2.28	104.21	106.82
3	D	761[B]	HDE	CMA-C3A-C4A	-2.28	108.83	112.68
2	C	760[A]	HDD	CMA-C3A-C4A	-2.27	121.97	125.42
3	B	761[B]	HDE	C1B-C2B-C3B	-2.26	104.22	106.82
2	D	760[A]	HDD	CBC-CAC-C3C	-2.26	116.22	127.53
3	D	761[B]	HDE	C1B-CHB-C4A	-2.25	121.43	125.81
3	D	761[B]	HDE	O1A-CGA-O2A	2.20	122.67	120.81
3	B	761[B]	HDE	O1A-CGA-CBA	2.20	112.18	110.17
2	B	760[A]	HDD	C4B-C3B-C2B	2.19	108.71	106.81
3	A	761[B]	HDE	CAB-C3B-C4B	-2.19	122.52	125.52
2	A	760[A]	HDD	C3C-C4C-NC	-2.16	107.98	109.80
2	D	760[A]	HDD	C2D-C1D-CHD	2.15	127.61	124.27
2	B	760[A]	HDD	CBB-CAB-C3B	-2.15	116.81	127.53
2	A	760[A]	HDD	CMB-C2B-C1B	2.14	128.49	124.73
2	A	760[A]	HDD	CMB-C2B-C3B	-2.11	123.31	128.43
3	A	761[B]	HDE	CAD-C3D-C2D	2.11	131.80	127.07
3	B	761[B]	HDE	O1A-CGA-O2A	2.11	122.59	120.81
3	C	761[B]	HDE	CHB-C1B-C2B	-2.09	121.36	127.43
3	B	761[B]	HDE	C4D-C3D-C2D	-2.09	103.64	106.87
3	A	761[B]	HDE	C2A-O1A-CGA	2.06	113.07	111.14
3	C	761[B]	HDE	CMD-C2D-C3D	2.05	129.97	125.62
3	D	761[B]	HDE	CMC-C2C-C3C	2.05	129.97	125.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	760[A]	HDD	C2C-C1C-NC	-2.04	106.87	110.14
2	A	760[A]	HDD	CMC-C2C-C1C	2.04	128.53	125.42
2	C	760[A]	HDD	CMA-C3A-C2A	2.02	129.90	125.62
3	D	761[B]	HDE	CAB-C3B-C2B	2.01	130.08	126.89
2	C	760[A]	HDD	C2D-C1D-CHD	2.01	127.40	124.27
2	B	760[A]	HDD	C1A-C2A-C3A	2.01	109.98	106.87

There are no chirality outliers.

All (40) 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
3	A	761[B]	HDE	C2C-C3C-CAC-CBC
3	D	761[B]	HDE	C2C-C3C-CAC-CBC
3	B	761[B]	HDE	C4B-C3B-CAB-CBB
3	D	761[B]	HDE	C4B-C3B-CAB-CBB
3	B	761[B]	HDE	C2B-C3B-CAB-CBB
3	A	761[B]	HDE	C4C-C3C-CAC-CBC
3	D	761[B]	HDE	C4C-C3C-CAC-CBC
3	A	761[B]	HDE	C4B-C3B-CAB-CBB
3	B	761[B]	HDE	C4C-C3C-CAC-CBC
3	C	761[B]	HDE	C4B-C3B-CAB-CBB
3	C	761[B]	HDE	C4C-C3C-CAC-CBC
3	A	761[B]	HDE	C2B-C3B-CAB-CBB
3	B	761[B]	HDE	C2C-C3C-CAC-CBC
3	C	761[B]	HDE	C2B-C3B-CAB-CBB
3	C	761[B]	HDE	C2C-C3C-CAC-CBC
3	D	761[B]	HDE	C2B-C3B-CAB-CBB
2	A	760[A]	HDD	C4C-C3C-CAC-CBC
2	D	760[A]	HDD	C4C-C3C-CAC-CBC
2	D	760[A]	HDD	CAA-CBA-CGA-O2A
3	A	761[B]	HDE	CAD-CBD-CGD-O1D
2	A	760[A]	HDD	CAA-CBA-CGA-O2A
2	C	760[A]	HDD	CAA-CBA-CGA-O1A
3	C	761[B]	HDE	CAD-CBD-CGD-O1D
3	A	761[B]	HDE	CAD-CBD-CGD-O2D
2	A	760[A]	HDD	C2C-C3C-CAC-CBC
2	D	760[A]	HDD	C2C-C3C-CAC-CBC
2	B	760[A]	HDD	CAA-CBA-CGA-O1A

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

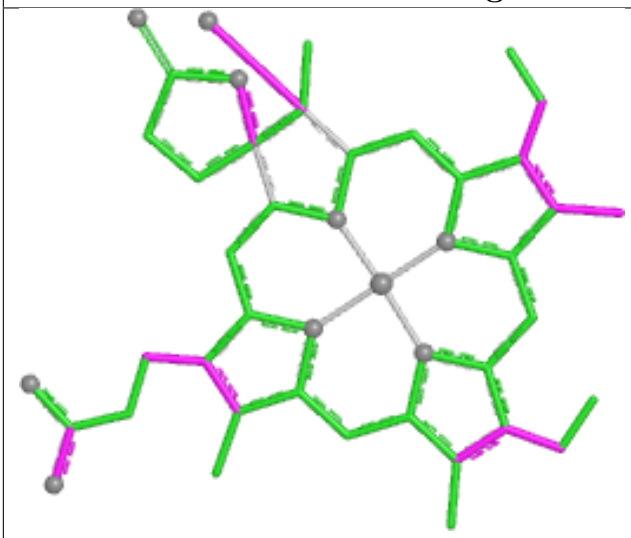
There are no ring outliers.

8 monomers are involved in 60 short contacts:

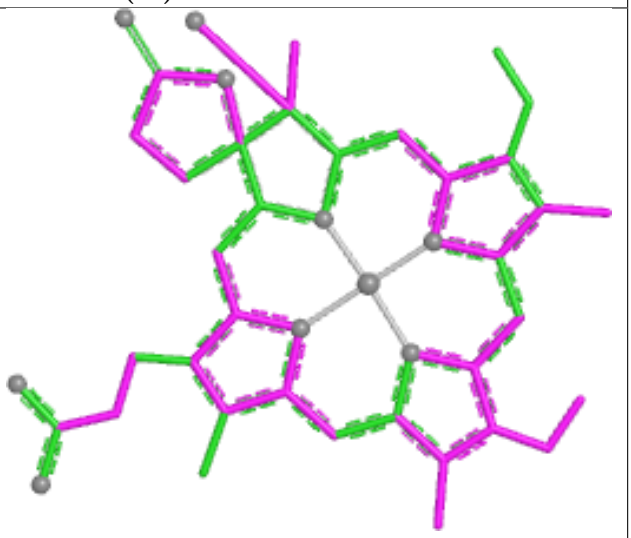
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	760[A]	HDD	7	0
2	C	760[A]	HDD	9	0
3	D	761[B]	HDE	6	0
2	B	760[A]	HDD	8	0
3	B	761[B]	HDE	10	0
3	C	761[B]	HDE	10	0
3	A	761[B]	HDE	8	0
2	D	760[A]	HDD	2	0

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

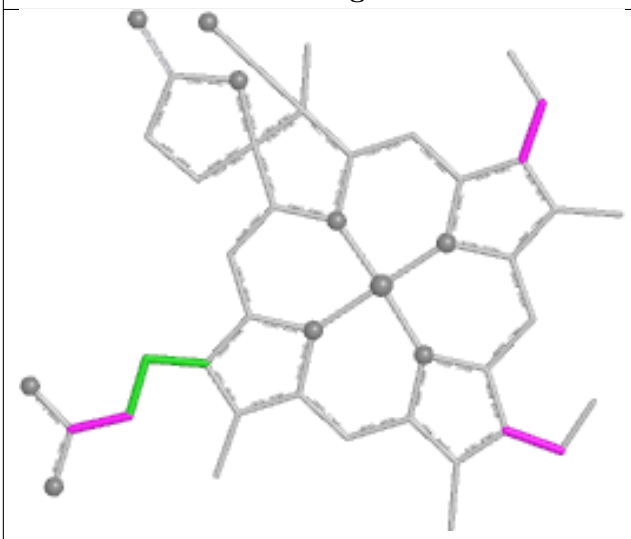
Ligand HDD A 760 (A)



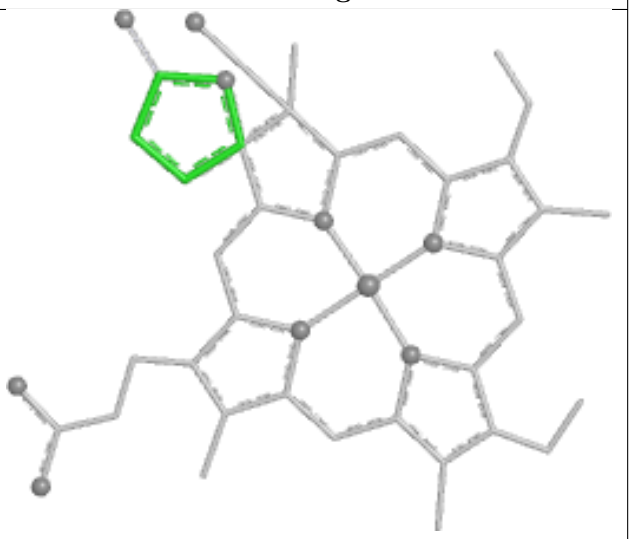
Bond lengths



Bond angles

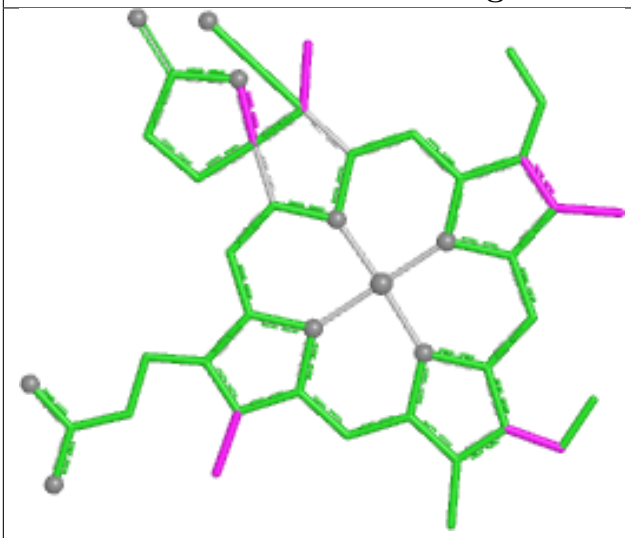


Torsions

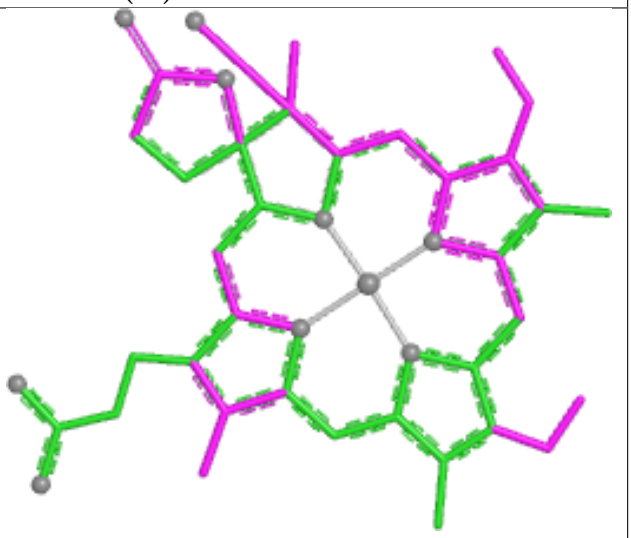


Rings

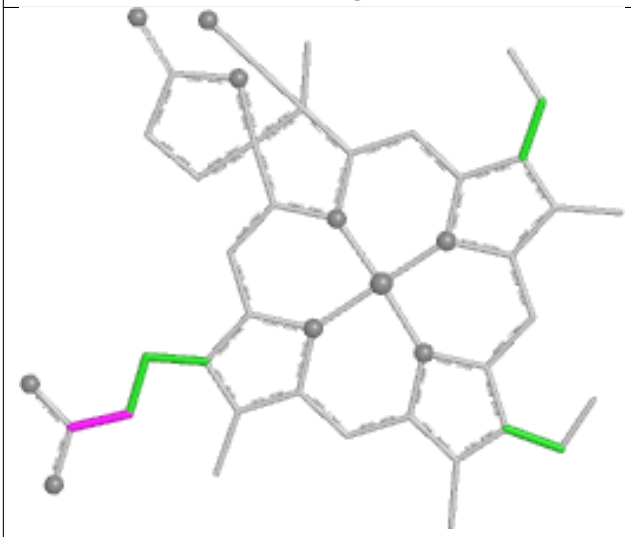
Ligand HDD C 760 (A)



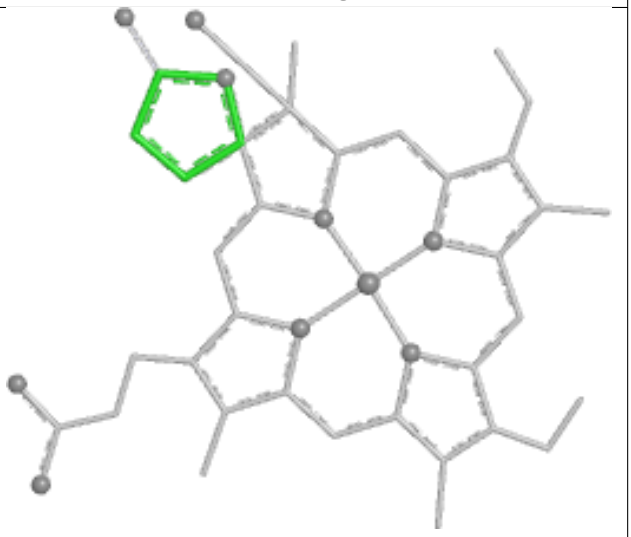
Bond lengths



Bond angles

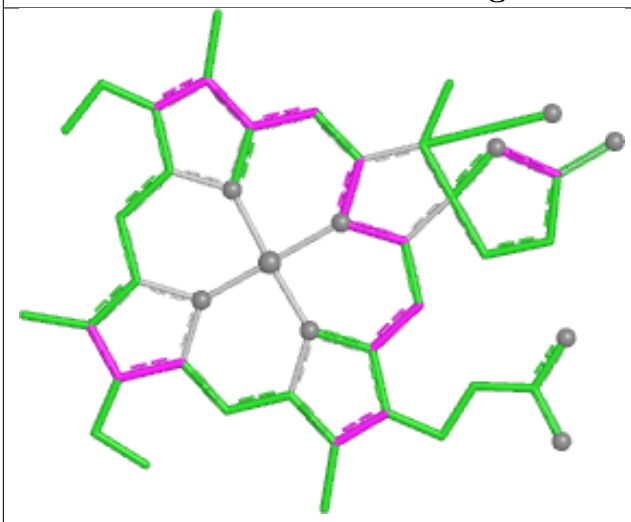


Torsions

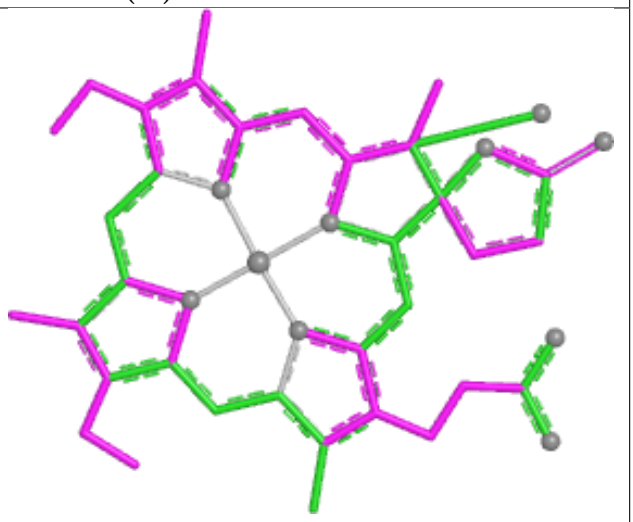


Rings

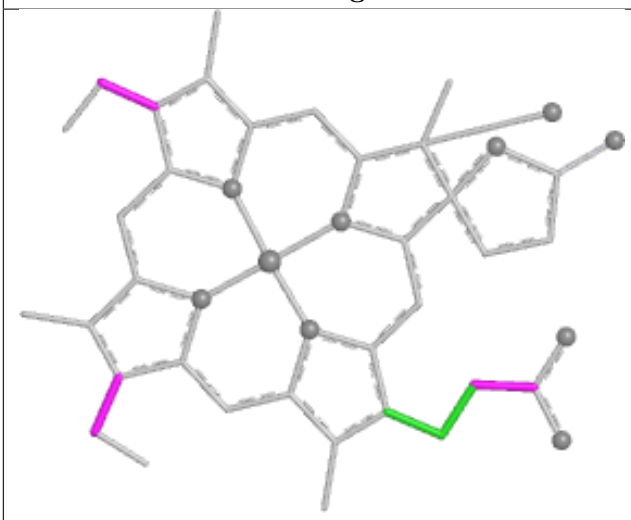
Ligand HDE D 761 (B)



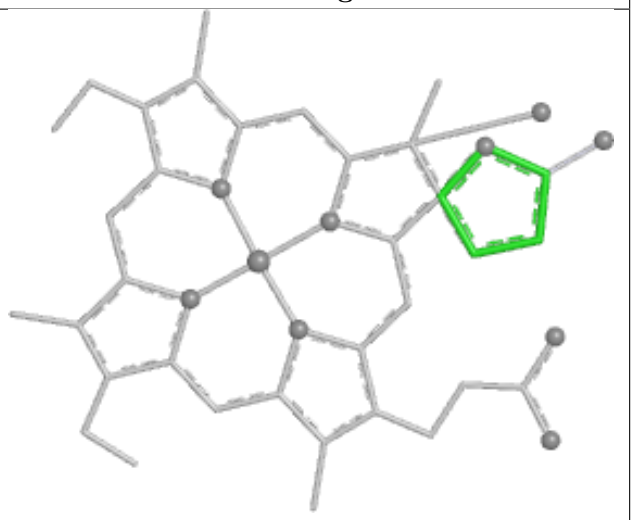
Bond lengths



Bond angles

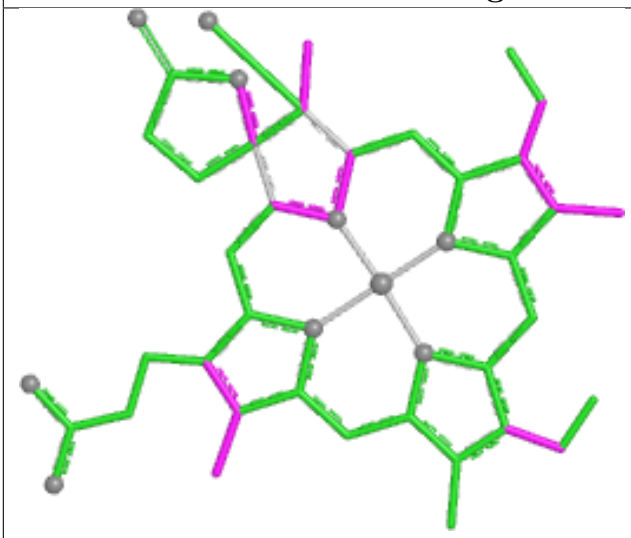


Torsions

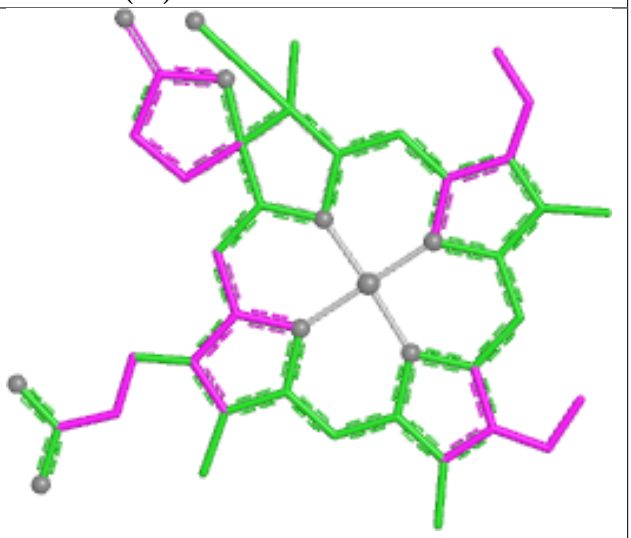


Rings

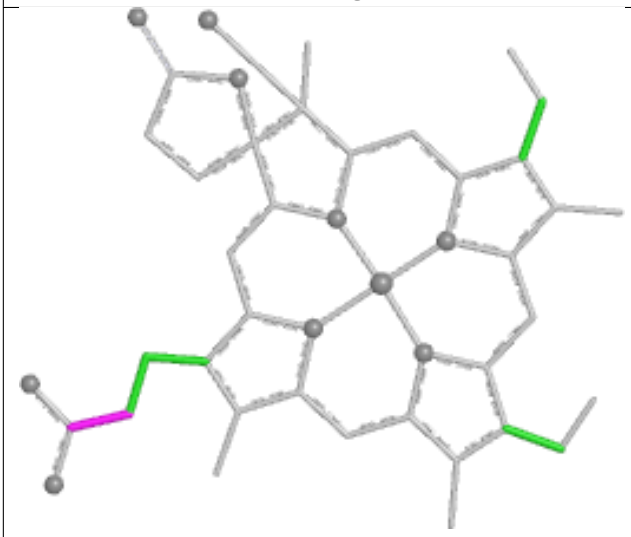
Ligand HDD B 760 (A)



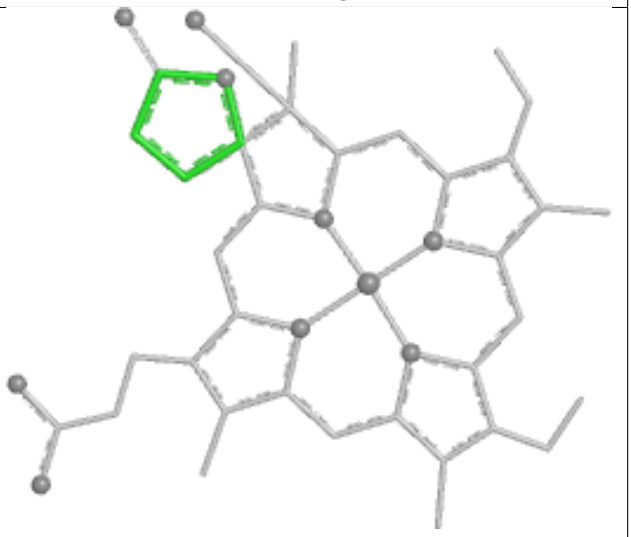
Bond lengths



Bond angles

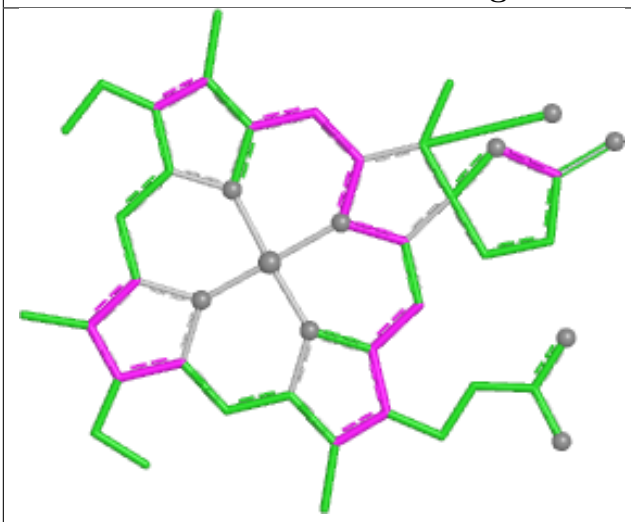


Torsions

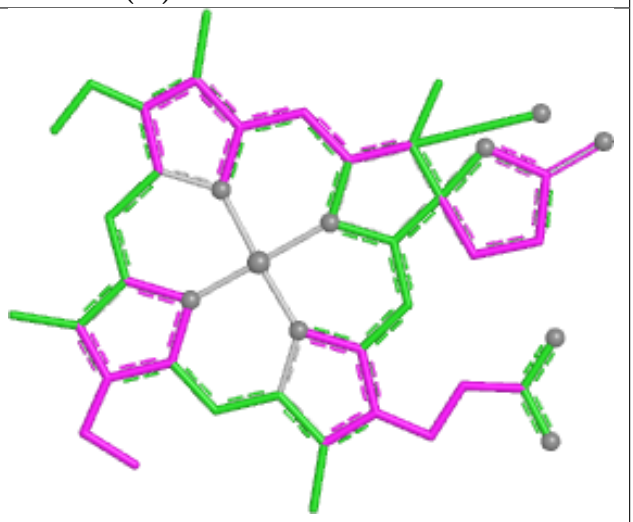


Rings

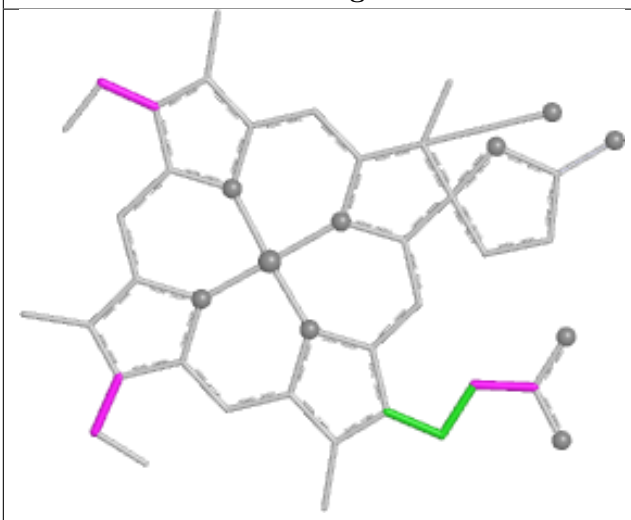
Ligand HDE B 761 (B)



Bond lengths



Bond angles



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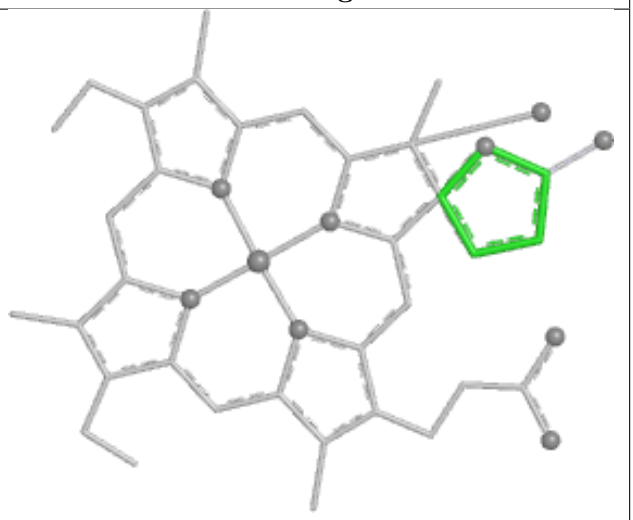
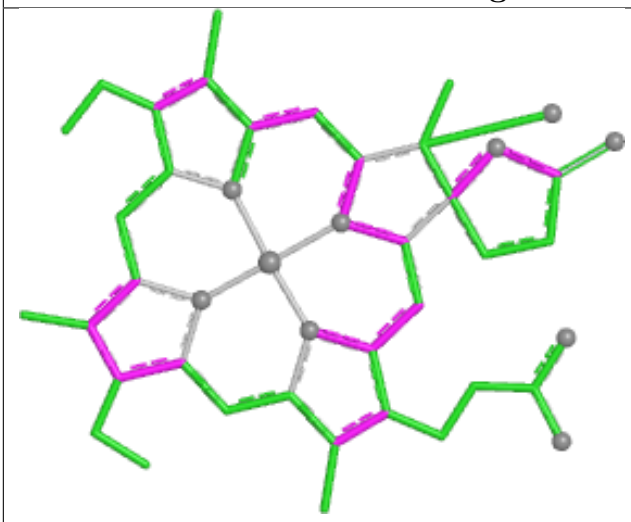
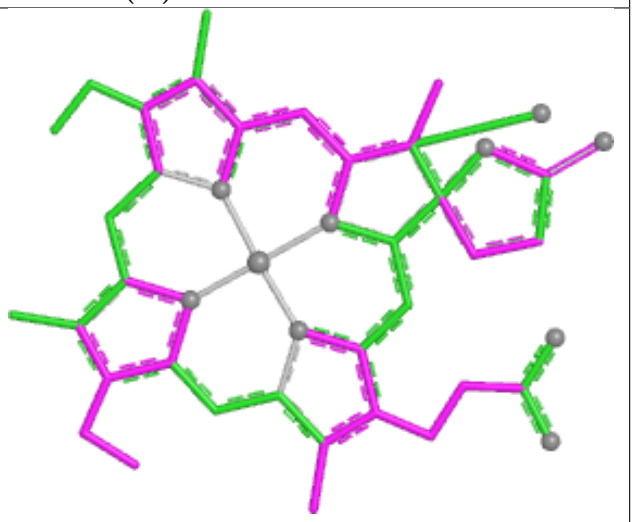


Rings

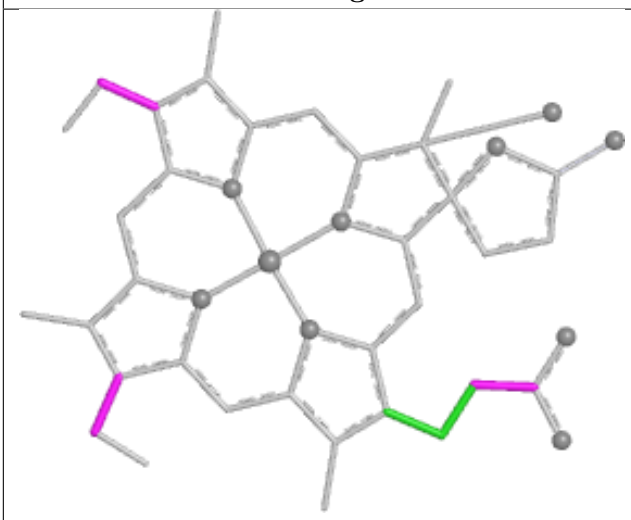
Ligand HDE C 761 (B)



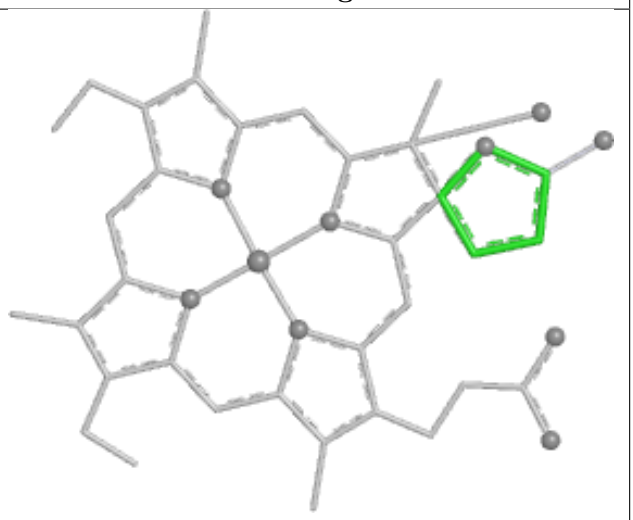
Bond lengths



Bond angles

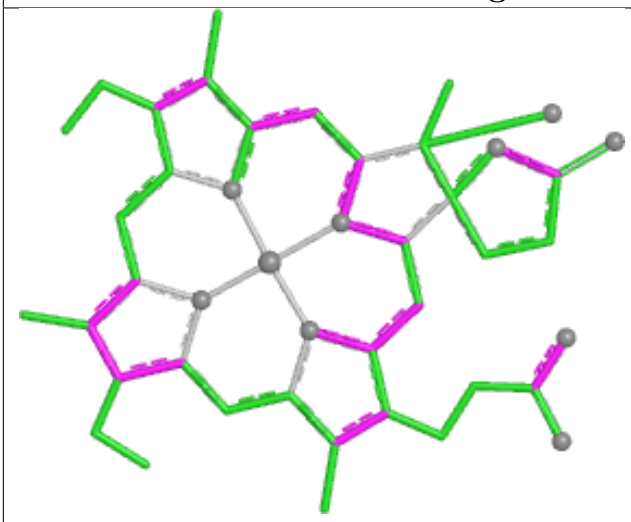


Torsions

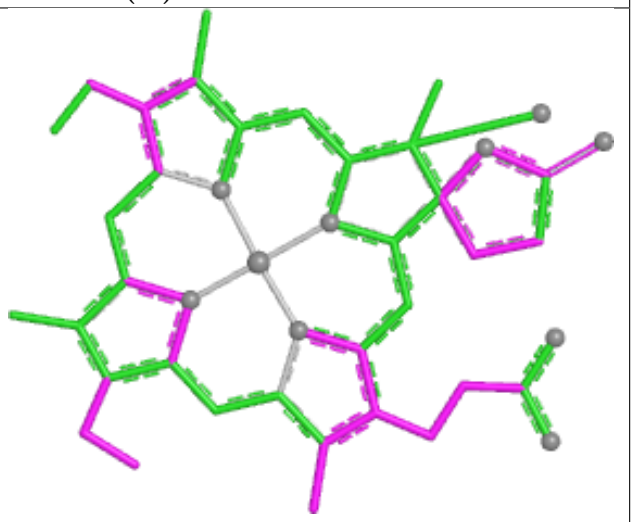


Rings

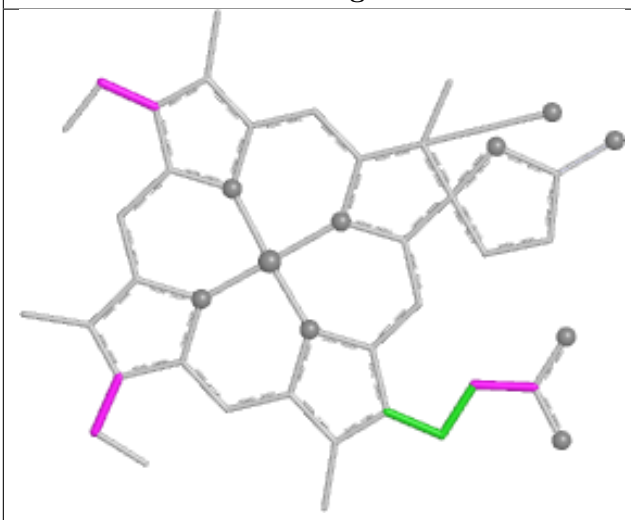
Ligand HDE A 761 (B)



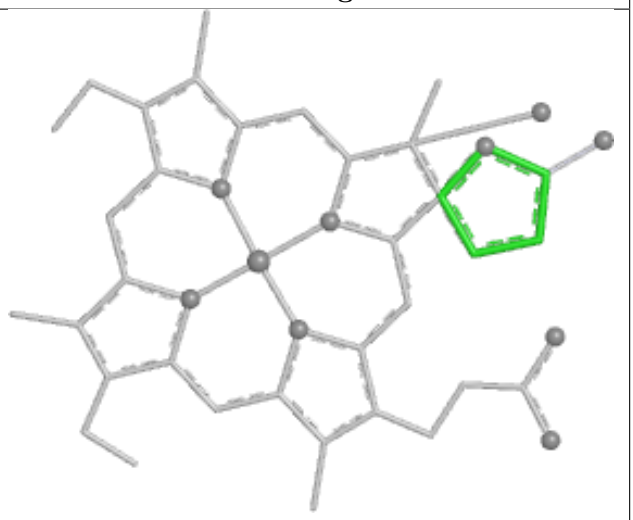
Bond lengths



Bond angles

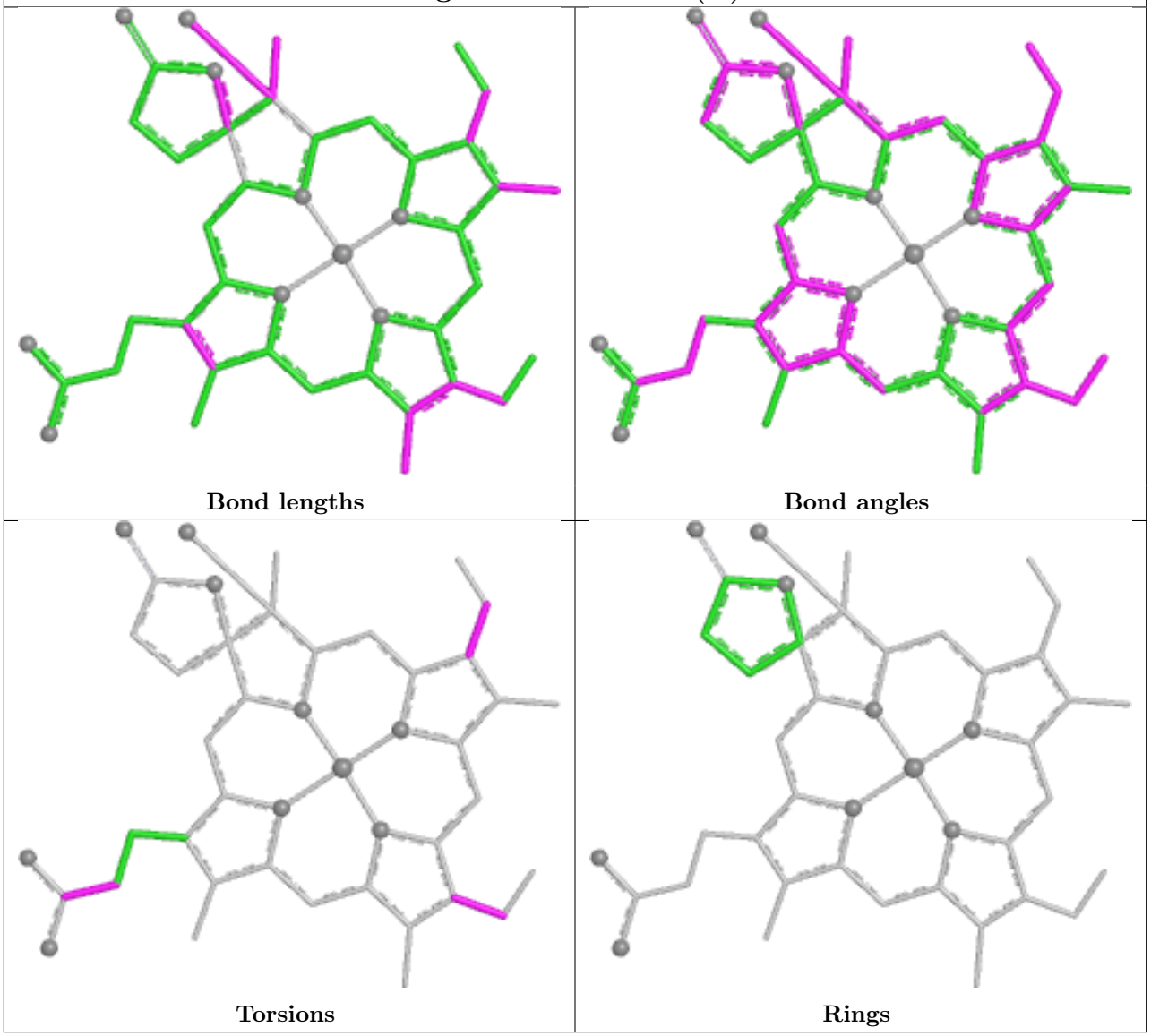


Torsions



Rings

Ligand HDD D 760 (A)



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	726/753 (96%)	-0.82	3 (0%)	88	89	3, 10, 27, 44	7 (0%)
1	B	726/753 (96%)	-0.71	1 (0%)	92	91	3, 12, 32, 48	7 (0%)
1	C	726/753 (96%)	-0.73	1 (0%)	92	91	2, 12, 31, 47	4 (0%)
1	D	726/753 (96%)	-0.82	1 (0%)	92	91	3, 10, 28, 44	10 (1%)
All	All	2904/3012 (96%)	-0.77	6 (0%)	91	91	2, 11, 30, 48	28 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	SER	3.1
1	D	28	SER	3.0
1	A	713	GLN	2.6
1	B	726	GLY	2.2
1	C	594	PRO	2.1
1	A	751	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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,

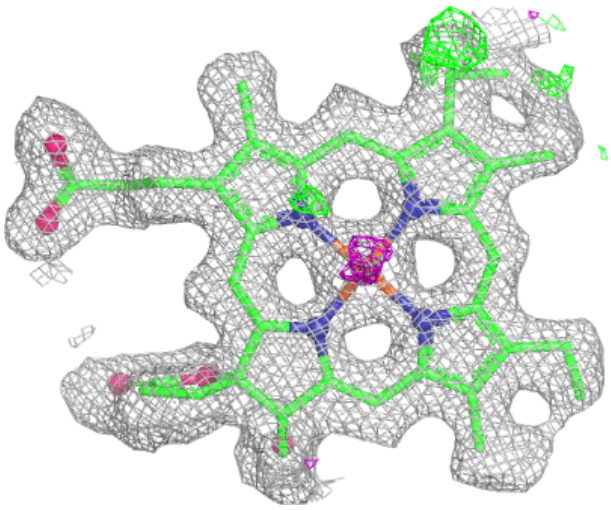
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

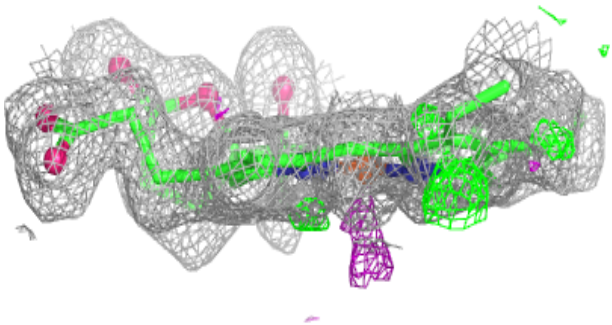
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	H2S	A	754	1/1	0.95	0.12	28,28,28,28	1
4	H2S	C	754	1/1	0.95	0.12	24,24,24,24	1
4	H2S	D	754	1/1	0.96	0.07	21,21,21,21	1
4	H2S	B	754	1/1	0.97	0.05	24,24,24,24	1
3	HDE	D	761[B]	44/44	0.98	0.06	3,9,14,16	44
2	HDD	C	760[A]	44/44	0.98	0.05	2,5,8,17	44
2	HDD	D	760[A]	44/44	0.98	0.05	2,4,9,14	44
3	HDE	B	761[B]	44/44	0.98	0.06	3,11,13,16	44
3	HDE	C	761[B]	44/44	0.98	0.05	3,11,14,15	44
2	HDD	B	760[A]	44/44	0.99	0.05	2,4,8,11	44
3	HDE	A	761[B]	44/44	0.99	0.05	2,8,11,12	44
2	HDD	A	760[A]	44/44	0.99	0.04	2,3,9,10	44

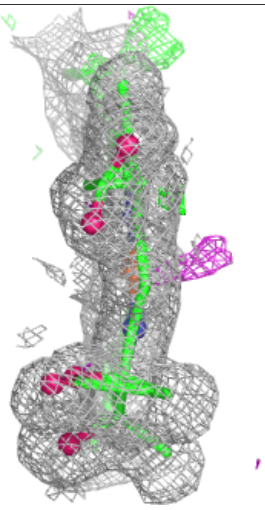
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HDE 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)

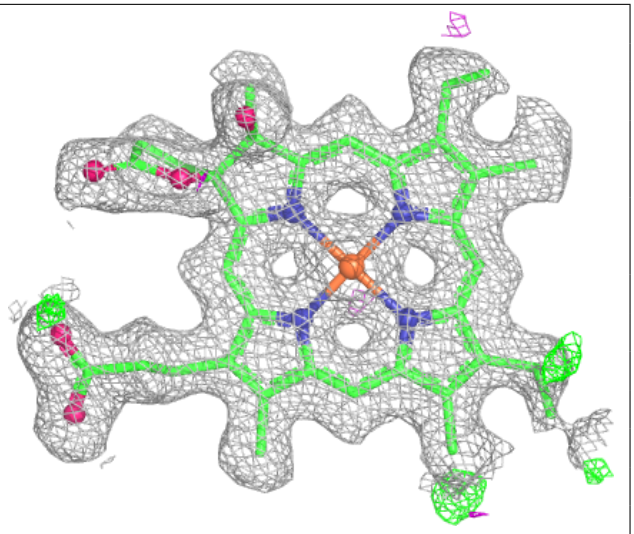


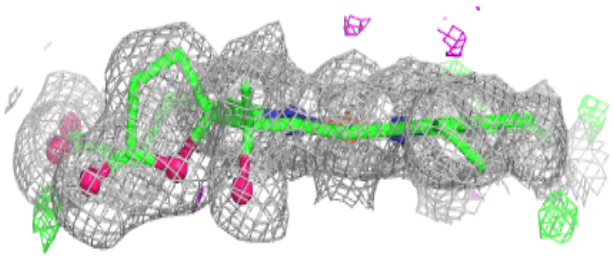


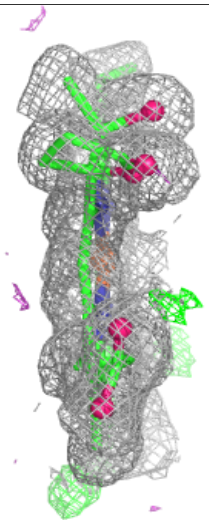


Electron density around HDD C 760 (A):

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

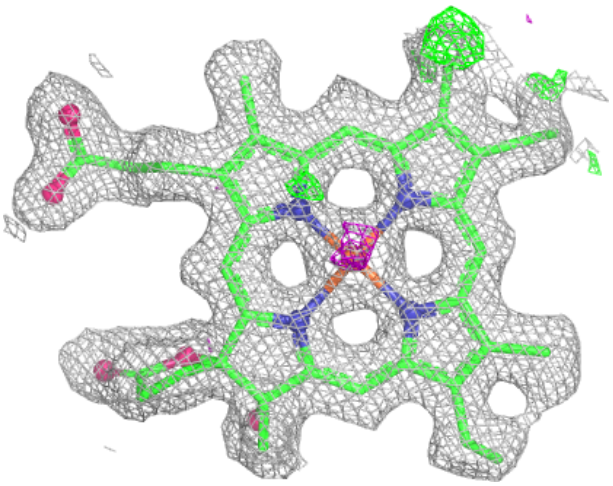


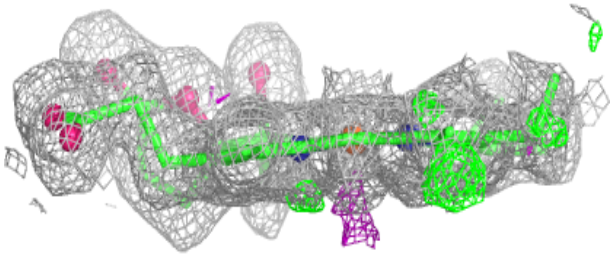


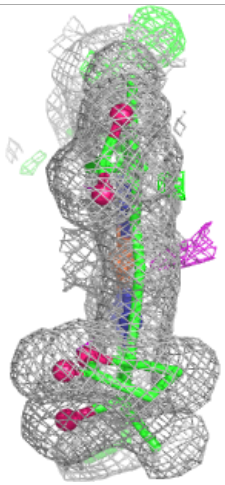


Electron density around HDD D 760 (A):

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

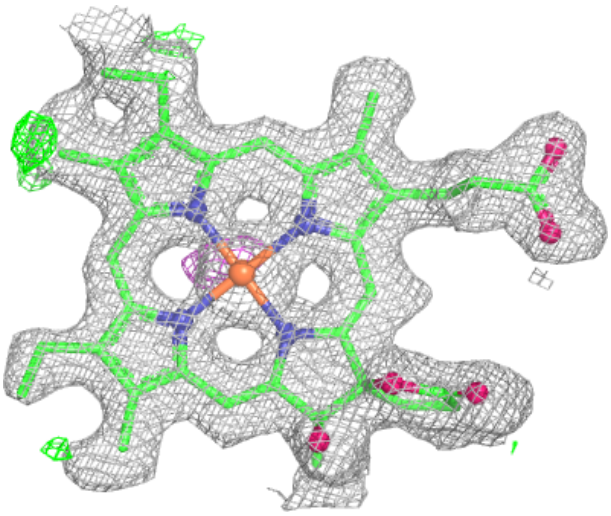


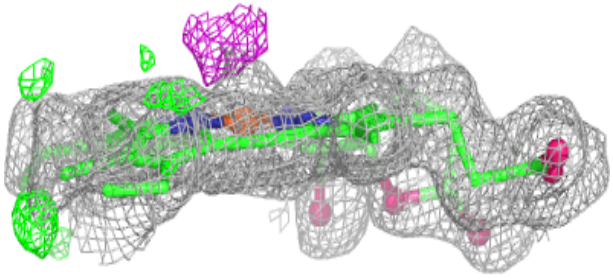


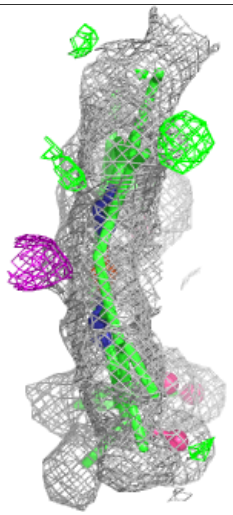


Electron density around HDE B 761 (B):

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

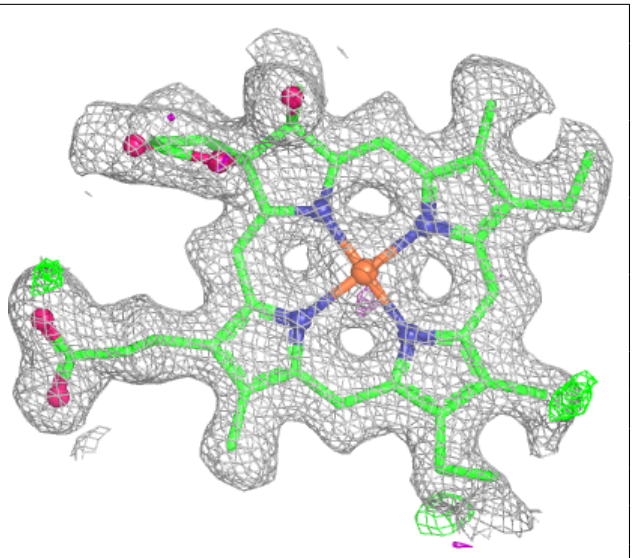


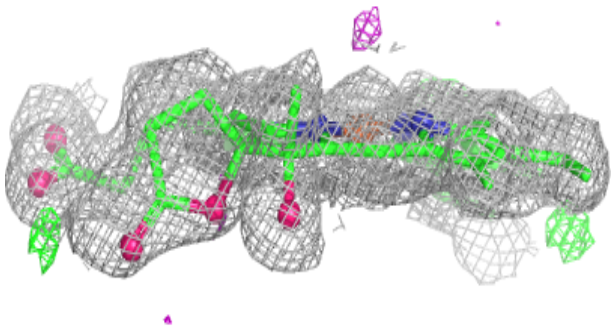


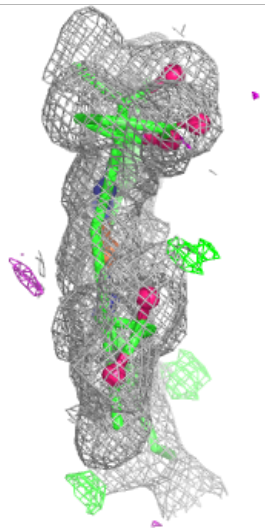


Electron density around HDE C 761 (B):

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

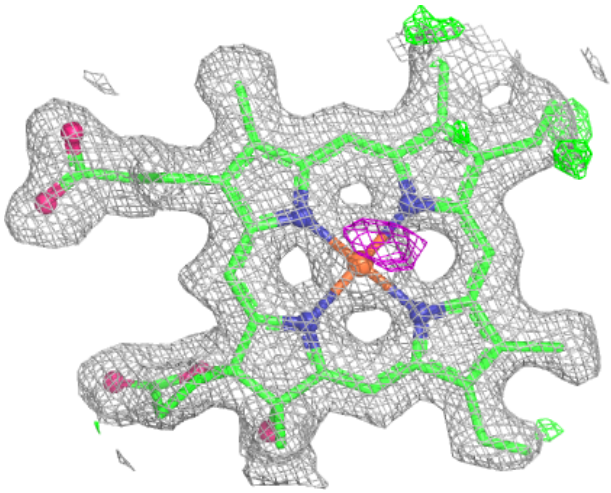


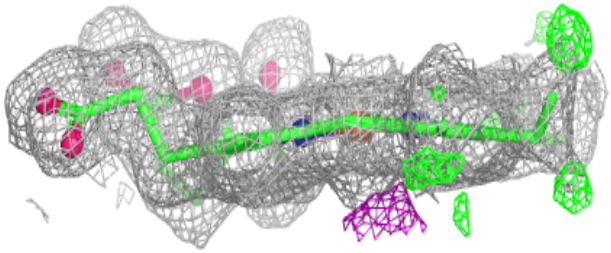


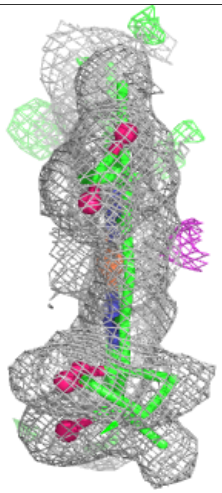


Electron density around HDD B 760 (A):

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

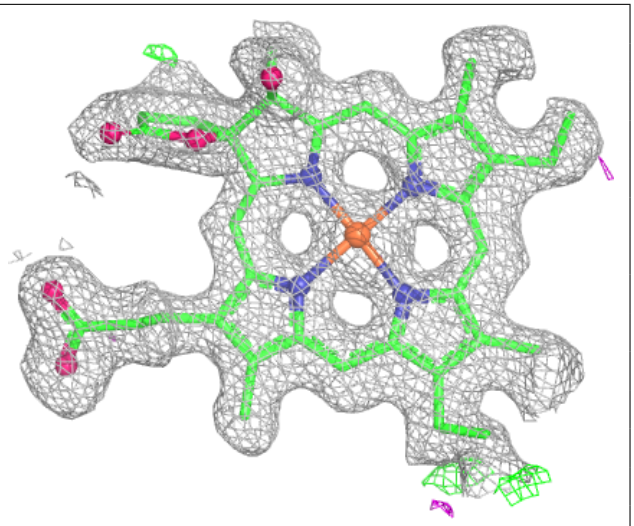


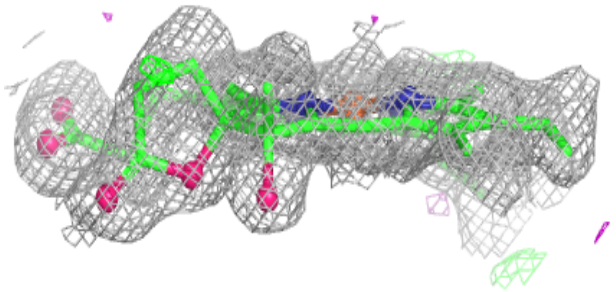


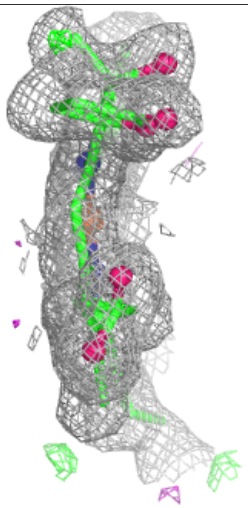


Electron density around HDE A 761 (B):

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

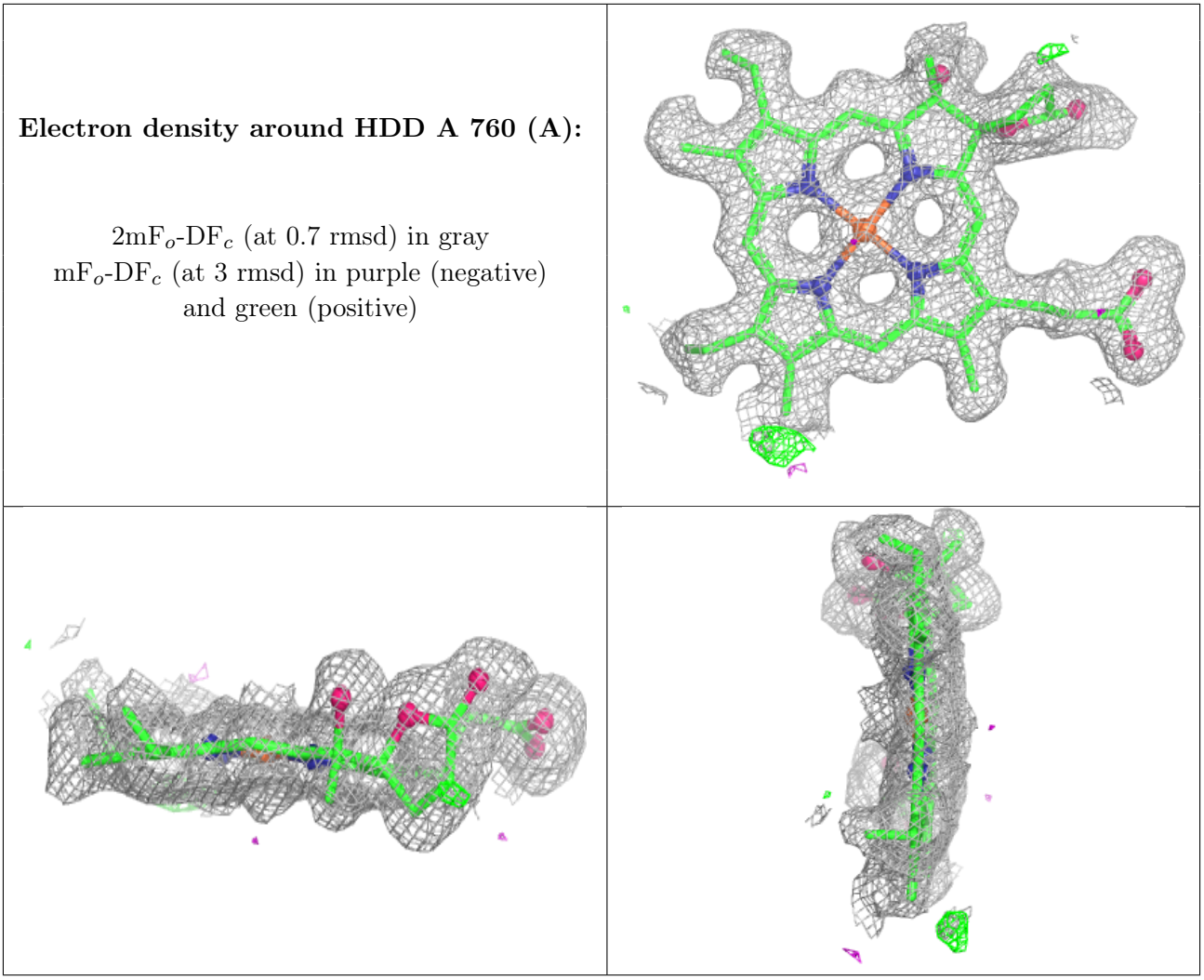






Electron density around HDD A 760 (A):

$2mF_o$-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

There are no such residues in this entry.