Full wwPDB X-ray Structure Validation Report (i)

Sep 5, 2023 – 07:13 PM EDT

PDB ID	:	4ENW
Title	:	Structure of the S234N variant of E. coli KatE
Authors	:	Loewen, P.C.; Jha, V.
Deposited on	:	2012-04-13
Resolution	:	1.90 Å(reported)

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

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

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

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

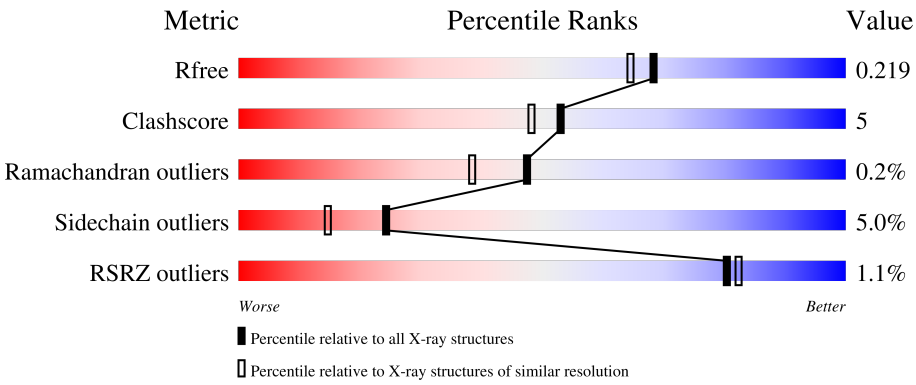
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	753	.% 85% 10% • •
1	B	753	2% 83% 11% • •
1	C	753	.% 82% 12% • •
1	D	753	.% 83% 12% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 25927 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

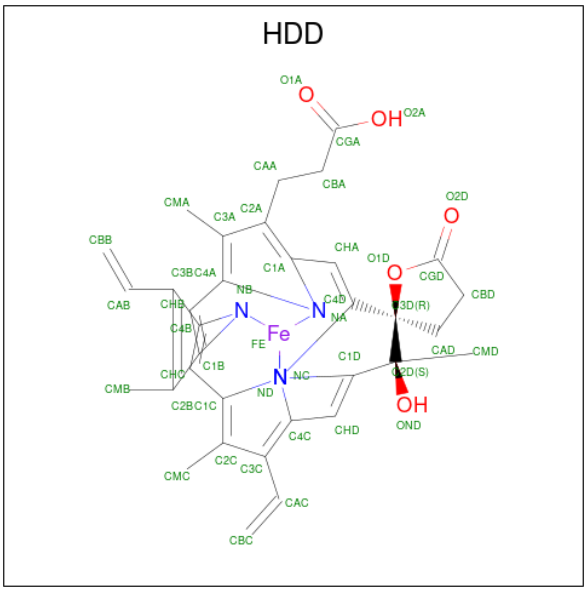
- Molecule 1 is a protein called Catalase HPII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	726	5747	3649	1007	1079	12	0	1	0
1	B	726	5747	3649	1007	1079	12	0	1	0
1	C	726	5752	3654	1007	1079	12	0	2	0
1	D	726	5753	3653	1008	1080	12	0	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	234	ASN	SER	engineered mutation	UNP P21179
B	234	ASN	SER	engineered mutation	UNP P21179
C	234	ASN	SER	engineered mutation	UNP P21179
D	234	ASN	SER	engineered mutation	UNP P21179

- Molecule 2 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (three-letter code: HDD) (formula: $C_{34}H_{32}FeN_4O_5$).



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

- Molecule 3 is water.

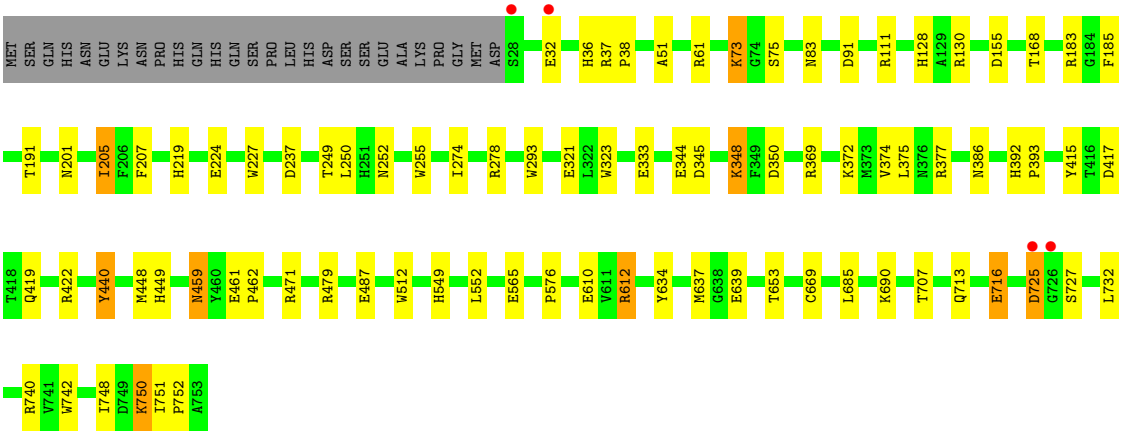
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	730	Total	O	0	0
			730	730		
3	B	629	Total	O	0	0
			629	629		
3	C	649	Total	O	0	0
			649	649		
3	D	744	Total	O	0	0
			744	744		

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.

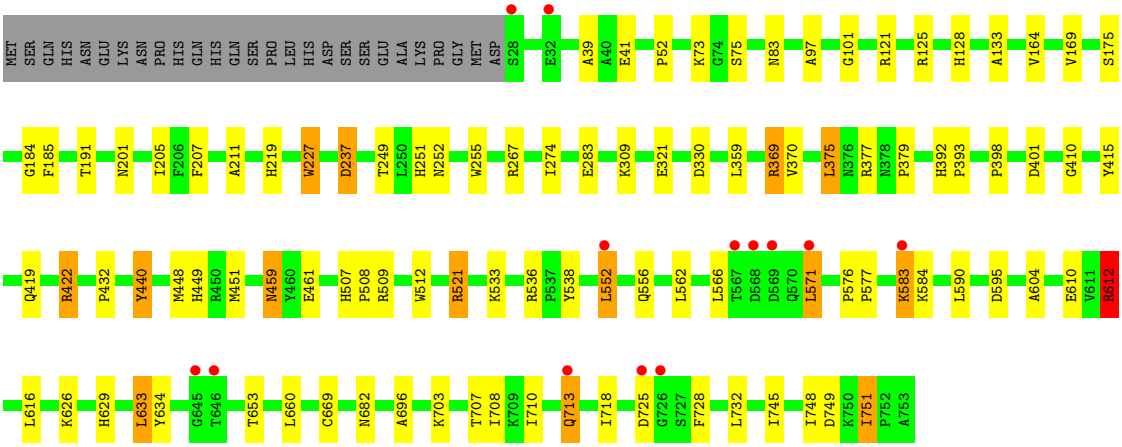
• Molecule 1: Catalase HPII

Chain A:



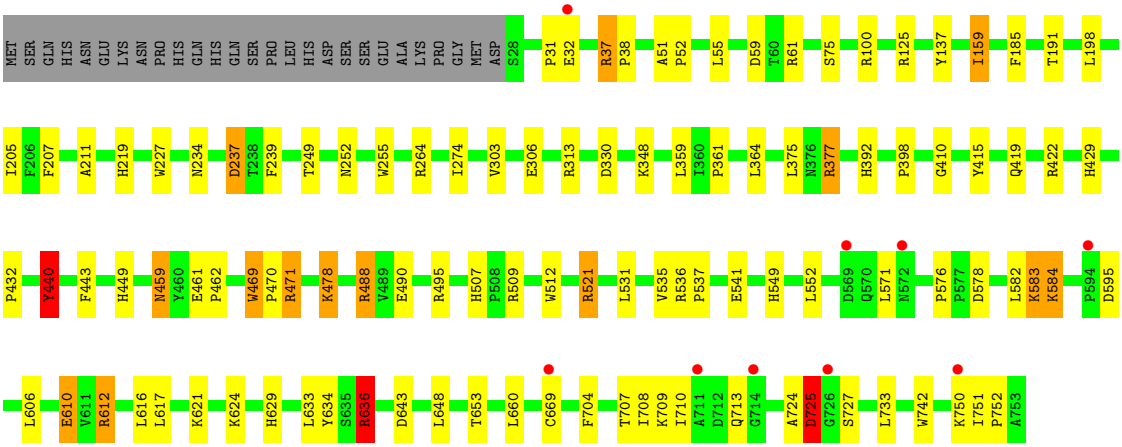
• Molecule 1: Catalase HPII

Chain B:



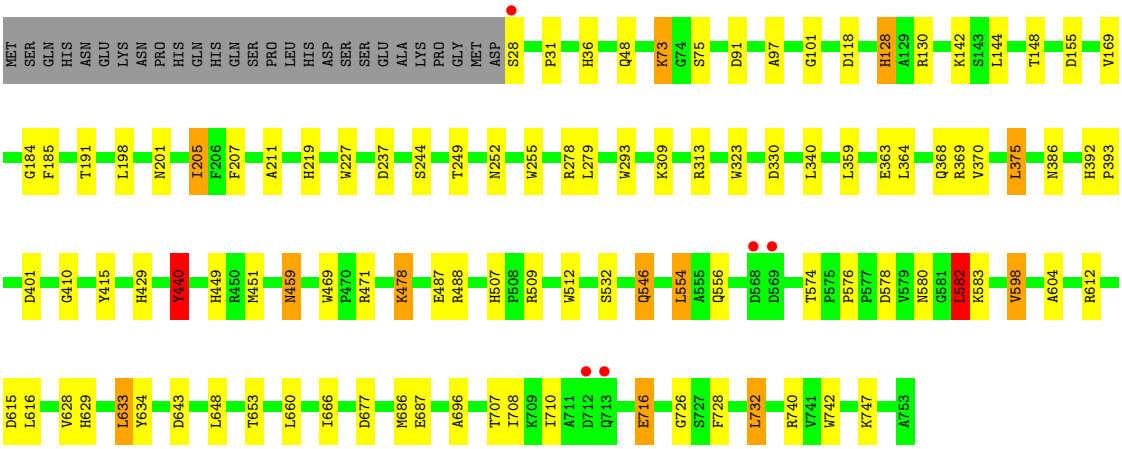
• Molecule 1: Catalase HPII

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	93.39Å 132.57Å 122.57Å 90.00° 109.23° 90.00°	Depositor
Resolution (Å)	35.13 – 1.90 35.13 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.4 (35.13-1.90) 93.4 (35.13-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	6.66 (at 1.89Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.175 , 0.221 0.174 , 0.219	Depositor DCC
R_{free} test set	10355 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	11.0	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	25927	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.00	8/5907 (0.1%)	0.97	12/8031 (0.1%)
1	B	0.97	4/5907 (0.1%)	0.96	7/8031 (0.1%)
1	C	0.97	5/5915 (0.1%)	0.96	15/8042 (0.2%)
1	D	1.02	8/5916 (0.1%)	0.98	14/8043 (0.2%)
All	All	0.99	25/23645 (0.1%)	0.97	48/32147 (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 (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	440	TYR	CE1-CZ	7.87	1.48	1.38
1	B	255	TRP	CD2-CE2	7.45	1.50	1.41
1	A	440	TYR	CE1-CZ	7.22	1.48	1.38
1	D	293	TRP	CD2-CE2	7.02	1.49	1.41
1	A	321	GLU	CD-OE1	6.69	1.33	1.25
1	D	323	TRP	CD2-CE2	6.51	1.49	1.41
1	C	469	TRP	CD2-CE2	6.44	1.49	1.41
1	A	742	TRP	CD2-CE2	6.32	1.49	1.41
1	A	323	TRP	CD2-CE2	6.18	1.48	1.41
1	A	344	GLU	CD-OE2	5.91	1.32	1.25
1	A	255	TRP	CD2-CE2	5.89	1.48	1.41
1	D	440	TYR	CE1-CZ	5.80	1.46	1.38
1	C	742	TRP	CD2-CE2	5.79	1.48	1.41
1	B	512	TRP	CD2-CE2	5.79	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	227	TRP	CD2-CE2	5.64	1.48	1.41
1	D	742	TRP	CD2-CE2	5.44	1.47	1.41
1	C	512	TRP	CD2-CE2	5.40	1.47	1.41
1	C	255	TRP	CD2-CE2	5.39	1.47	1.41
1	D	469	TRP	CD2-CE2	5.33	1.47	1.41
1	D	512	TRP	CD2-CE2	5.28	1.47	1.41
1	D	128	HIS	CB-CG	5.28	1.59	1.50
1	A	512	TRP	CD2-CE2	5.25	1.47	1.41
1	D	255	TRP	CD2-CE2	5.22	1.47	1.41
1	C	440	TYR	CE1-CZ	5.22	1.45	1.38
1	A	293	TRP	CD2-CE2	5.15	1.47	1.41

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	478	LYS	CD-CE-NZ	10.06	134.84	111.70
1	C	471	ARG	NE-CZ-NH2	-9.57	115.51	120.30
1	B	121	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	B	422	ARG	NE-CZ-NH1	8.05	124.33	120.30
1	B	401	ASP	CB-CG-OD2	8.00	125.50	118.30
1	C	636	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	B	401	ASP	CB-CG-OD1	-7.27	111.76	118.30
1	B	375	LEU	CB-CG-CD1	7.06	123.00	111.00
1	A	740	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	377	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	130	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	B	590	LEU	CB-CG-CD2	-6.57	99.83	111.00
1	C	636	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	A	479	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	A	350	ASP	CB-CG-OD1	-6.42	112.52	118.30
1	D	582	LEU	CB-CG-CD1	6.31	121.73	111.00
1	A	471	ARG	NE-CZ-NH1	-6.29	117.15	120.30
1	D	740	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	D	401	ASP	CB-CG-OD2	6.07	123.76	118.30
1	C	377	ARG	NE-CZ-NH1	-5.99	117.30	120.30
1	D	375	LEU	CB-CG-CD2	5.97	121.14	111.00
1	A	372	LYS	CD-CE-NZ	-5.95	98.02	111.70
1	A	155	ASP	CB-CG-OD2	5.88	123.60	118.30
1	D	155	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	250	LEU	CB-CG-CD1	-5.80	101.14	111.00
1	C	313	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	B	121	ARG	NE-CZ-NH2	-5.73	117.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	478	LYS	CB-CG-CD	5.72	126.47	111.60
1	C	348	LYS	CD-CE-NZ	-5.72	98.55	111.70
1	C	495	ARG	NE-CZ-NH1	-5.63	117.48	120.30
1	D	554	LEU	CB-CG-CD2	5.60	120.53	111.00
1	A	183	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	685	LEU	CB-CG-CD1	-5.54	101.58	111.00
1	C	264	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	C	313	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	C	595	ASP	CB-CG-OD2	5.47	123.22	118.30
1	D	471	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	A	111	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	C	100	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	C	725	ASP	N-CA-C	5.37	125.51	111.00
1	D	401	ASP	CB-CG-OD1	-5.26	113.57	118.30
1	D	130	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	D	740	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	C	552[A]	LEU	CB-CG-CD2	5.15	119.75	111.00
1	C	552[B]	LEU	CB-CG-CD2	5.15	119.75	111.00
1	D	615	ASP	CB-CG-OD2	5.14	122.93	118.30
1	D	643	ASP	CB-CG-OD1	5.11	122.90	118.30
1	C	471	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5747	0	5582	50	0
1	B	5747	0	5582	70	0
1	C	5752	0	5593	73	1
1	D	5753	0	5589	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	44	0	31	4	0
2	B	44	0	31	6	0
2	C	44	0	31	5	0
2	D	44	0	31	3	0
3	A	730	0	0	7	0
3	B	629	0	0	11	1
3	C	649	0	0	15	0
3	D	744	0	0	11	0
All	All	25927	0	22470	245	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (245) 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:392:HIS:ND1	1:A:415:TYR:CB	1.71	1.54
1:D:392:HIS:ND1	1:D:415:TYR:CB	1.69	1.53
1:B:392:HIS:ND1	1:B:415:TYR:CB	1.72	1.49
1:C:392:HIS:ND1	1:C:415:TYR:CB	1.71	1.49
1:D:449[B]:HIS:CE1	3:D:1637:HOH:O	1.76	1.37
3:B:1463:HOH:O	1:D:73:LYS:HD3	1.33	1.27
1:D:449[B]:HIS:NE2	3:D:1637:HOH:O	1.66	1.21
1:C:521:ARG:HH11	1:C:521:ARG:CG	1.54	1.20
1:D:392:HIS:CE1	1:D:415:TYR:HB2	1.78	1.17
1:A:392:HIS:CE1	1:A:415:TYR:HB2	1.80	1.17
1:C:392:HIS:CE1	1:C:415:TYR:HB2	1.79	1.17
1:C:521:ARG:NH1	1:C:521:ARG:HG2	1.29	1.15
1:B:392:HIS:CE1	1:B:415:TYR:HB2	1.83	1.13
1:C:392:HIS:ND1	1:C:415:TYR:HB2	0.77	1.09
1:B:392:HIS:ND1	1:B:415:TYR:HB2	0.77	1.09
1:B:369:ARG:HG2	3:B:1296:HOH:O	1.51	1.08
1:A:392:HIS:ND1	1:A:415:TYR:HB2	0.75	1.08
1:D:392:HIS:ND1	1:D:415:TYR:HB2	0.75	1.07
1:A:392:HIS:CG	1:A:415:TYR:HB2	1.95	1.00
1:C:440:TYR:HD1	3:C:1353:HOH:O	1.42	1.00
1:D:392:HIS:CG	1:D:415:TYR:HB2	1.98	0.97
1:A:716:GLU:HG2	3:A:1302:HOH:O	1.64	0.96
1:A:449[B]:HIS:CG	1:C:449[B]:HIS:CG	2.34	0.95
1:B:392:HIS:CG	1:B:415:TYR:HB2	2.01	0.94
1:C:392:HIS:CG	1:C:415:TYR:HB2	2.00	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:710:ILE:HD13	1:B:718:ILE:HG13	1.51	0.93
1:A:639:GLU:HG3	3:A:1479:HOH:O	1.70	0.92
1:A:716:GLU:CG	3:A:1302:HOH:O	2.18	0.89
1:B:708:ILE:HD12	1:B:710:ILE:HD11	1.52	0.89
1:B:708:ILE:HD12	1:B:710:ILE:CD1	2.03	0.88
1:B:583:LYS:NZ	1:B:583:LYS:H	1.73	0.86
1:C:521:ARG:CG	1:C:521:ARG:NH1	2.20	0.86
1:A:449[B]:HIS:CG	1:C:449[B]:HIS:ND1	2.04	0.86
1:C:610:GLU:OE1	1:C:643:ASP:HA	1.76	0.86
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.61	0.83
1:C:612:ARG:HH11	1:C:612:ARG:HG3	1.45	0.81
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.63	0.79
1:A:449[B]:HIS:ND1	1:C:449[B]:HIS:CG	2.09	0.78
1:C:612:ARG:HH11	1:C:612:ARG:CG	1.98	0.74
1:D:629:HIS:HD2	3:D:1259:HOH:O	1.70	0.74
1:A:274:ILE:HD12	2:A:801:HDD:HMB1	1.68	0.73
1:C:521:ARG:HH11	1:C:521:ARG:HG2	0.65	0.73
1:D:598:VAL:HG13	1:D:628:VAL:CG2	2.19	0.73
1:A:73:LYS:HE2	1:C:440:TYR:O	1.89	0.72
1:D:368:GLN:OE1	3:D:1555:HOH:O	2.07	0.71
1:A:690:LYS:HG3	1:A:751:ILE:HD11	1.72	0.70
1:A:392:HIS:ND1	1:A:415:TYR:CG	2.58	0.70
1:C:549:HIS:NE2	3:C:1506:HOH:O	2.23	0.70
1:A:751:ILE:HD12	1:A:751:ILE:O	1.92	0.69
1:B:419:GLN:HE22	1:B:422:ARG:HH21	1.41	0.68
1:B:583:LYS:H	1:B:583:LYS:HZ2	1.41	0.67
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.77	0.67
1:B:612:ARG:NH1	1:B:669:CYS:SG	2.68	0.67
1:C:488:ARG:HD3	3:C:1429:HOH:O	1.94	0.67
1:C:636:ARG:HD3	3:C:1478:HOH:O	1.93	0.66
1:C:583:LYS:O	1:C:584:LYS:HB3	1.96	0.66
1:C:751:ILE:HG13	1:C:752:PRO:HD2	1.79	0.65
1:B:556:GLN:HG2	1:B:566:LEU:HD23	1.78	0.65
1:C:274:ILE:HD12	2:C:801:HDD:HMB1	1.79	0.64
1:B:552:LEU:CD2	1:B:571:LEU:HD12	2.27	0.63
1:C:629:HIS:HD2	3:C:1201:HOH:O	1.79	0.63
2:B:801:HDD:HBC1	2:B:801:HDD:HMC1	1.79	0.63
1:C:469:TRP:CE3	1:C:471:ARG:HG3	2.34	0.63
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.29	0.63
1:B:710:ILE:CD1	1:B:718:ILE:HG13	2.28	0.62
1:C:612:ARG:NH1	1:C:612:ARG:HB2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:578:ASP:HB2	1:C:582:LEU:O	1.99	0.62
1:B:583:LYS:H	1:B:583:LYS:HZ3	1.45	0.61
1:D:392:HIS:ND1	1:D:415:TYR:HB3	2.05	0.61
2:A:801:HDD:HMB1	2:A:801:HDD:HBB1	1.82	0.61
1:C:392:HIS:ND1	1:C:415:TYR:CG	2.64	0.61
1:D:598:VAL:HG13	1:D:628:VAL:HG22	1.83	0.60
1:B:708:ILE:HD12	1:B:710:ILE:HD12	1.83	0.60
1:C:125:ARG:HB3	2:C:801:HDD:HBD1	1.84	0.59
1:D:708:ILE:HG13	1:D:710:ILE:HG12	1.83	0.59
1:B:125:ARG:HB3	2:B:801:HDD:HBD1	1.85	0.58
1:B:629:HIS:HD2	3:B:1159:HOH:O	1.86	0.58
1:A:345:ASP:HA	1:A:348:LYS:HG3	1.86	0.58
1:C:37:ARG:NH1	3:C:1345:HOH:O	2.33	0.58
1:C:727:SER:HA	3:C:1477:HOH:O	2.03	0.58
1:D:716:GLU:HG3	3:D:938:HOH:O	2.04	0.57
1:C:583:LYS:HG2	3:C:1501:HOH:O	2.04	0.57
1:A:36:HIS:CD2	1:A:36:HIS:H	2.23	0.56
1:D:392:HIS:ND1	1:D:415:TYR:CG	2.66	0.56
1:D:509:ARG:HD2	1:D:576:PRO:HD2	1.86	0.56
1:C:704:PHE:O	1:C:707:THR:HG22	2.06	0.56
3:B:1463:HOH:O	1:D:73:LYS:CD	2.16	0.55
1:D:392:HIS:CG	1:D:415:TYR:CB	2.75	0.54
1:C:38:PRO:HG2	1:C:51:ALA:HB2	1.88	0.54
1:B:211:ALA:CB	1:B:410:GLY:HA3	2.37	0.54
1:D:556:GLN:NE2	3:D:1572:HOH:O	2.39	0.54
1:B:509:ARG:HD2	1:B:576:PRO:HD2	1.90	0.54
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.91	0.54
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.12	0.53
1:A:725:ASP:OD1	1:A:727:SER:HB3	2.08	0.53
1:B:612:ARG:HB2	1:B:612:ARG:CZ	2.38	0.53
1:B:521:ARG:CB	1:B:521:ARG:HH21	2.20	0.53
1:C:359:LEU:H	1:C:507:HIS:HD2	1.57	0.53
1:B:448:MET:HG3	1:B:449[B]:HIS:CD2	2.43	0.53
1:B:274:ILE:HD12	2:B:801:HDD:HMB1	1.91	0.53
1:C:584:LYS:NZ	3:C:1286:HOH:O	2.25	0.53
1:C:541:GLU:HG2	3:C:1544:HOH:O	2.09	0.53
1:C:634:TYR:O	1:C:653:THR:HA	2.09	0.52
1:D:359:LEU:H	1:D:507:HIS:HD2	1.57	0.52
1:A:392:HIS:CG	1:A:415:TYR:CB	2.74	0.51
2:C:801:HDD:HBD2	3:C:1083:HOH:O	2.10	0.51
1:C:52:PRO:HG2	1:C:55:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.94	0.50
1:C:612:ARG:CG	1:C:612:ARG:NH1	2.67	0.50
1:D:278:ARG:HH12	1:D:487:GLU:CD	2.15	0.50
1:B:459:ASN:HD22	1:B:459:ASN:H	1.59	0.50
1:C:612:ARG:HH11	1:C:612:ARG:CB	2.25	0.50
1:D:201:ASN:CG	2:D:801:HDD:HMB2	2.32	0.50
1:B:309:LYS:HD2	1:B:660:LEU:HD11	1.93	0.50
1:A:750:LYS:HE3	1:D:677:ASP:HB3	1.93	0.49
1:B:392:HIS:ND1	1:B:415:TYR:CA	2.68	0.49
1:D:205:ILE:H	1:D:205:ILE:HD13	1.78	0.49
1:A:610:GLU:HG3	3:A:1513:HOH:O	2.11	0.49
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.95	0.49
1:B:533:LYS:HD2	3:B:1456:HOH:O	2.12	0.49
1:A:91:ASP:OD1	1:C:461:GLU:OE1	2.30	0.49
1:B:708:ILE:CD1	1:B:710:ILE:HD12	2.41	0.49
1:C:440:TYR:CD1	3:C:1353:HOH:O	2.31	0.49
1:D:578:ASP:OD1	1:D:583:LYS:HE3	2.12	0.49
1:B:52:PRO:HG3	3:D:1191:HOH:O	2.13	0.49
1:C:478:LYS:HB2	3:C:1532:HOH:O	2.13	0.49
1:B:359:LEU:H	1:B:507:HIS:HD2	1.60	0.49
1:B:39:ALA:HB1	1:B:41:GLU:HG2	1.95	0.48
1:C:392:HIS:CG	1:C:415:TYR:CB	2.78	0.48
1:A:448:MET:O	1:A:449[B]:HIS:HB2	2.14	0.48
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.29	0.48
1:B:392:HIS:CG	1:B:415:TYR:CB	2.79	0.48
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.43	0.48
1:C:361:PRO:HD2	1:C:364:LEU:HD12	1.96	0.48
1:C:207:PHE:O	1:C:249:THR:HA	2.12	0.47
1:D:459:ASN:HD22	1:D:459:ASN:H	1.62	0.47
1:C:610:GLU:HG3	1:C:610:GLU:O	2.14	0.47
1:A:128:HIS:HA	1:A:168:THR:O	2.15	0.47
1:A:201:ASN:CG	2:A:801:HDD:HMB2	2.35	0.47
1:B:175:SER:HB2	3:B:1096:HOH:O	2.15	0.47
1:B:552:LEU:HD13	1:B:552:LEU:O	2.14	0.47
1:C:211:ALA:CB	1:C:410:GLY:HA3	2.45	0.47
1:C:359:LEU:H	1:C:507:HIS:CD2	2.33	0.47
1:D:478:LYS:HE3	3:D:1499:HOH:O	2.14	0.47
1:D:634:TYR:O	1:D:653:THR:HA	2.14	0.47
1:B:251:HIS:HA	1:B:508:PRO:HG3	1.96	0.47
1:D:363:GLU:HB2	1:D:582:LEU:HD21	1.97	0.47
1:B:128:HIS:CE1	1:B:169:VAL:HG22	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:612:ARG:NH2	1:C:669:CYS:SG	2.88	0.47
1:A:207:PHE:O	1:A:249:THR:HA	2.14	0.47
1:B:184:GLY:HA3	2:B:801:HDD:HMA2	1.97	0.46
1:C:704:PHE:O	1:C:707:THR:CG2	2.63	0.46
1:A:419:GLN:HE22	1:A:422:ARG:HH11	1.63	0.46
1:B:696:ALA:HB1	1:B:728:PHE:CZ	2.50	0.46
1:C:461:GLU:HB2	1:C:462:PRO:HA	1.98	0.46
1:C:509:ARG:HD2	1:C:576:PRO:HD2	1.97	0.46
1:A:612:ARG:HH11	1:A:669:CYS:CB	2.29	0.46
1:B:392:HIS:ND1	1:B:415:TYR:CG	2.69	0.46
1:B:451:MET:HE2	1:D:451:MET:HE1	1.97	0.46
1:B:538:TYR:CD2	1:C:31:PRO:HG3	2.51	0.46
1:D:313:ARG:HG3	1:D:660:LEU:HD12	1.98	0.46
1:A:61:ARG:HD2	3:A:1626:HOH:O	2.15	0.46
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.31	0.46
1:A:61:ARG:HG2	1:A:61:ARG:HH11	1.81	0.46
1:A:549:HIS:O	1:A:576:PRO:HD3	2.15	0.46
2:C:801:HDD:HMC1	2:C:801:HDD:HBC1	1.98	0.45
1:B:393:PRO:HD2	1:B:415:TYR:CD2	2.51	0.45
1:B:748:ILE:O	1:B:751:ILE:HG22	2.16	0.45
1:C:612:ARG:NH1	1:C:612:ARG:CB	2.79	0.45
1:D:309:LYS:HE2	1:D:687:GLU:OE2	2.16	0.45
1:A:83:ASN:HB3	1:C:429:HIS:CG	2.52	0.45
1:D:31:PRO:HD2	1:D:36:HIS:HB3	1.99	0.45
1:D:666:ILE:HD11	1:D:732:LEU:CD1	2.47	0.45
1:D:207:PHE:O	1:D:249:THR:HA	2.15	0.45
1:A:637:MET:HG3	1:D:532:SER:HB2	1.97	0.44
1:C:237:ASP:OD2	1:C:536:ARG:HG3	2.17	0.44
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.32	0.44
1:C:330:ASP:OD1	1:C:629:HIS:CE1	2.66	0.44
1:B:448:MET:O	1:B:449[B]:HIS:HB2	2.18	0.44
2:B:801:HDD:HBD2	3:B:1039:HOH:O	2.18	0.44
1:C:419:GLN:HE22	1:C:422:ARG:HH11	1.65	0.44
1:C:459:ASN:H	1:C:459:ASN:HD22	1.66	0.44
1:B:552:LEU:HD13	1:B:552:LEU:C	2.38	0.43
1:D:364:LEU:HD11	1:D:580:ASN:HB2	2.01	0.43
1:D:393:PRO:HD2	1:D:415:TYR:CG	2.53	0.43
2:D:801:HDD:HBD2	3:D:1139:HOH:O	2.18	0.43
1:A:333:GLU:HG2	1:A:374:VAL:HG22	2.00	0.43
1:C:440:TYR:OH	3:C:1135:HOH:O	2.20	0.43
1:D:244:SER:HA	1:D:546[B]:GLN:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:443:PHE:CZ	1:C:470:PRO:HD2	2.54	0.43
1:B:73:LYS:NZ	3:B:1232:HOH:O	2.51	0.43
1:A:205:ILE:HD13	1:A:205:ILE:H	1.84	0.43
1:B:267:ARG:HD2	3:B:1132:HOH:O	2.19	0.43
1:B:745:ILE:O	1:B:748:ILE:HG12	2.19	0.43
1:C:137:TYR:HB2	1:C:159:ILE:HD12	2.01	0.43
1:C:490:GLU:OE1	1:D:488:ARG:NH2	2.45	0.43
1:D:386:ASN:OD1	1:D:386:ASN:C	2.57	0.43
1:D:440:TYR:CD2	1:D:440:TYR:C	2.92	0.43
1:A:386:ASN:OD1	1:A:386:ASN:C	2.57	0.42
1:A:459:ASN:HD22	1:A:459:ASN:H	1.65	0.42
1:A:461:GLU:HA	1:A:462:PRO:C	2.38	0.42
1:A:634:TYR:O	1:A:653:THR:HA	2.18	0.42
1:B:133:ALA:HA	1:B:164:VAL:O	2.19	0.42
1:B:419:GLN:HE22	1:B:422:ARG:NH2	2.13	0.42
1:A:224:GLU:OE1	3:A:1024:HOH:O	2.22	0.42
1:A:751:ILE:HA	1:A:752:PRO:HD3	1.97	0.42
1:D:28:SER:N	3:D:1638:HOH:O	2.53	0.42
1:D:148:THR:HB	1:D:279:LEU:HB3	2.02	0.42
1:D:184:GLY:HA3	2:D:801:HDD:HMA2	2.00	0.42
1:A:748:ILE:O	1:A:751:ILE:HG13	2.19	0.42
1:B:97:ALA:O	1:B:101:GLY:HA3	2.19	0.42
1:B:634:TYR:O	1:B:653:THR:HA	2.19	0.42
1:D:128:HIS:CE1	1:D:169:VAL:HG22	2.55	0.42
1:C:303:VAL:O	1:C:306:GLU:HB3	2.19	0.42
1:B:201:ASN:CG	2:B:801:HDD:HMB2	2.40	0.42
1:D:97:ALA:O	1:D:101:GLY:HA3	2.19	0.42
1:D:696:ALA:HB1	1:D:728:PHE:CZ	2.55	0.42
1:B:713:GLN:NE2	1:B:713:GLN:H	2.18	0.42
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.35	0.42
1:A:38:PRO:HG2	1:A:51:ALA:HB2	2.02	0.42
1:B:521:ARG:HH21	1:B:521:ARG:HB2	1.83	0.42
1:D:686:MET:HG3	1:D:707:THR:HG22	2.00	0.42
1:A:393:PRO:HD2	1:A:415:TYR:CD2	2.55	0.41
1:B:461:GLU:OE1	1:D:91:ASP:OD1	2.38	0.41
2:C:801:HDD:HMB1	2:C:801:HDD:HBB1	2.01	0.41
1:C:234:ASN:HB3	1:C:239:PHE:CD2	2.56	0.41
2:A:801:HDD:HMC1	2:A:801:HDD:CBC	2.50	0.41
1:B:207:PHE:O	1:B:249:THR:HA	2.20	0.41
3:B:1330:HOH:O	1:D:449[A]:HIS:HE1	2.03	0.41
1:C:535:VAL:O	1:C:537:PRO:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:LEU:HD11	1:B:556:GLN:OE1	2.21	0.41
1:B:604:ALA:HB1	1:B:633:LEU:HD22	2.01	0.41
1:A:417:ASP:OD2	1:D:118:ASP:OD1	2.38	0.41
1:D:144:LEU:HD11	1:D:370:VAL:HG13	2.03	0.41
1:D:726:GLY:O	3:D:1500:HOH:O	2.22	0.41
1:B:577:PRO:HG2	3:B:1457:HOH:O	2.20	0.41
1:D:309:LYS:CE	1:D:687:GLU:OE2	2.69	0.41
1:C:624:LYS:HE2	3:C:1438:HOH:O	2.20	0.41
1:D:359:LEU:H	1:D:507:HIS:CD2	2.37	0.40
1:B:83:ASN:HB3	1:D:429:HIS:CG	2.55	0.40
1:A:36:HIS:HE1	3:A:1350:HOH:O	2.04	0.40
1:A:637:MET:CG	1:D:532:SER:HB2	2.51	0.40
1:B:583:LYS:O	1:B:584:LYS:HB3	2.21	0.40
1:D:604:ALA:HB1	1:D:633:LEU:HD22	2.04	0.40
1:B:237:ASP:OD2	1:B:536:ARG:HG3	2.20	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:ASP:CB	3:B:1526:HOH:O[2_545]	2.00	0.20

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	725/753 (96%)	706 (97%)	18 (2%)	1 (0%)	51 42
1	B	725/753 (96%)	702 (97%)	20 (3%)	3 (0%)	34 24
1	C	726/753 (96%)	710 (98%)	15 (2%)	1 (0%)	51 42
1	D	726/753 (96%)	704 (97%)	21 (3%)	1 (0%)	51 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2902/3012 (96%)	2822 (97%)	74 (2%)	6 (0%)	47 38

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	725	ASP
1	B	612	ARG
1	D	75	SER
1	A	75	SER
1	B	75	SER
1	C	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	612/636 (96%)	589 (96%)	23 (4%)	33 24
1	B	612/636 (96%)	579 (95%)	33 (5%)	22 13
1	C	613/636 (96%)	574 (94%)	39 (6%)	17 8
1	D	613/636 (96%)	585 (95%)	28 (5%)	27 17
All	All	2450/2544 (96%)	2327 (95%)	123 (5%)	24 15

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	37	ARG
1	A	73	LYS
1	A	185	PHE
1	A	191	THR
1	A	205	ILE
1	A	227	TRP
1	A	237	ASP
1	A	252	ASN

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Mol	Chain	Res	Type
1	A	348	LYS
1	A	369	ARG
1	A	375	LEU
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	565	GLU
1	A	612	ARG
1	A	707	THR
1	A	713	GLN
1	A	716	GLU
1	A	725	ASP
1	A	732	LEU
1	A	750	LYS
1	B	185	PHE
1	B	191	THR
1	B	205	ILE
1	B	227	TRP
1	B	237	ASP
1	B	252	ASN
1	B	283	GLU
1	B	321	GLU
1	B	369	ARG
1	B	370	VAL
1	B	375	LEU
1	B	377	ARG
1	B	379	PRO
1	B	398	PRO
1	B	432	PRO
1	B	440	TYR
1	B	459	ASN
1	B	521	ARG
1	B	552	LEU
1	B	562	LEU
1	B	571	LEU
1	B	583	LYS
1	B	595	ASP
1	B	610	GLU
1	B	612	ARG
1	B	616	LEU
1	B	626	LYS
1	B	633	LEU

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Mol	Chain	Res	Type
1	B	703	LYS
1	B	713	GLN
1	B	732	LEU
1	B	749	ASP
1	B	751	ILE
1	C	32	GLU
1	C	37	ARG
1	C	61	ARG
1	C	159	ILE
1	C	185	PHE
1	C	191	THR
1	C	198	LEU
1	C	205	ILE
1	C	227	TRP
1	C	237	ASP
1	C	252	ASN
1	C	375	LEU
1	C	377	ARG
1	C	398	PRO
1	C	432	PRO
1	C	440	TYR
1	C	459	ASN
1	C	478	LYS
1	C	488	ARG
1	C	521	ARG
1	C	531	LEU
1	C	571	LEU
1	C	583	LYS
1	C	584	LYS
1	C	606	LEU
1	C	610	GLU
1	C	612	ARG
1	C	616	LEU
1	C	617	LEU
1	C	621	LYS
1	C	633	LEU
1	C	636	ARG
1	C	648	LEU
1	C	660	LEU
1	C	709	LYS
1	C	713	GLN
1	C	725	ASP

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Mol	Chain	Res	Type
1	C	733	LEU
1	C	750	LYS
1	D	48	GLN
1	D	73	LYS
1	D	142	LYS
1	D	185	PHE
1	D	191	THR
1	D	198	LEU
1	D	205	ILE
1	D	227	TRP
1	D	237	ASP
1	D	252	ASN
1	D	340	LEU
1	D	369	ARG
1	D	375	LEU
1	D	440	TYR
1	D	459	ASN
1	D	546[A]	GLN
1	D	546[B]	GLN
1	D	554	LEU
1	D	574	THR
1	D	582	LEU
1	D	598	VAL
1	D	612	ARG
1	D	616	LEU
1	D	633	LEU
1	D	648	LEU
1	D	716	GLU
1	D	732	LEU
1	D	747	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	252	ASN
1	A	419	GLN
1	A	459	ASN
1	A	515	GLN
1	A	713	GLN
1	B	252	ASN
1	B	419	GLN

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Mol	Chain	Res	Type
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	B	713	GLN
1	C	252	ASN
1	C	368	GLN
1	C	419	GLN
1	C	459	ASN
1	C	507	HIS
1	C	556	GLN
1	C	572	ASN
1	C	629	HIS
1	C	671	ASN
1	D	48	GLN
1	D	252	ASN
1	D	419	GLN
1	D	459	ASN
1	D	507	HIS
1	D	556	GLN
1	D	629	HIS
1	D	671	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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	B	801	1,3	41,52,52	1.72	9 (21%)	31,89,89	3.08	15 (48%)
2	HDD	C	801	1	41,52,52	1.67	6 (14%)	31,89,89	2.32	13 (41%)
2	HDD	A	801	1,3	41,52,52	1.58	10 (24%)	31,89,89	2.80	13 (41%)
2	HDD	D	801	1,3	41,52,52	1.65	10 (24%)	31,89,89	2.37	12 (38%)

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	B	801	1,3	-	2/5/89/89	0/1/9/9
2	HDD	C	801	1	-	2/5/89/89	0/1/9/9
2	HDD	A	801	1,3	-	2/5/89/89	0/1/9/9
2	HDD	D	801	1,3	-	2/5/89/89	0/1/9/9

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	HDD	C3C-C2C	6.35	1.49	1.40
2	A	801	HDD	O1D-CGD	5.38	1.44	1.35
2	B	801	HDD	O1D-C3D	4.52	1.54	1.46
2	D	801	HDD	C3B-C2B	3.82	1.45	1.40
2	D	801	HDD	O1D-CGD	3.66	1.41	1.35
2	B	801	HDD	O1D-CGD	3.66	1.41	1.35
2	C	801	HDD	C4A-CHB	3.53	1.50	1.41
2	B	801	HDD	C2A-C3A	3.49	1.48	1.37
2	B	801	HDD	C3C-C2C	3.38	1.45	1.40
2	B	801	HDD	C3B-C2B	3.18	1.44	1.40
2	D	801	HDD	C4C-CHD	3.09	1.49	1.41
2	D	801	HDD	C2A-C3A	3.03	1.46	1.37
2	C	801	HDD	O1D-CGD	2.91	1.40	1.35
2	D	801	HDD	OND-C2D	2.91	1.48	1.42
2	C	801	HDD	C2B-C1B	2.86	1.49	1.42
2	D	801	HDD	C3C-C2C	2.79	1.44	1.40
2	A	801	HDD	C3B-C2B	2.76	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HDD	C3C-C2C	2.74	1.44	1.40
2	B	801	HDD	C4A-CHB	2.72	1.48	1.41
2	C	801	HDD	C2A-C3A	2.62	1.45	1.37
2	A	801	HDD	OND-C2D	2.61	1.47	1.42
2	D	801	HDD	C1C-CHC	2.55	1.48	1.41
2	D	801	HDD	C1A-CHA	2.44	1.47	1.41
2	A	801	HDD	C4C-CHD	2.38	1.47	1.41
2	B	801	HDD	C2B-C1B	2.33	1.47	1.42
2	A	801	HDD	C2B-C1B	2.31	1.47	1.42
2	D	801	HDD	C2B-C1B	2.31	1.47	1.42
2	A	801	HDD	C2A-C3A	2.28	1.44	1.37
2	B	801	HDD	C4C-CHD	2.16	1.47	1.41
2	B	801	HDD	C1C-CHC	2.13	1.46	1.41
2	A	801	HDD	C1C-CHC	2.13	1.46	1.41
2	A	801	HDD	C1A-CHA	2.11	1.46	1.41
2	D	801	HDD	C4A-CHB	2.10	1.46	1.41
2	C	801	HDD	C1C-CHC	2.09	1.46	1.41
2	A	801	HDD	O2A-CGA	-2.07	1.23	1.30

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	HDD	O1D-CGD-O2D	8.68	128.55	120.80
2	A	801	HDD	O1D-CGD-O2D	8.01	127.95	120.80
2	B	801	HDD	O1D-CGD-CBD	-6.28	103.86	110.19
2	A	801	HDD	OND-C2D-CMD	-5.95	98.63	109.59
2	A	801	HDD	O1D-CGD-CBD	-5.91	104.23	110.19
2	D	801	HDD	C4A-C3A-C2A	-5.86	102.92	107.00
2	B	801	HDD	C4A-C3A-C2A	-5.33	103.29	107.00
2	C	801	HDD	O1D-CGD-O2D	4.97	125.23	120.80
2	C	801	HDD	OND-C2D-CMD	-4.65	101.02	109.59
2	B	801	HDD	OND-C2D-CMD	-4.44	101.41	109.59
2	D	801	HDD	O1D-CGD-O2D	4.30	124.64	120.80
2	C	801	HDD	C4A-C3A-C2A	-4.28	104.02	107.00
2	B	801	HDD	C2D-C1D-CHD	-4.19	117.36	124.28
2	D	801	HDD	CMB-C2B-C3B	4.16	132.46	124.68
2	B	801	HDD	CAA-CBA-CGA	-4.08	102.33	113.76
2	D	801	HDD	CAA-CBA-CGA	-4.00	102.53	113.76
2	A	801	HDD	CMB-C2B-C3B	3.94	132.05	124.68
2	C	801	HDD	CAA-CBA-CGA	-3.84	103.00	113.76
2	D	801	HDD	C2D-C1D-CHD	-3.73	118.12	124.28
2	A	801	HDD	C4C-CHD-C1D	-3.67	122.85	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	HDD	C2D-C1D-CHD	-3.60	118.34	124.28
2	D	801	HDD	OND-C2D-CMD	-3.59	102.98	109.59
2	A	801	HDD	CAA-CBA-CGA	-3.49	103.99	113.76
2	B	801	HDD	CMC-C2C-C3C	3.47	131.17	124.68
2	A	801	HDD	CMC-C2C-C1C	3.42	133.72	128.46
2	D	801	HDD	C4C-CHD-C1D	-3.40	123.39	130.12
2	A	801	HDD	C4A-C3A-C2A	-3.37	104.65	107.00
2	B	801	HDD	CBA-CAA-C2A	-3.33	106.93	112.62
2	C	801	HDD	CMA-C3A-C2A	3.32	131.19	124.94
2	C	801	HDD	CMC-C2C-C3C	3.24	130.75	124.68
2	B	801	HDD	O1D-C3D-C4D	3.24	114.83	108.25
2	B	801	HDD	CAD-CBD-CGD	3.24	109.57	104.56
2	B	801	HDD	C1A-CHA-C4D	-3.17	123.85	130.12
2	C	801	HDD	C2D-C1D-CHD	-3.09	119.17	124.28
2	B	801	HDD	CMB-C2B-C3B	2.72	129.77	124.68
2	C	801	HDD	CBA-CAA-C2A	-2.71	108.00	112.62
2	D	801	HDD	C1A-CHA-C4D	-2.69	124.80	130.12
2	C	801	HDD	C4C-CHD-C1D	-2.63	124.91	130.12
2	B	801	HDD	C3D-C4D-CHA	-2.59	116.64	124.34
2	B	801	HDD	C4C-CHD-C1D	-2.53	125.10	130.12
2	C	801	HDD	CMA-C3A-C4A	-2.45	124.70	128.46
2	D	801	HDD	CMC-C2C-C1C	2.44	132.21	128.46
2	C	801	HDD	C3D-C4D-CHA	-2.38	117.27	124.34
2	C	801	HDD	C2B-C3B-C4B	2.23	108.45	106.90
2	C	801	HDD	CMB-C2B-C3B	2.20	128.79	124.68
2	D	801	HDD	C3D-C4D-CHA	-2.18	117.85	124.34
2	A	801	HDD	C3D-C4D-CHA	-2.18	117.86	124.34
2	A	801	HDD	C1A-CHA-C4D	-2.18	125.81	130.12
2	D	801	HDD	CMA-C3A-C2A	2.12	128.95	124.94
2	D	801	HDD	CBA-CAA-C2A	-2.11	109.02	112.62
2	B	801	HDD	CMA-C3A-C2A	2.09	128.89	124.94
2	A	801	HDD	CHD-C1D-ND	2.06	127.22	124.20
2	A	801	HDD	O1D-C3D-CAD	-2.05	99.15	103.01

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	HDD	CAA-CBA-CGA-O1A
2	D	801	HDD	CAA-CBA-CGA-O2A
2	A	801	HDD	CAA-CBA-CGA-O2A
2	B	801	HDD	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
2	B	801	HDD	CAA-CBA-CGA-O2A
2	C	801	HDD	CAA-CBA-CGA-O1A
2	D	801	HDD	CAA-CBA-CGA-O1A
2	C	801	HDD	CAA-CBA-CGA-O2A

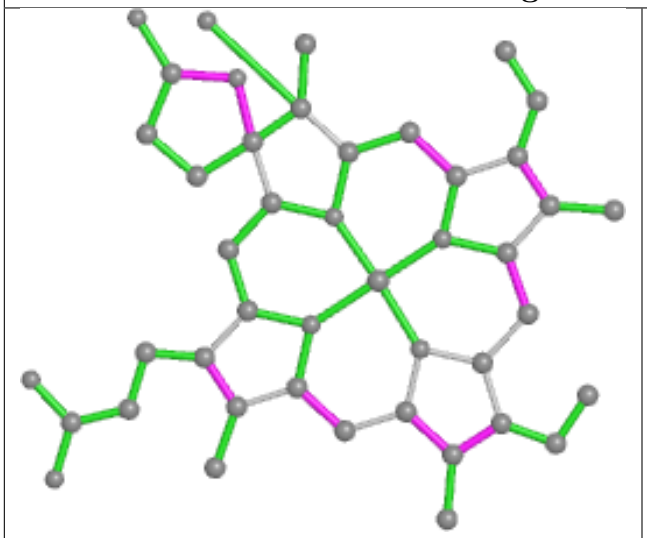
There are no ring outliers.

4 monomers are involved in 18 short contacts:

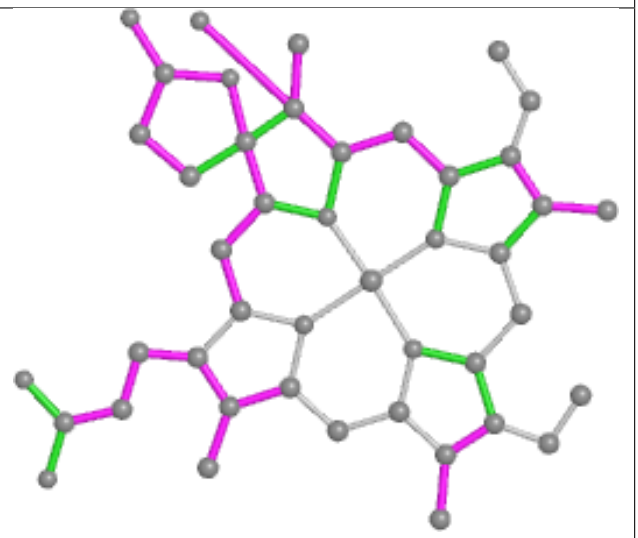
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	HDD	6	0
2	C	801	HDD	5	0
2	A	801	HDD	4	0
2	D	801	HDD	3	0

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.

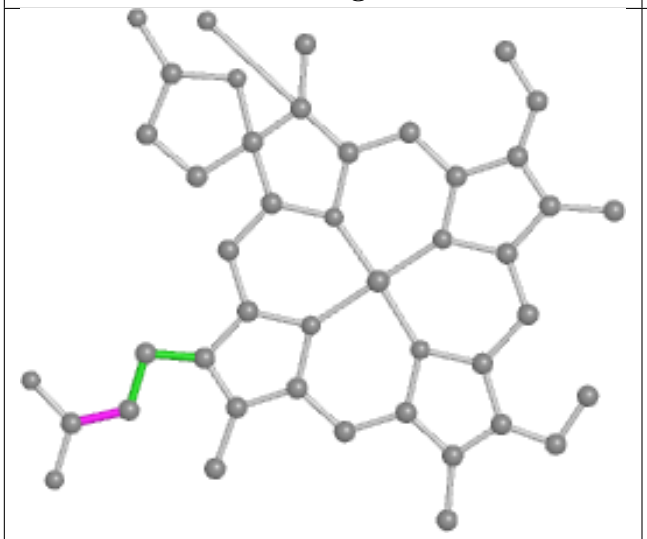
Ligand HDD B 801



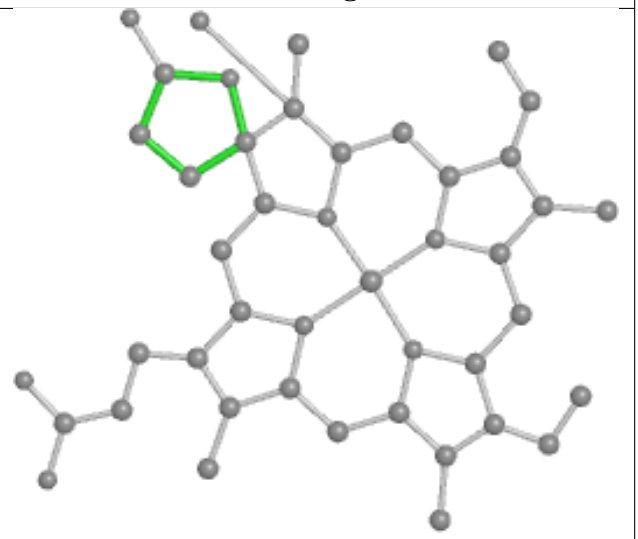
Bond lengths



Bond angles

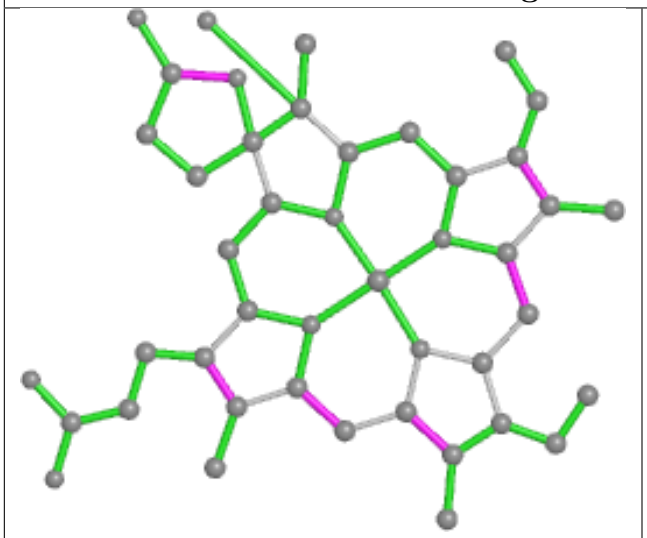


Torsions

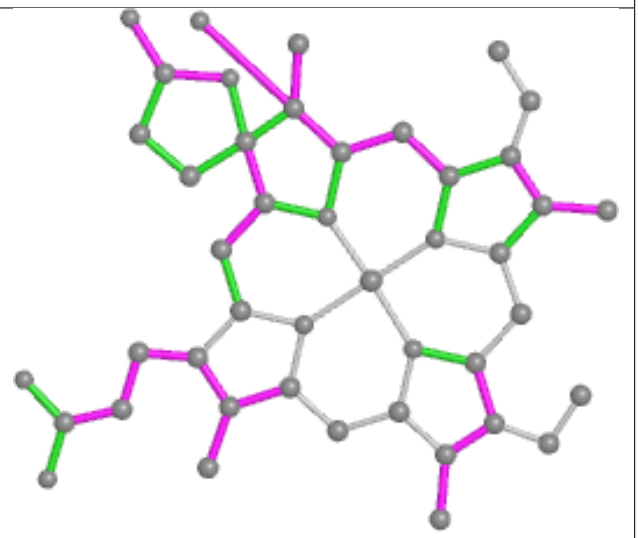


Rings

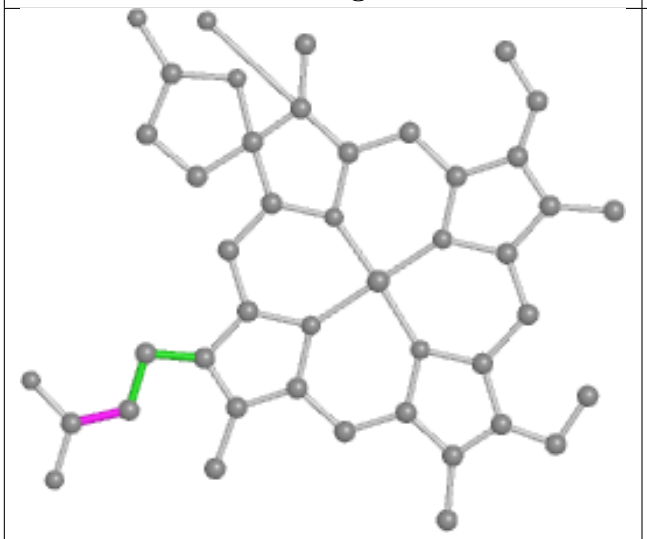
Ligand HDD C 801



Bond lengths



Bond angles



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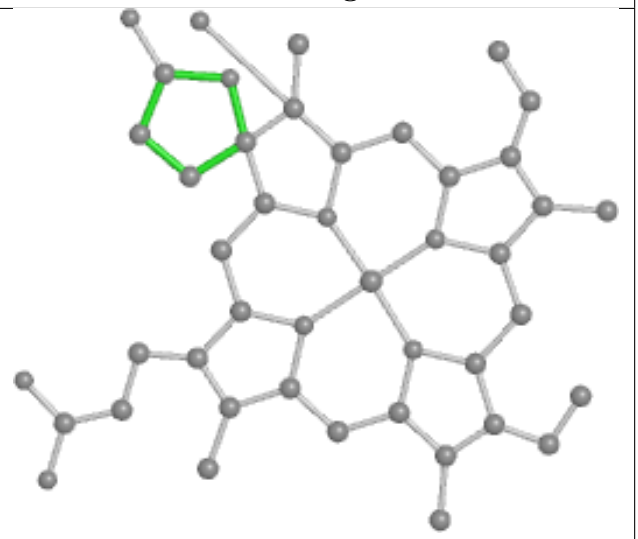
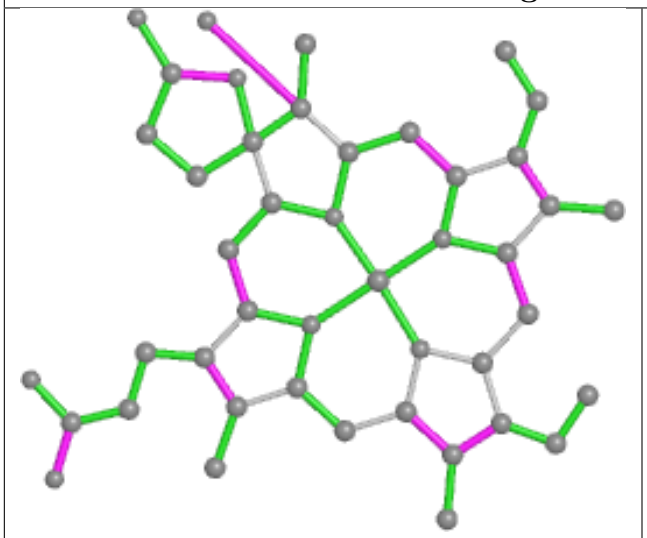
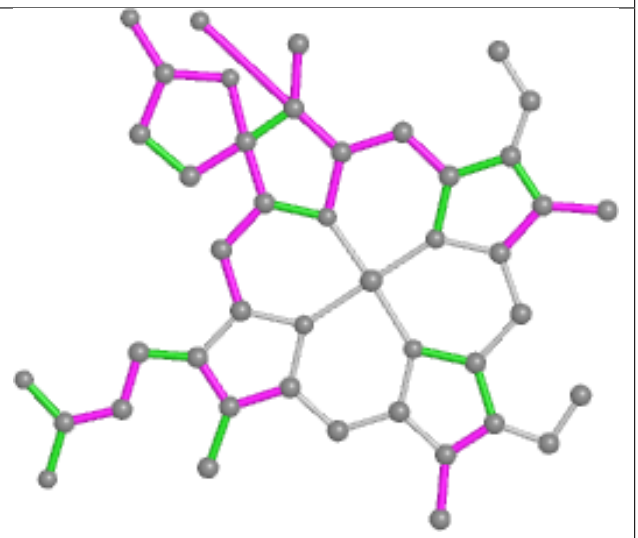


Rings

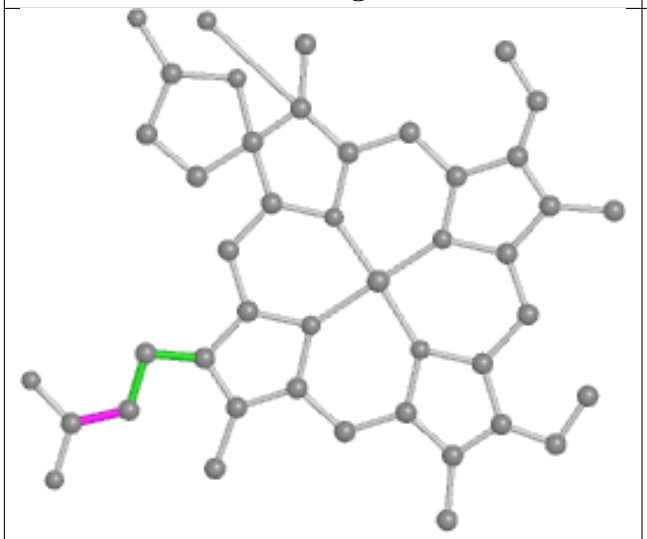
Ligand HDD A 801



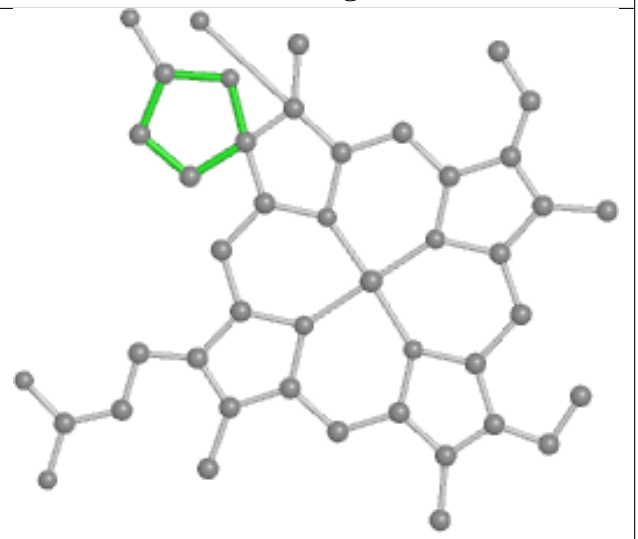
Bond lengths



Bond angles

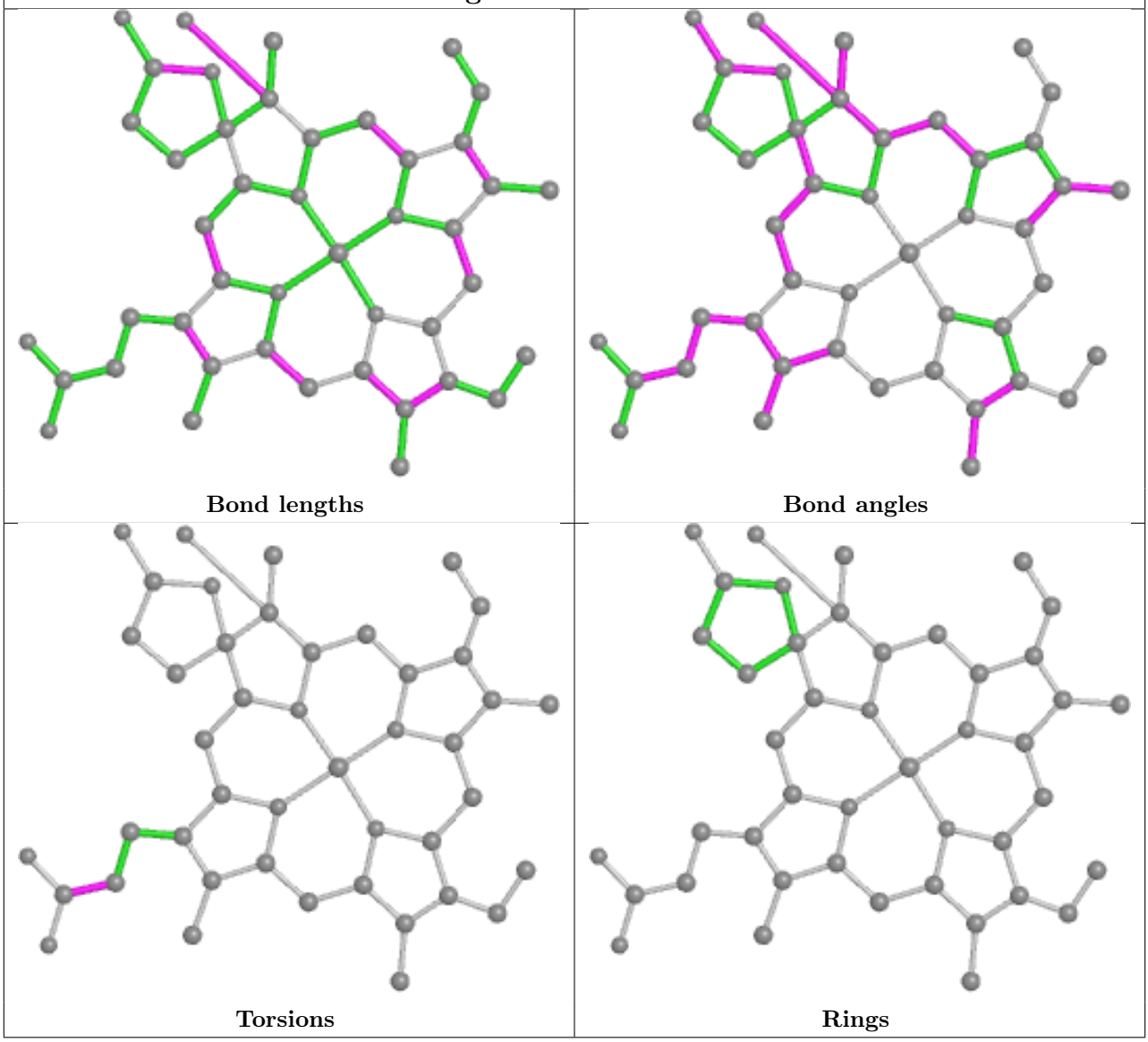


Torsions



Rings

Ligand HDD D 801



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	726/753 (96%)	-0.55	4 (0%)	89	90	5, 12, 26, 51	1 (0%)
1	B	726/753 (96%)	-0.44	13 (1%)	68	71	6, 13, 35, 56	1 (0%)
1	C	726/753 (96%)	-0.44	9 (1%)	79	81	6, 13, 33, 52	1 (0%)
1	D	726/753 (96%)	-0.50	5 (0%)	87	88	5, 12, 29, 54	1 (0%)
All	All	2904/3012 (96%)	-0.48	31 (1%)	80	82	5, 12, 32, 56	4 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	713	GLN	3.5
1	B	726	GLY	3.4
1	B	28	SER	3.3
1	B	32	GLU	3.3
1	D	28	SER	3.2
1	D	712	ASP	3.1
1	D	713	GLN	3.1
1	A	726	GLY	3.1
1	C	594	PRO	3.0
1	B	568	ASP	2.9
1	C	750	LYS	2.8
1	B	569	ASP	2.8
1	A	32	GLU	2.8
1	C	711	ALA	2.7
1	C	726	GLY	2.7
1	A	725	ASP	2.6
1	B	552	LEU	2.6
1	A	28	SER	2.5
1	C	32	GLU	2.3
1	C	569	ASP	2.3
1	B	645	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	568	ASP	2.2
1	B	583	LYS	2.2
1	C	669	CYS	2.2
1	C	572	ASN	2.2
1	D	569	ASP	2.1
1	B	567	THR	2.1
1	B	725	ASP	2.1
1	B	571	LEU	2.0
1	B	646	THR	2.0
1	C	714	GLY	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 monosaccharides in this entry.

6.4 Ligands (i)

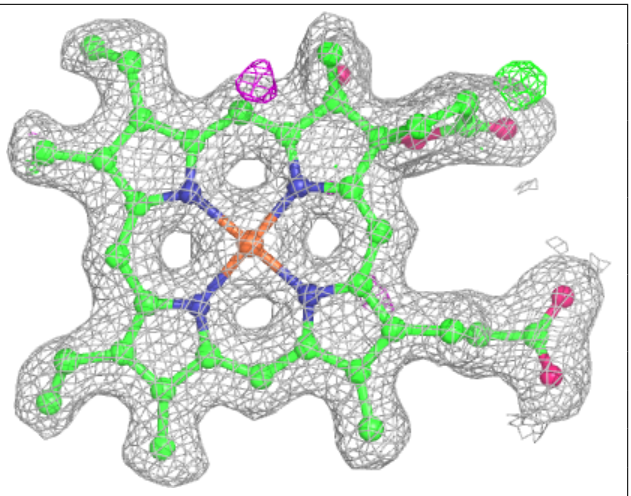
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

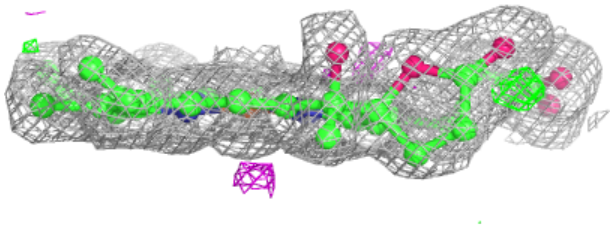
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HDD	A	801	44/44	0.98	0.11	5,8,11,12	0
2	HDD	B	801	44/44	0.98	0.08	6,9,11,12	0
2	HDD	C	801	44/44	0.98	0.09	7,8,13,17	0
2	HDD	D	801	44/44	0.98	0.09	6,7,12,14	0

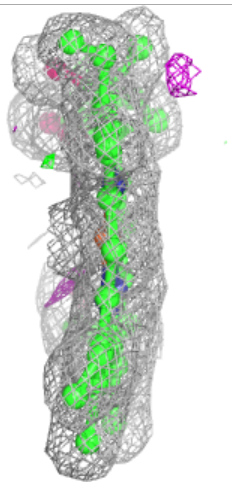
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HDD A 801:

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

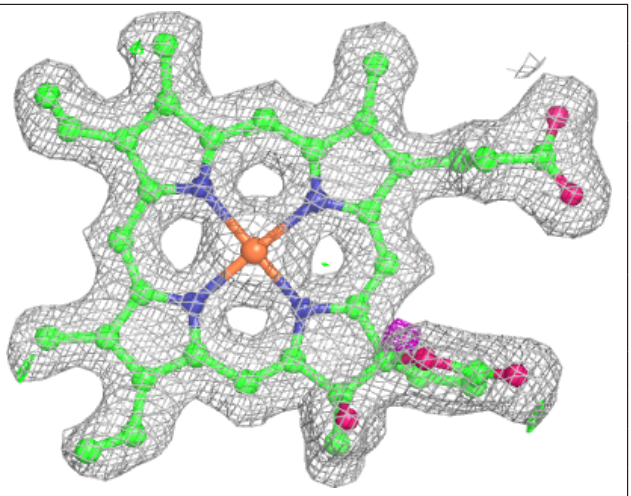


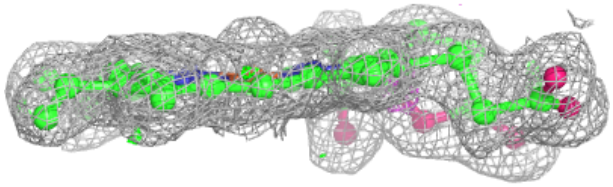


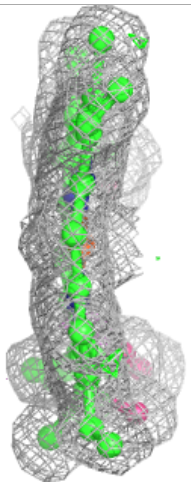


Electron density around HDD B 801:

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

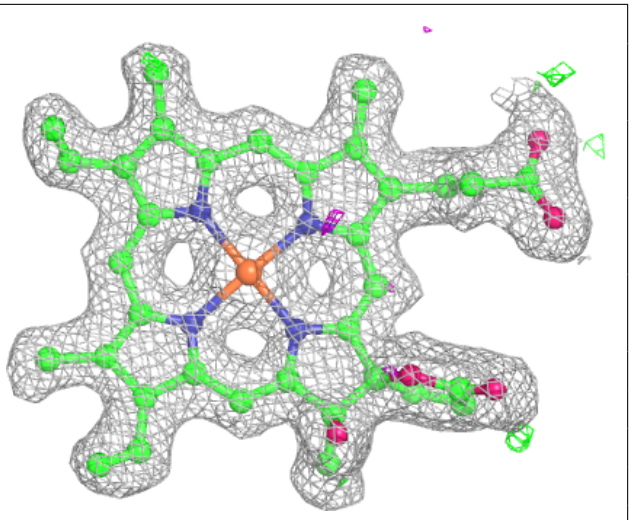


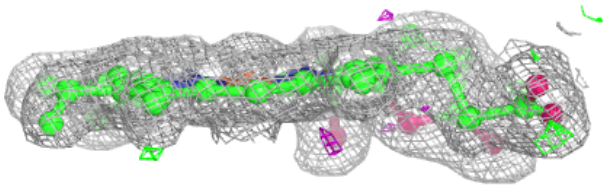


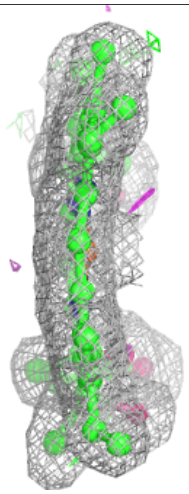


Electron density around HDD C 801:

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

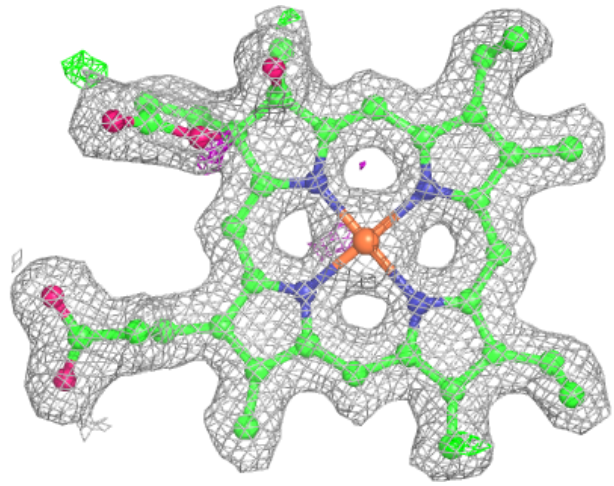


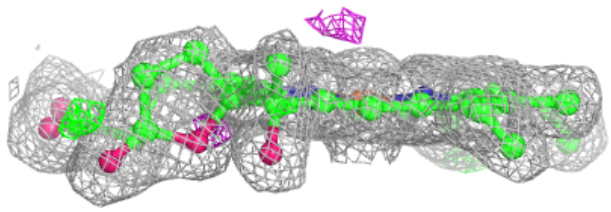


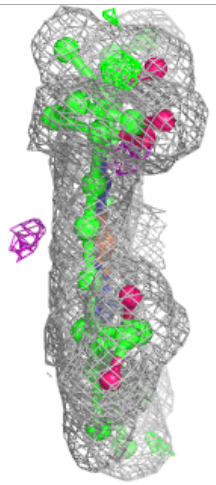


Electron density around HDD D 801:

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.