Full wwPDB X-ray Structure Validation Report (i)

Aug 7, 2023 – 09:55 PM EDT

PDB ID	:	1P81
Title	:	Crystal structure of the D181E variant of catalase HPII from E. coli
Authors	:	Chelikani, P.; Carpena, X.; Fita, I.; Loewen, P.C.
Deposited on	:	2003-05-06
Resolution	:	1.81 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:

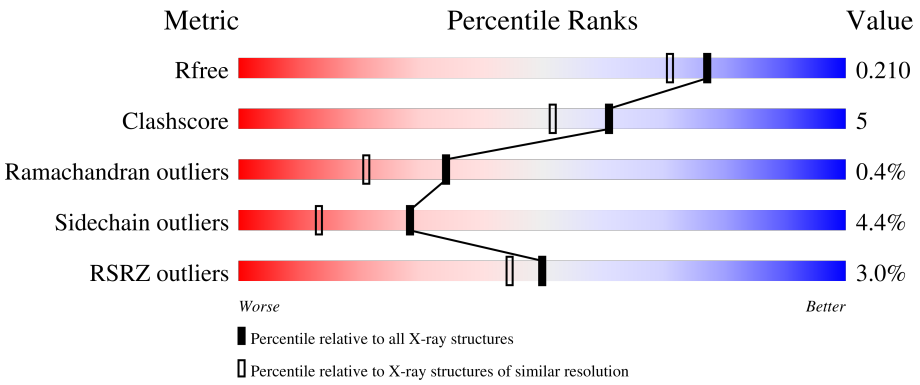
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.81 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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	3% 86% 10%
1	B	753	3% 81% 13%
1	C	753	2% 84% 10%
1	D	753	3% 81% 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 26236 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.

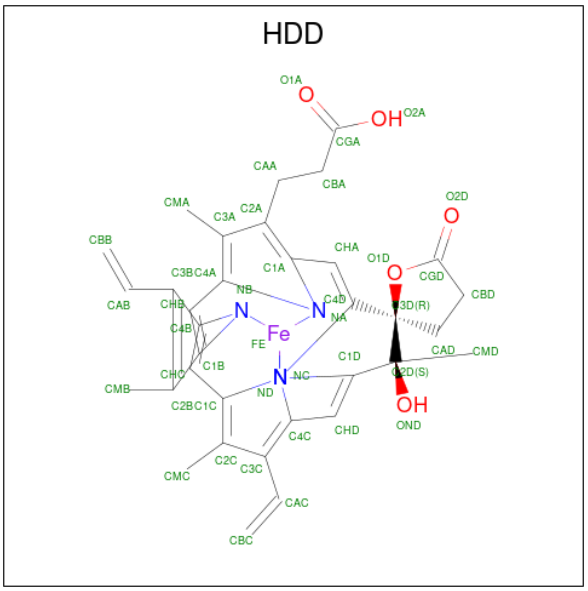
- Molecule 1 is a protein called Catalase HPII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	727	5747	3648	1005	1082	12	0	0	0
1	B	727	5747	3648	1005	1082	12	0	0	0
1	C	727	5747	3648	1005	1082	12	0	0	0
1	D	727	5747	3648	1005	1082	12	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	GLU	ASP	engineered mutation	UNP P21179
B	181	GLU	ASP	engineered mutation	UNP P21179
C	181	GLU	ASP	engineered mutation	UNP P21179
D	181	GLU	ASP	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.

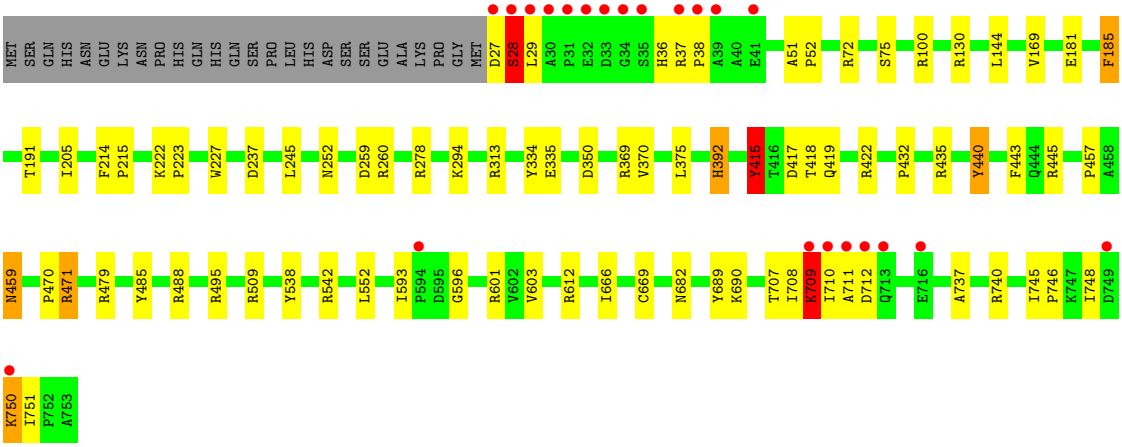
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	815	Total	O	0	0
			815	815		
3	B	702	Total	O	0	0
			702	702		
3	C	768	Total	O	0	0
			768	768		
3	D	787	Total	O	0	0
			787	787		

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.

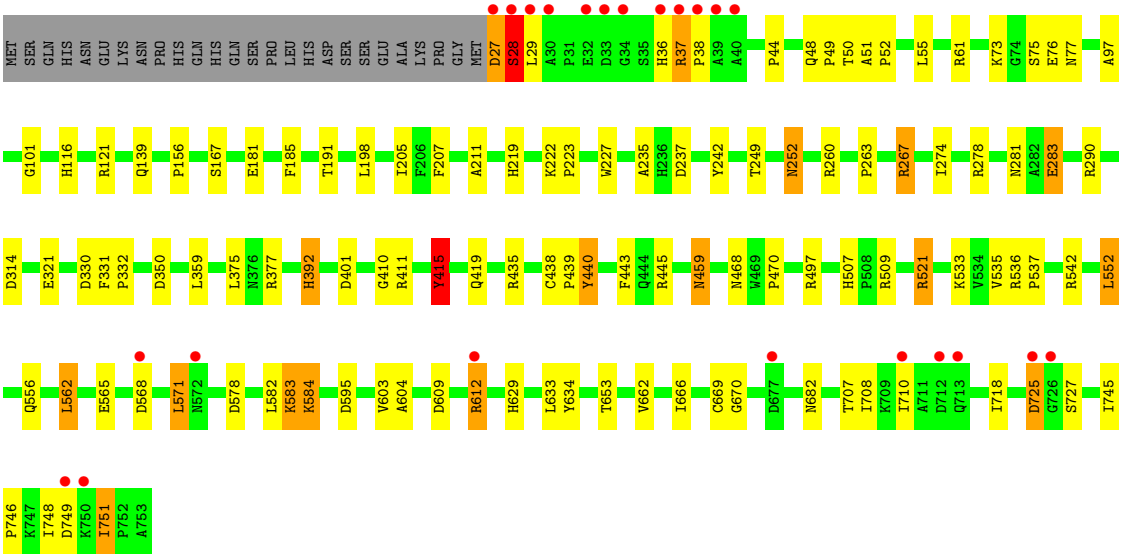
- Molecule 1: Catalase HPII

Chain A:



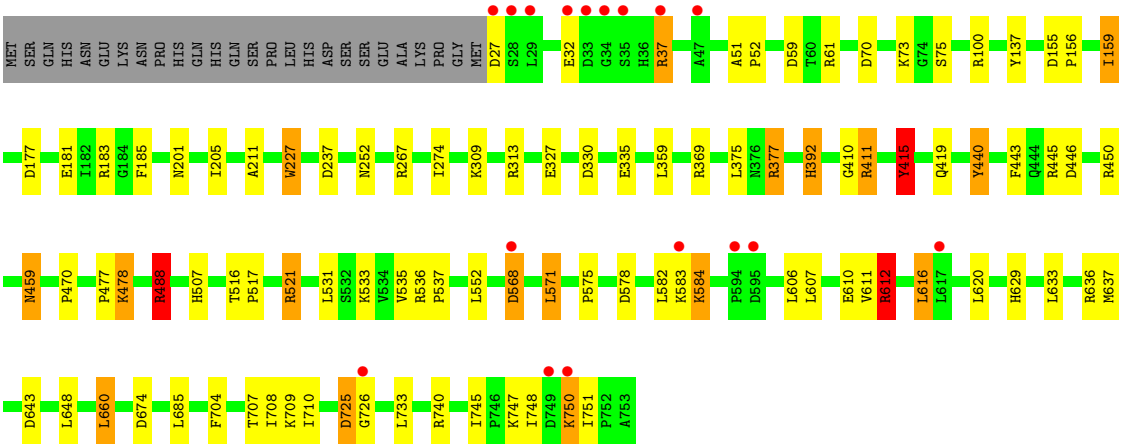
- Molecule 1: Catalase HPII

Chain B:



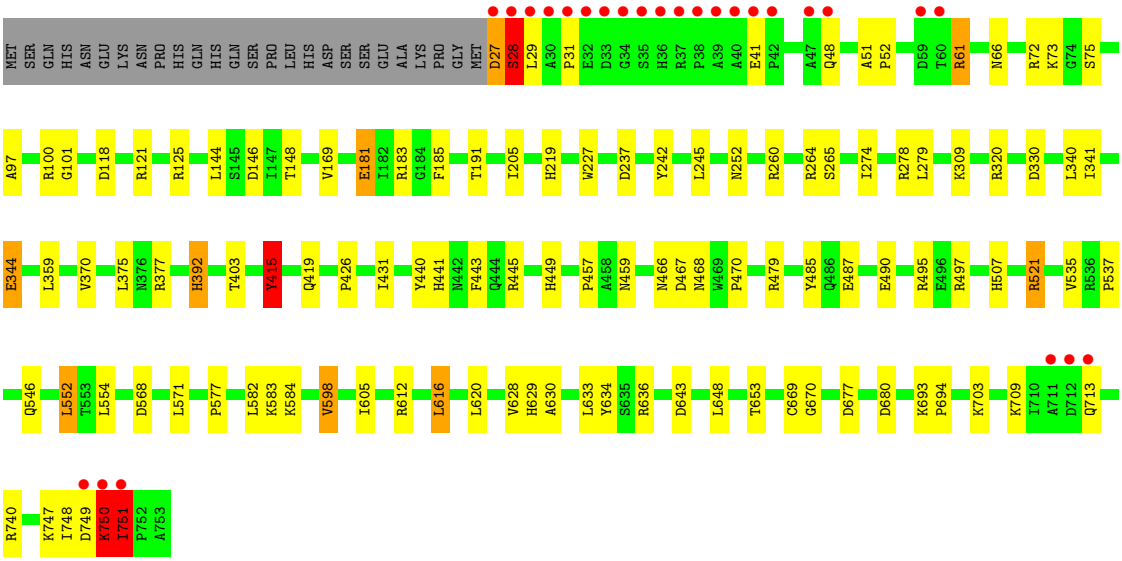
- Molecule 1: Catalase HPII

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	93.38Å 132.86Å 122.04Å 90.00° 109.50° 90.00°	Depositor
Resolution (Å)	29.90 – 1.81 17.97 – 1.81	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.90-1.81) 98.7 (17.97-1.81)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 1.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.172 , 0.216 0.171 , 0.210	Depositor DCC
R_{free} test set	12587 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	13.9	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 61.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	26236	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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	0.58	0/5903	1.24	31/8025 (0.4%)
1	B	0.56	0/5903	1.23	34/8025 (0.4%)
1	C	0.57	0/5903	1.23	28/8025 (0.3%)
1	D	0.58	0/5903	1.33	47/8025 (0.6%)
All	All	0.57	0/23612	1.26	140/32100 (0.4%)

There are no bond length outliers.

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	612	ARG	CD-NE-CZ	30.17	165.83	123.60
1	B	521	ARG	NE-CZ-NH1	14.58	127.59	120.30
1	D	740	ARG	NE-CZ-NH1	12.87	126.74	120.30
1	D	61	ARG	NE-CZ-NH1	-12.16	114.22	120.30
1	D	61	ARG	NE-CZ-NH2	11.55	126.08	120.30
1	D	612	ARG	NE-CZ-NH2	10.81	125.71	120.30
1	C	445	ARG	NE-CZ-NH1	10.54	125.57	120.30
1	D	740	ARG	NE-CZ-NH2	-10.15	115.22	120.30
1	A	488	ARG	NE-CZ-NH2	-10.05	115.27	120.30
1	D	521	ARG	NE-CZ-NH2	9.76	125.18	120.30
1	D	260	ARG	NE-CZ-NH2	-9.71	115.44	120.30
1	C	313	ARG	NE-CZ-NH1	9.67	125.14	120.30
1	C	377	ARG	NE-CZ-NH1	-9.35	115.62	120.30
1	B	27	ASP	CB-CG-OD2	-9.15	110.06	118.30
1	A	471	ARG	NE-CZ-NH2	8.96	124.78	120.30
1	B	435	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	A	479	ARG	CD-NE-CZ	8.49	135.49	123.60
1	C	636	ARG	NE-CZ-NH1	-8.46	116.07	120.30
1	A	509	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	A	479	ARG	NE-CZ-NH2	-8.19	116.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	320	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	C	59	ASP	CB-CG-OD1	7.94	125.44	118.30
1	C	636	ARG	NE-CZ-NH2	7.89	124.24	120.30
1	B	440	TYR	CB-CG-CD2	-7.86	116.28	121.00
1	D	449	HIS	CA-CB-CG	7.81	126.88	113.60
1	B	267	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	C	488	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	D	677	ASP	CB-CG-OD2	7.62	125.16	118.30
1	C	726	GLY	N-CA-C	-7.42	94.54	113.10
1	B	445	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	C	568	ASP	CB-CG-OD1	-7.28	111.75	118.30
1	A	542	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	B	445	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	D	497	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	D	377	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	B	440	TYR	CB-CG-CD1	7.00	125.20	121.00
1	B	392	HIS	CG-ND1-CE1	6.98	117.97	108.20
1	B	121	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	A	495	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	D	415	TYR	CB-CG-CD1	-6.83	116.90	121.00
1	B	435	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	D	320	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	C	392	HIS	CG-ND1-CE1	6.77	117.68	108.20
1	B	28	SER	N-CA-CB	6.77	120.65	110.50
1	C	440	TYR	CB-CG-CD1	6.76	125.05	121.00
1	A	130	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	A	435	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	D	479	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	A	471	ARG	NE-CZ-NH1	-6.70	116.95	120.30
1	D	100	ARG	CG-CD-NE	6.67	125.82	111.80
1	D	344	GLU	CA-CB-CG	6.61	127.94	113.40
1	B	260	ARG	NE-CZ-NH2	6.56	123.58	120.30
1	D	121	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	D	445	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	B	350	ASP	CB-CG-OD1	-6.46	112.49	118.30
1	D	61	ARG	CD-NE-CZ	6.45	132.63	123.60
1	A	440	TYR	CB-CG-CD1	6.42	124.85	121.00
1	D	260	ARG	NH1-CZ-NH2	6.42	126.46	119.40
1	B	278	ARG	CD-NE-CZ	6.33	132.47	123.60
1	B	401	ASP	CB-CG-OD2	6.30	123.97	118.30
1	C	536	ARG	NE-CZ-NH1	-6.28	117.16	120.30
1	A	350	ASP	CB-CG-OD1	-6.23	112.70	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	125	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	D	636	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	259	ASP	CB-CG-OD2	6.04	123.74	118.30
1	B	242	TYR	CB-CG-CD2	-6.03	117.38	121.00
1	C	440	TYR	CB-CG-CD2	-6.01	117.39	121.00
1	B	27	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	440	TYR	CB-CG-CD2	-5.94	117.44	121.00
1	A	479	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	B	121	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	C	725	ASP	N-CA-CB	5.94	121.28	110.60
1	D	568	ASP	CB-CG-OD2	5.93	123.64	118.30
1	C	740	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	C	70	ASP	CB-CG-OD2	5.92	123.63	118.30
1	D	264	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	A	445	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	D	495	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	C	740	ARG	CD-NE-CZ	5.86	131.81	123.60
1	A	392	HIS	CG-ND1-CE1	5.86	116.40	108.20
1	A	130	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	B	415	TYR	CA-CB-CG	5.85	124.52	113.40
1	C	446	ASP	CB-CG-OD2	5.84	123.56	118.30
1	C	327	GLU	OE1-CD-OE2	-5.84	116.29	123.30
1	A	278	ARG	NE-CZ-NH1	-5.79	117.40	120.30
1	A	485	TYR	CB-CG-CD1	-5.75	117.55	121.00
1	A	601	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	D	445	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	A	415	TYR	CB-CG-CD1	-5.67	117.60	121.00
1	B	283	GLU	CB-CG-CD	5.66	129.49	114.20
1	A	260	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	D	643	ASP	CB-CG-OD1	5.62	123.36	118.30
1	D	709	LYS	CA-CB-CG	5.62	125.76	113.40
1	A	28	SER	N-CA-CB	-5.61	102.09	110.50
1	D	183	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	B	609	ASP	CB-CG-OD2	5.55	123.30	118.30
1	D	479	ARG	CD-NE-CZ	5.54	131.35	123.60
1	D	521	ARG	CG-CD-NE	5.50	123.36	111.80
1	B	419	GLN	CG-CD-OE1	-5.50	110.60	121.60
1	C	450	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	C	674	ASP	CB-CG-OD2	5.48	123.23	118.30
1	C	177	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	100	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	D	485	TYR	CB-CG-CD1	-5.46	117.73	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	467	ASP	CB-CG-OD1	5.45	123.20	118.30
1	D	680	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	334	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	D	377	ARG	NH1-CZ-NH2	5.43	125.37	119.40
1	B	61	ARG	NE-CZ-NH2	5.40	123.00	120.30
1	D	612	ARG	CG-CD-NE	5.39	123.12	111.80
1	D	419	GLN	CG-CD-OE1	-5.39	110.83	121.60
1	C	419	GLN	CB-CG-CD	-5.37	97.64	111.60
1	D	521	ARG	CD-NE-CZ	-5.34	116.12	123.60
1	C	419	GLN	CG-CD-OE1	-5.32	110.96	121.60
1	D	403	THR	N-CA-CB	5.32	120.41	110.30
1	C	183	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	A	422	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	A	740	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	D	265	SER	N-CA-CB	-5.26	102.61	110.50
1	A	419	GLN	CB-CG-CD	-5.25	97.94	111.60
1	B	167	SER	N-CA-CB	-5.25	102.63	110.50
1	C	411	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	D	72	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	D	27	ASP	CB-CG-OD1	5.22	123.00	118.30
1	D	392	HIS	CG-ND1-CE1	5.22	115.51	108.20
1	B	419	GLN	CB-CG-CD	-5.22	98.03	111.60
1	B	497	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	B	377	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	C	415	TYR	CA-CB-CG	5.16	123.19	113.40
1	B	542	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	C	612	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	D	457	PRO	N-CA-CB	5.12	109.45	103.30
1	B	536	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	A	72	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	509	ARG	NE-CZ-NH1	-5.07	117.76	120.30
1	D	242	TYR	CB-CG-CD2	-5.06	117.96	121.00
1	B	290	ARG	N-CA-CB	5.05	119.69	110.60
1	B	542	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	B	314	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	185	PHE	CB-CG-CD2	-5.01	117.29	120.80

There are no chirality outliers.

There are no planarity outliers.

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	5580	43	0
1	B	5747	0	5580	66	0
1	C	5747	0	5580	52	0
1	D	5747	0	5580	52	0
2	A	44	0	31	5	0
2	B	44	0	31	4	0
2	C	44	0	31	6	0
2	D	44	0	31	2	0
3	A	815	0	0	6	1
3	B	702	0	0	6	1
3	C	768	0	0	9	0
3	D	787	0	0	7	0
All	All	26236	0	22444	206	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 (206) 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:B:392:HIS:ND1	1:B:415:TYR:HB2	1.38	1.39
1:A:392:HIS:ND1	1:A:415:TYR:HB2	1.40	1.35
1:C:392:HIS:ND1	1:C:415:TYR:HB2	1.42	1.32
1:D:392:HIS:ND1	1:D:415:TYR:HB2	1.39	1.31
1:C:392:HIS:ND1	1:C:415:TYR:CB	2.33	0.89
1:A:392:HIS:ND1	1:A:415:TYR:CB	2.34	0.86
1:B:392:HIS:ND1	1:B:415:TYR:CB	2.34	0.85
1:D:392:HIS:ND1	1:D:415:TYR:CB	2.35	0.80
1:D:750:LYS:HD3	1:D:751:ILE:H	1.48	0.77
1:B:583:LYS:H	1:B:583:LYS:NZ	1.82	0.77
2:C:760:HDD:HBC1	2:C:760:HDD:HMC1	1.66	0.76
1:C:392:HIS:CG	1:C:415:TYR:HB2	2.22	0.75
1:B:710:ILE:HD13	1:B:718:ILE:HG13	1.69	0.74
1:C:748:ILE:O	1:C:751:ILE:HG22	1.89	0.73
2:A:760:HDD:HMC1	2:A:760:HDD:HBC1	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:ARG:HG3	3:C:3862:HOH:O	1.94	0.67
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.24	0.67
1:A:181:GLU:HG2	3:A:4194:HOH:O	1.94	0.67
1:D:27:ASP:O	1:D:28:SER:HB2	1.94	0.66
1:A:392:HIS:CG	1:A:415:TYR:HB2	2.29	0.66
1:A:28:SER:HB2	1:D:245:LEU:HD13	1.78	0.65
1:B:267:ARG:HG3	3:B:2872:HOH:O	1.95	0.65
1:B:533:LYS:HE2	3:B:4201:HOH:O	1.96	0.65
1:B:51:ALA:HB1	1:B:52:PRO:HD2	1.79	0.64
1:B:521:ARG:NH2	1:B:745:ILE:HD13	2.13	0.63
1:B:583:LYS:O	1:B:584:LYS:HB3	1.98	0.63
1:D:392:HIS:CG	1:D:415:TYR:HB2	2.28	0.62
1:A:690:LYS:HG3	1:A:751:ILE:HD11	1.80	0.62
1:D:552:LEU:HD11	1:D:571:LEU:HD23	1.81	0.62
1:A:709:LYS:HA	1:A:709:LYS:HE3	1.81	0.62
1:C:552:LEU:HD21	1:C:571:LEU:HD12	1.83	0.61
1:D:546:GLN:HG3	3:D:3688:HOH:O	2.00	0.61
1:A:245:LEU:HD13	1:D:29:LEU:HD13	1.84	0.60
1:B:552:LEU:HD22	1:B:556:GLN:HG3	1.82	0.60
1:B:612:ARG:HD3	1:B:670:GLY:HA2	1.82	0.60
2:B:760:HDD:HMC1	2:B:760:HDD:HBC1	1.83	0.60
1:C:745:ILE:HD13	3:C:3866:HOH:O	2.00	0.60
1:C:274:ILE:HD12	2:C:760:HDD:HMB1	1.84	0.59
1:C:583:LYS:O	1:C:584:LYS:HB3	2.02	0.59
1:C:521:ARG:HG2	3:C:3866:HOH:O	2.03	0.59
1:B:748:ILE:O	1:B:751:ILE:HG22	2.03	0.59
1:B:281:ASN:OD1	1:B:283:GLU:HG3	2.03	0.59
2:A:760:HDD:HMB1	2:A:760:HDD:HBB1	1.85	0.58
1:A:748:ILE:O	1:A:751:ILE:HG13	2.03	0.58
1:C:477:PRO:HB2	1:C:478:LYS:HD3	1.86	0.58
1:A:750:LYS:O	1:A:750:LYS:HE3	2.04	0.57
1:D:431:ILE:HD11	3:D:4022:HOH:O	2.04	0.57
1:B:37:ARG:HD2	3:B:3832:HOH:O	2.04	0.57
1:D:51:ALA:HB1	1:D:52:PRO:HD2	1.88	0.56
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.20	0.56
1:B:583:LYS:H	1:B:583:LYS:HZ3	1.53	0.56
1:D:629:HIS:HD2	3:D:2510:HOH:O	1.88	0.56
1:A:51:ALA:HB1	1:A:52:PRO:HD2	1.88	0.55
1:B:359:LEU:H	1:B:507:HIS:HD2	1.52	0.55
1:D:750:LYS:HD3	1:D:751:ILE:N	2.20	0.55
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:578:ASP:HB2	1:C:582:LEU:O	2.07	0.55
1:D:583:LYS:NZ	1:D:583:LYS:HB2	2.22	0.55
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.89	0.54
1:D:535:VAL:O	1:D:537:PRO:HD3	2.06	0.54
1:A:36:HIS:CD2	1:A:36:HIS:H	2.26	0.54
1:B:392:HIS:CG	1:B:415:TYR:HB2	2.34	0.53
1:C:535:VAL:O	1:C:537:PRO:HD3	2.08	0.53
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.90	0.53
1:B:521:ARG:NH2	1:B:745:ILE:HG21	2.24	0.53
1:B:535:VAL:O	1:B:537:PRO:HD3	2.09	0.53
1:B:634:TYR:O	1:B:653:THR:HA	2.08	0.53
1:A:708:ILE:O	1:A:710:ILE:HG22	2.09	0.52
1:C:610:GLU:OE1	1:C:643:ASP:HA	2.09	0.52
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.92	0.52
1:D:274:ILE:HD12	2:D:760:HDD:HMB1	1.92	0.52
1:C:443:PHE:CZ	1:C:470:PRO:HD2	2.45	0.52
1:B:603:VAL:HG11	1:B:666:ILE:HD12	1.92	0.51
1:C:704:PHE:O	1:C:707:THR:HG22	2.11	0.51
1:D:61:ARG:HH11	1:D:66:ASN:HA	1.76	0.51
1:A:443:PHE:CZ	1:A:470:PRO:HD2	2.45	0.51
2:C:760:HDD:HMB1	2:C:760:HDD:HBB1	1.93	0.51
1:B:583:LYS:H	1:B:583:LYS:HZ2	1.55	0.51
1:C:359:LEU:H	1:C:507:HIS:HD2	1.59	0.51
1:D:443:PHE:CZ	1:D:470:PRO:HD2	2.46	0.51
2:B:760:HDD:HBB1	2:B:760:HDD:HMB1	1.92	0.50
1:D:748:ILE:O	1:D:751:ILE:HG22	2.12	0.50
1:A:751:ILE:O	1:A:751:ILE:HD12	2.12	0.50
1:B:708:ILE:HG13	1:B:710:ILE:HD12	1.93	0.50
1:A:682:ASN:HB3	1:A:707:THR:HG21	1.94	0.50
3:A:3472:HOH:O	1:C:27:ASP:HB3	2.10	0.50
1:A:457:PRO:HG2	1:C:37:ARG:HH21	1.77	0.50
1:A:144:LEU:HD11	1:A:370:VAL:HG13	1.94	0.50
1:D:577:PRO:HG2	3:D:4041:HOH:O	2.11	0.50
1:B:578:ASP:HB3	1:B:582:LEU:O	2.11	0.49
1:A:538:TYR:CE2	1:D:31:PRO:HG3	2.47	0.49
1:B:629:HIS:HD2	3:B:1690:HOH:O	1.95	0.49
1:C:629:HIS:HD2	3:C:2098:HOH:O	1.95	0.49
1:A:689:TYR:OH	1:A:710:ILE:HG21	2.13	0.49
1:C:745:ILE:O	1:C:748:ILE:HG12	2.12	0.49
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.96	0.49
1:C:607:LEU:HD22	1:C:611:VAL:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:ILE:HG13	3:D:3967:HOH:O	2.14	0.48
1:D:616:LEU:HD22	1:D:620:LEU:HG	1.95	0.48
1:B:76:GLU:O	1:B:77:ASN:HB2	2.14	0.48
1:A:27:ASP:O	1:A:28:SER:C	2.51	0.48
1:A:603:VAL:HG11	1:A:666:ILE:HD12	1.96	0.48
1:D:61:ARG:NH1	1:D:66:ASN:HA	2.29	0.48
1:C:747:LYS:HE2	3:C:3968:HOH:O	2.13	0.47
1:B:50:THR:HG21	1:C:227:TRP:CZ3	2.49	0.47
1:B:222:LYS:HB3	1:B:223:PRO:HD2	1.96	0.47
1:B:443:PHE:CZ	1:B:470:PRO:HD2	2.48	0.47
2:A:760:HDD:HBC1	2:A:760:HDD:CMC	2.42	0.47
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.96	0.47
1:A:457:PRO:HG2	1:C:37:ARG:NH2	2.29	0.47
1:B:745:ILE:O	1:B:748:ILE:HG12	2.15	0.47
1:D:278:ARG:HH12	1:D:487:GLU:CD	2.17	0.47
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.30	0.47
1:D:144:LEU:HD11	1:D:370:VAL:HG13	1.96	0.47
1:A:745:ILE:N	1:A:746:PRO:HD2	2.30	0.47
1:B:274:ILE:HD12	2:B:760:HDD:HMB1	1.96	0.47
3:A:1180:HOH:O	1:C:52:PRO:HG3	2.15	0.46
1:B:29:LEU:HG	3:B:3519:HOH:O	2.14	0.46
1:A:612:ARG:HE	1:A:669:CYS:HB3	1.79	0.46
3:B:1590:HOH:O	1:D:52:PRO:HG3	2.16	0.46
1:B:359:LEU:H	1:B:507:HIS:CD2	2.31	0.46
1:B:604:ALA:HB2	1:B:662:VAL:HG11	1.97	0.46
1:B:52:PRO:HG2	1:B:55:LEU:HD12	1.97	0.46
1:C:612:ARG:CZ	1:C:612:ARG:HB2	2.45	0.46
1:A:471:ARG:CZ	1:C:27:ASP:HA	2.46	0.45
1:C:211:ALA:CB	1:C:410:GLY:HA3	2.46	0.45
1:A:294:LYS:NZ	3:A:2181:HOH:O	2.49	0.45
2:A:760:HDD:HMC1	2:A:760:HDD:CBC	2.44	0.45
1:D:359:LEU:H	1:D:507:HIS:HD2	1.64	0.45
1:A:750:LYS:HE3	1:A:750:LYS:C	2.36	0.45
1:B:562:LEU:HA	1:C:637:MET:HB2	1.99	0.45
1:B:725:ASP:OD2	1:B:727:SER:N	2.49	0.45
1:A:612:ARG:NH2	3:A:4124:HOH:O	2.49	0.45
1:B:521:ARG:HH21	1:B:745:ILE:HD13	1.78	0.45
1:C:359:LEU:H	1:C:507:HIS:CD2	2.35	0.45
1:D:634:TYR:O	1:D:653:THR:HA	2.17	0.45
1:C:51:ALA:HB1	1:C:52:PRO:HD2	1.98	0.44
1:C:309:LYS:HB3	1:C:660:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:521:ARG:HH11	1:D:521:ARG:HD3	1.56	0.44
1:D:146:ASP:HB2	3:D:3343:HOH:O	2.18	0.44
1:B:468:ASN:HD22	1:D:27:ASP:N	2.14	0.44
2:D:760:HDD:HMB1	2:D:760:HDD:HBB1	1.98	0.44
1:B:411:ARG:HG2	2:B:760:HDD:C2C	2.47	0.44
1:D:598:VAL:HG13	1:D:628:VAL:CG2	2.48	0.44
1:A:38:PRO:HG2	1:A:51:ALA:HB2	1.99	0.44
1:C:73:LYS:HD2	3:C:3629:HOH:O	2.17	0.43
1:C:616:LEU:O	1:C:620:LEU:HG	2.18	0.43
1:D:669:CYS:SG	1:D:670:GLY:N	2.89	0.43
2:C:760:HDD:HMC1	2:C:760:HDD:CBC	2.45	0.43
1:A:418:THR:HG21	2:A:760:HDD:HBD2	2.00	0.43
1:B:459:ASN:H	1:B:459:ASN:HD22	1.67	0.43
1:D:583:LYS:O	1:D:584:LYS:HB3	2.19	0.43
1:B:48:GLN:HB3	1:B:49:PRO:HD2	2.01	0.43
1:D:552:LEU:HD11	1:D:571:LEU:CD2	2.49	0.43
1:A:603:VAL:HG11	1:A:666:ILE:CD1	2.49	0.43
1:B:29:LEU:HD12	1:D:468:ASN:HB2	2.00	0.42
1:D:605:ILE:HD12	1:D:630:ALA:HB1	2.00	0.42
1:A:335:GLU:OE1	1:A:369:ARG:HD3	2.19	0.42
1:A:294:LYS:NZ	3:A:1383:HOH:O	2.51	0.42
1:C:516:THR:HB	1:C:517:PRO:CD	2.49	0.42
1:B:438:CYS:HB2	1:B:439:PRO:HD2	2.00	0.42
1:B:521:ARG:HH21	1:B:521:ARG:HD2	1.60	0.42
1:B:745:ILE:HB	1:B:746:PRO:HD3	2.01	0.42
1:B:669:CYS:SG	1:B:670:GLY:N	2.90	0.42
1:C:155:ASP:HA	1:C:156:PRO:HD2	1.86	0.42
1:D:278:ARG:HH21	1:D:278:ARG:HD2	1.74	0.42
1:B:521:ARG:HH21	1:B:745:ILE:HG21	1.85	0.42
1:B:207:PHE:O	1:B:249:THR:HA	2.20	0.42
1:A:313:ARG:NH1	1:D:309:LYS:HD2	2.35	0.41
1:A:417:ASP:OD2	1:D:118:ASP:OD1	2.38	0.41
1:B:44:PRO:HB3	1:B:629:HIS:CD2	2.56	0.41
1:C:533:LYS:NZ	3:C:3181:HOH:O	2.53	0.41
1:B:252:ASN:HD22	1:B:252:ASN:HA	1.61	0.41
1:A:214:PHE:HB3	1:A:215:PRO:HD3	2.02	0.41
1:A:169:VAL:HB	1:A:181:GLU:OE2	2.20	0.41
1:B:211:ALA:CB	1:B:410:GLY:HA3	2.51	0.41
1:C:411:ARG:HG2	2:C:760:HDD:C2C	2.51	0.41
1:C:750:LYS:HA	1:C:750:LYS:HD3	1.86	0.41
1:D:703:LYS:HE2	3:D:3690:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:GLN:HG2	1:B:156:PRO:O	2.20	0.41
1:C:516:THR:HB	1:C:517:PRO:HD2	2.03	0.41
1:C:37:ARG:NH1	3:C:2821:HOH:O	2.54	0.41
1:C:201:ASN:CG	2:C:760:HDD:HMB2	2.41	0.41
1:A:222:LYS:HB3	1:A:223:PRO:HD2	2.02	0.41
1:B:36:HIS:H	1:B:36:HIS:HD1	1.67	0.41
1:B:37:ARG:HA	1:B:38:PRO:HD3	1.88	0.41
1:B:97:ALA:O	1:B:101:GLY:HA3	2.20	0.41
1:C:100:ARG:HH11	1:C:100:ARG:HD3	1.78	0.41
1:C:751:ILE:HD12	3:C:3317:HOH:O	2.20	0.41
1:D:97:ALA:O	1:D:101:GLY:HA3	2.21	0.41
1:D:169:VAL:HB	1:D:181:GLU:OE2	2.21	0.41
1:D:693:LYS:HA	1:D:694:PRO:HD3	1.86	0.41
1:A:37:ARG:HA	1:A:38:PRO:HD3	1.89	0.41
1:A:596:GLY:HA3	1:A:737:ALA:O	2.21	0.41
1:C:488:ARG:HE	1:C:488:ARG:HB2	1.59	0.40
1:B:37:ARG:NH1	1:D:466:ASN:OD1	2.54	0.40
1:B:116:HIS:CD2	1:D:426:PRO:HB2	2.57	0.40
1:B:235:ALA:HB1	1:B:533:LYS:HD3	2.03	0.40
1:B:331:PHE:HA	1:B:332:PRO:HD3	1.89	0.40
1:A:708:ILE:O	1:A:709:LYS:C	2.59	0.40
1:B:211:ALA:HB3	1:B:410:GLY:HA3	2.02	0.40
1:C:32:GLU:HA	1:C:32:GLU:OE1	2.21	0.40
1:D:148:THR:HB	1:D:279:LEU:HB3	2.03	0.40
1:B:73:LYS:HD3	1:D:441:HIS:CD2	2.56	0.40
1:D:552:LEU:HD22	1:D:552:LEU:HA	1.85	0.40
1:C:335:GLU:OE2	1:C:369:ARG:NH2	2.55	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)
3:A:1050:HOH:O	3:B:3904:HOH:O[2_747]	1.45	0.75

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%)	699 (96%)	22 (3%)	4 (1%)	25	12
1	B	725/753 (96%)	699 (96%)	22 (3%)	4 (1%)	25	12
1	C	725/753 (96%)	703 (97%)	21 (3%)	1 (0%)	51	37
1	D	725/753 (96%)	700 (97%)	21 (3%)	4 (1%)	25	12
All	All	2900/3012 (96%)	2801 (97%)	86 (3%)	13 (0%)	34	21

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	709	LYS
1	B	28	SER
1	D	28	SER
1	D	750	LYS
1	D	751	ILE
1	B	725	ASP
1	A	75	SER
1	A	711	ALA
1	C	75	SER
1	B	75	SER
1	B	584	LYS
1	D	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%)	595 (97%)	17 (3%)	43	29
1	B	612/636 (96%)	584 (95%)	28 (5%)	27	12
1	C	612/636 (96%)	579 (95%)	33 (5%)	22	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	612/636 (96%)	582 (95%)	30 (5%)	25	10
All	All	2448/2544 (96%)	2340 (96%)	108 (4%)	28	13

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	185	PHE
1	A	191	THR
1	A	205	ILE
1	A	227	TRP
1	A	237	ASP
1	A	252	ASN
1	A	375	LEU
1	A	415	TYR
1	A	432	PRO
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	593	ILE
1	A	709	LYS
1	A	712	ASP
1	A	750	LYS
1	B	27	ASP
1	B	28	SER
1	B	37	ARG
1	B	181	GLU
1	B	185	PHE
1	B	191	THR
1	B	198	LEU
1	B	205	ILE
1	B	227	TRP
1	B	237	ASP
1	B	252	ASN
1	B	263	PRO
1	B	321	GLU
1	B	375	LEU
1	B	415	TYR
1	B	440	TYR
1	B	459	ASN
1	B	552	LEU
1	B	562	LEU

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Mol	Chain	Res	Type
1	B	565	GLU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	595	ASP
1	B	612	ARG
1	B	633	LEU
1	B	749	ASP
1	B	751	ILE
1	C	37	ARG
1	C	61	ARG
1	C	159	ILE
1	C	181	GLU
1	C	185	PHE
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	415	TYR
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	568	ASP
1	C	571	LEU
1	C	575	PRO
1	C	584	LYS
1	C	606	LEU
1	C	612	ARG
1	C	616	LEU
1	C	633	LEU
1	C	648	LEU
1	C	660	LEU
1	C	685	LEU
1	C	709	LYS
1	C	725	ASP
1	C	733	LEU
1	C	750	LYS

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Mol	Chain	Res	Type
1	D	28	SER
1	D	41	GLU
1	D	48	GLN
1	D	73	LYS
1	D	181	GLU
1	D	185	PHE
1	D	191	THR
1	D	205	ILE
1	D	227	TRP
1	D	237	ASP
1	D	252	ASN
1	D	340	LEU
1	D	344	GLU
1	D	375	LEU
1	D	415	TYR
1	D	440	TYR
1	D	459	ASN
1	D	490	GLU
1	D	552	LEU
1	D	554	LEU
1	D	582	LEU
1	D	598	VAL
1	D	616	LEU
1	D	633	LEU
1	D	648	LEU
1	D	713	GLN
1	D	747	LYS
1	D	749	ASP
1	D	750	LYS
1	D	751	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	252	ASN
1	A	459	ASN
1	A	515	GLN
1	A	713	GLN
1	B	157	ASN
1	B	252	ASN
1	B	459	ASN

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Mol	Chain	Res	Type
1	B	507	HIS
1	B	629	HIS
1	C	252	ASN
1	C	459	ASN
1	C	507	HIS
1	C	556	GLN
1	C	629	HIS
1	C	671	ASN
1	D	48	GLN
1	D	252	ASN
1	D	449	HIS
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	D	760	1,3	41,52,52	3.50	16 (39%)	31,89,89	4.84	22 (70%)
2	HDD	B	760	1,3	41,52,52	3.24	18 (43%)	31,89,89	5.12	23 (74%)
2	HDD	C	760	1,3	41,52,52	3.45	18 (43%)	31,89,89	4.54	22 (70%)
2	HDD	A	760	1,3	41,52,52	3.44	19 (46%)	31,89,89	4.57	21 (67%)

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

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

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	760	HDD	CMD-C2D	11.39	1.69	1.53
2	B	760	HDD	C3D-C2D	-11.06	1.27	1.55
2	C	760	HDD	C3D-C2D	-10.95	1.28	1.55
2	A	760	HDD	C3D-C2D	-10.55	1.29	1.55
2	D	760	HDD	C3D-C2D	-10.53	1.29	1.55
2	C	760	HDD	CAD-C3D	-10.23	1.35	1.53
2	A	760	HDD	CAD-C3D	10.04	1.71	1.53
2	B	760	HDD	O1D-C3D	7.89	1.59	1.46
2	C	760	HDD	O1D-C3D	7.54	1.59	1.46
2	A	760	HDD	O1D-C3D	7.17	1.58	1.46
2	D	760	HDD	O1D-C3D	6.88	1.57	1.46
2	B	760	HDD	CMD-C2D	6.56	1.62	1.53
2	A	760	HDD	OND-C2D	5.71	1.53	1.42
2	C	760	HDD	FE-ND	5.49	2.17	1.95
2	D	760	HDD	FE-ND	5.38	2.16	1.95
2	D	760	HDD	OND-C2D	5.36	1.53	1.42
2	A	760	HDD	FE-ND	5.31	2.16	1.95
2	C	760	HDD	CHA-C4D	5.22	1.44	1.36
2	D	760	HDD	CHA-C4D	5.19	1.44	1.36
2	A	760	HDD	CHA-C4D	5.00	1.44	1.36
2	B	760	HDD	OND-C2D	4.81	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	760	HDD	CHA-C4D	4.70	1.43	1.36
2	B	760	HDD	C3C-C2C	-4.42	1.34	1.40
2	C	760	HDD	OND-C2D	4.27	1.51	1.42
2	A	760	HDD	C3C-C2C	-4.27	1.34	1.40
2	D	760	HDD	C3C-C2C	-4.21	1.34	1.40
2	B	760	HDD	FE-ND	3.96	2.11	1.95
2	C	760	HDD	C3B-CAB	3.82	1.55	1.47
2	D	760	HDD	C3B-C2B	-3.64	1.35	1.40
2	B	760	HDD	CAD-C3D	3.57	1.60	1.53
2	C	760	HDD	C3C-C2C	-3.55	1.35	1.40
2	B	760	HDD	C3B-C2B	-3.50	1.35	1.40
2	D	760	HDD	O1D-CGD	-3.47	1.30	1.35
2	C	760	HDD	C3B-C2B	-3.29	1.35	1.40
2	A	760	HDD	C3C-CAC	3.28	1.54	1.47
2	B	760	HDD	O1D-CGD	-3.16	1.30	1.35
2	A	760	HDD	C3B-C2B	-3.14	1.36	1.40
2	D	760	HDD	C3B-CAB	3.07	1.54	1.47
2	B	760	HDD	C3B-CAB	3.03	1.54	1.47
2	B	760	HDD	C3C-CAC	2.93	1.53	1.47
2	C	760	HDD	CBA-CGA	2.84	1.57	1.50
2	C	760	HDD	C2B-C1B	2.84	1.49	1.42
2	D	760	HDD	C3C-CAC	2.81	1.53	1.47
2	D	760	HDD	C2B-C1B	2.80	1.48	1.42
2	C	760	HDD	CMC-C2C	2.80	1.57	1.51
2	C	760	HDD	CMD-C2D	2.80	1.57	1.53
2	C	760	HDD	C4A-NA	2.79	1.41	1.36
2	A	760	HDD	CBA-CGA	2.76	1.57	1.50
2	B	760	HDD	CBA-CGA	2.70	1.56	1.50
2	A	760	HDD	C4A-NA	2.67	1.41	1.36
2	A	760	HDD	C3B-CAB	2.67	1.53	1.47
2	A	760	HDD	O1D-CGD	-2.65	1.31	1.35
2	D	760	HDD	C4A-NA	2.62	1.41	1.36
2	A	760	HDD	C2B-C1B	2.59	1.48	1.42
2	B	760	HDD	C2B-C1B	2.59	1.48	1.42
2	D	760	HDD	CMC-C2C	2.58	1.57	1.51
2	C	760	HDD	C1C-NC	2.57	1.41	1.36
2	A	760	HDD	CMC-C2C	2.56	1.57	1.51
2	C	760	HDD	C3C-CAC	2.53	1.53	1.47
2	B	760	HDD	C4A-NA	2.49	1.41	1.36
2	D	760	HDD	CBA-CGA	2.43	1.56	1.50
2	A	760	HDD	O2A-CGA	-2.41	1.22	1.30
2	B	760	HDD	CMC-C2C	2.40	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	760	HDD	FE-NB	2.39	2.16	1.96
2	C	760	HDD	O1D-CGD	-2.37	1.31	1.35
2	A	760	HDD	C1C-NC	2.34	1.41	1.36
2	B	760	HDD	C1D-ND	2.18	1.41	1.37
2	B	760	HDD	CAA-C2A	2.14	1.55	1.52
2	D	760	HDD	FE-NB	2.14	2.14	1.96
2	A	760	HDD	CAA-C2A	2.11	1.55	1.52
2	C	760	HDD	FE-NB	2.05	2.13	1.96

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	760	HDD	OND-C2D-CMD	-13.27	85.17	109.59
2	B	760	HDD	C2B-C3B-C4B	12.86	115.88	106.90
2	D	760	HDD	C2B-C3B-C4B	12.18	115.40	106.90
2	A	760	HDD	C2B-C3B-C4B	11.88	115.20	106.90
2	D	760	HDD	OND-C2D-CMD	-11.69	88.06	109.59
2	C	760	HDD	C2B-C3B-C4B	11.25	114.75	106.90
2	C	760	HDD	CHD-C1D-ND	9.68	138.38	124.20
2	B	760	HDD	CHD-C1D-ND	9.62	138.31	124.20
2	A	760	HDD	CHD-C1D-ND	9.00	137.39	124.20
2	A	760	HDD	O1D-CGD-CBD	-8.28	101.83	110.19
2	C	760	HDD	OND-C2D-CMD	-7.87	95.10	109.59
2	D	760	HDD	CHD-C1D-ND	7.47	135.16	124.20
2	D	760	HDD	O1D-CGD-O2D	7.47	127.47	120.80
2	B	760	HDD	C4C-CHD-C1D	-7.06	116.14	130.12
2	B	760	HDD	C3B-C4B-NB	-7.03	97.68	110.94
2	C	760	HDD	C4C-CHD-C1D	-6.92	116.42	130.12
2	A	760	HDD	C4C-CHD-C1D	-6.87	116.51	130.12
2	D	760	HDD	O1D-C3D-CAD	-6.84	90.15	103.01
2	D	760	HDD	C4C-CHD-C1D	-6.72	116.80	130.12
2	C	760	HDD	O1D-CGD-CBD	-6.65	103.48	110.19
2	D	760	HDD	O1D-CGD-CBD	-6.27	103.86	110.19
2	D	760	HDD	C3B-C4B-NB	-6.19	99.26	110.94
2	C	760	HDD	C3B-C4B-NB	-6.10	99.42	110.94
2	A	760	HDD	C3B-C4B-NB	-6.08	99.47	110.94
2	B	760	HDD	O1D-C3D-CAD	-5.96	91.81	103.01
2	C	760	HDD	C4A-C3A-C2A	-5.75	102.99	107.00
2	A	760	HDD	C3C-C4C-NC	-5.56	102.02	109.21
2	C	760	HDD	CHA-C4D-ND	-5.48	116.17	124.20
2	A	760	HDD	CHA-C4D-ND	-5.28	116.46	124.20
2	B	760	HDD	C4A-C3A-C2A	-5.12	103.44	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	760	HDD	CHA-C4D-ND	-4.95	116.95	124.20
2	A	760	HDD	O2A-CGA-O1A	4.87	135.43	123.30
2	B	760	HDD	C2D-C1D-CHD	-4.84	116.28	124.28
2	A	760	HDD	CMA-C3A-C4A	-4.77	121.13	128.46
2	A	760	HDD	O1D-C3D-CAD	-4.77	94.05	103.01
2	D	760	HDD	C3C-C4C-NC	-4.61	103.25	109.21
2	D	760	HDD	CHA-C4D-ND	-4.54	117.55	124.20
2	A	760	HDD	C4A-C3A-C2A	-4.48	103.88	107.00
2	D	760	HDD	CMD-C2D-C1D	4.25	120.19	112.63
2	C	760	HDD	O2A-CGA-O1A	4.21	133.79	123.30
2	B	760	HDD	O1D-CGD-O2D	4.21	124.56	120.80
2	A	760	HDD	OND-C2D-CMD	-4.18	101.89	109.59
2	A	760	HDD	CMA-C3A-C2A	4.14	132.75	124.94
2	B	760	HDD	O1D-CGD-CBD	-4.12	106.03	110.19
2	A	760	HDD	O1D-CGD-O2D	3.99	124.36	120.80
2	C	760	HDD	CMA-C3A-C2A	3.88	132.26	124.94
2	B	760	HDD	CMC-C2C-C1C	-3.85	122.55	128.46
2	D	760	HDD	O2A-CGA-O1A	3.84	132.88	123.30
2	B	760	HDD	C3C-C4C-NC	-3.81	104.28	109.21
2	D	760	HDD	O1A-CGA-CBA	-3.69	111.23	123.08
2	C	760	HDD	CAA-CBA-CGA	-3.66	103.50	113.76
2	C	760	HDD	C2D-C1D-CHD	-3.65	118.25	124.28
2	C	760	HDD	O1D-C3D-C4D	-3.64	100.86	108.25
2	A	760	HDD	O1A-CGA-CBA	-3.63	111.42	123.08
2	C	760	HDD	O1D-C3D-CAD	-3.56	96.32	103.01
2	A	760	HDD	C3D-C4D-CHA	3.52	134.80	124.34
2	A	760	HDD	CAA-CBA-CGA	-3.51	103.93	113.76
2	C	760	HDD	O1D-CGD-O2D	3.50	123.92	120.80
2	B	760	HDD	CMA-C3A-C4A	-3.49	123.09	128.46
2	C	760	HDD	C3D-C4D-CHA	3.48	134.68	124.34
2	C	760	HDD	C3C-C4C-NC	-3.48	104.71	109.21
2	B	760	HDD	CMA-C3A-C2A	3.43	131.40	124.94
2	C	760	HDD	O1A-CGA-CBA	-3.29	112.52	123.08
2	B	760	HDD	CMB-C2B-C3B	3.22	130.70	124.68
2	B	760	HDD	O1A-CGA-CBA	-3.21	112.77	123.08
2	B	760	HDD	O2A-CGA-O1A	3.19	131.25	123.30
2	B	760	HDD	O1D-C3D-C4D	-3.15	101.84	108.25
2	D	760	HDD	C4A-C3A-C2A	-3.13	104.82	107.00
2	A	760	HDD	C2D-C1D-CHD	-3.11	119.15	124.28
2	D	760	HDD	CAA-CBA-CGA	-2.87	105.71	113.76
2	A	760	HDD	OND-C2D-C3D	-2.86	103.33	110.45
2	B	760	HDD	CAA-CBA-CGA	-2.86	105.73	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	760	HDD	O1D-C3D-C4D	-2.85	102.47	108.25
2	C	760	HDD	OND-C2D-C3D	-2.80	103.48	110.45
2	A	760	HDD	O1D-C3D-C4D	-2.75	102.67	108.25
2	D	760	HDD	OND-C2D-C3D	-2.74	103.63	110.45
2	B	760	HDD	CMC-C2C-C3C	2.71	129.74	124.68
2	D	760	HDD	C2D-C1D-CHD	-2.67	119.87	124.28
2	B	760	HDD	CMD-C2D-C1D	2.64	117.33	112.63
2	B	760	HDD	C3D-C4D-CHA	2.64	132.19	124.34
2	C	760	HDD	CMA-C3A-C4A	-2.54	124.56	128.46
2	D	760	HDD	CMB-C2B-C3B	2.53	129.42	124.68
2	C	760	HDD	CMB-C2B-C3B	2.51	129.37	124.68
2	D	760	HDD	CBA-CAA-C2A	2.44	116.79	112.62
2	D	760	HDD	C3D-C4D-CHA	2.39	131.42	124.34
2	A	760	HDD	CMB-C2B-C3B	2.36	129.09	124.68
2	D	760	HDD	C1A-CHA-C4D	-2.33	125.50	130.12
2	C	760	HDD	OND-C2D-C1D	-2.18	107.50	111.92

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	760	HDD	CAA-CBA-CGA-O1A
2	D	760	HDD	CAA-CBA-CGA-O2A
2	B	760	HDD	CAA-CBA-CGA-O2A
2	C	760	HDD	CAA-CBA-CGA-O2A
2	A	760	HDD	CAA-CBA-CGA-O1A
2	C	760	HDD	CAA-CBA-CGA-O1A
2	A	760	HDD	CAA-CBA-CGA-O2A
2	D	760	HDD	CAA-CBA-CGA-O1A

There are no ring outliers.

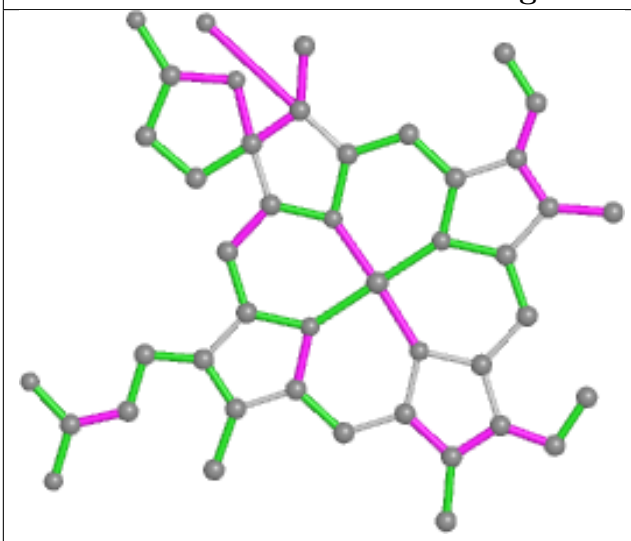
4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	760	HDD	2	0
2	B	760	HDD	4	0
2	C	760	HDD	6	0
2	A	760	HDD	5	0

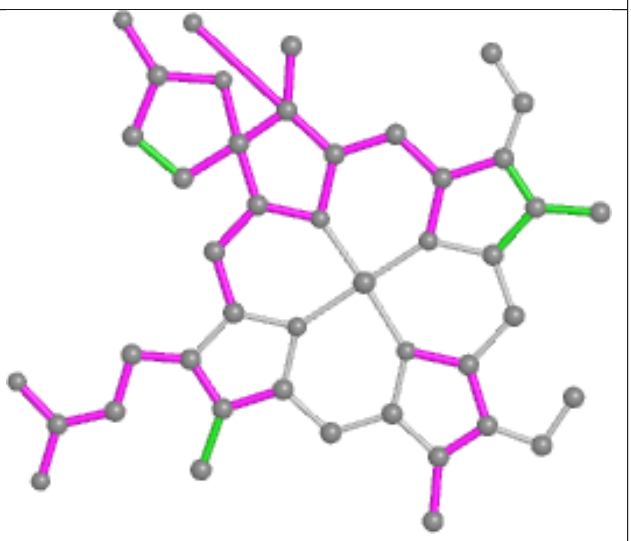
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

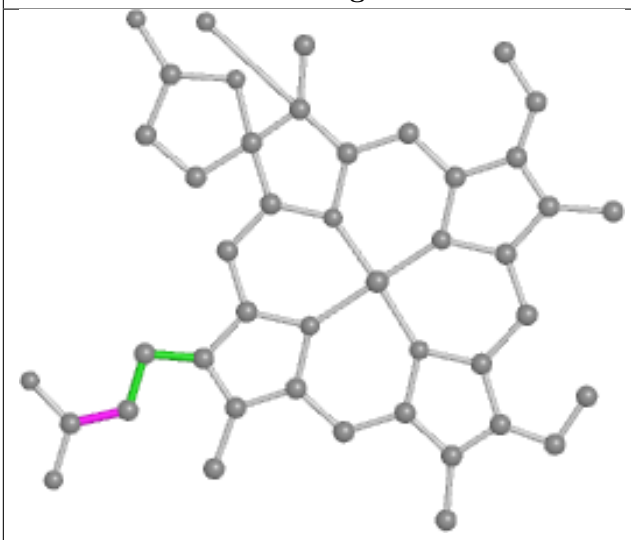
Ligand HDD D 760



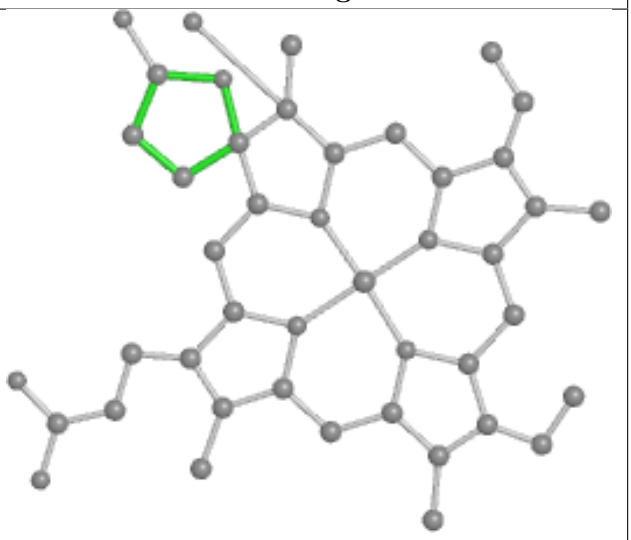
Bond lengths



Bond angles

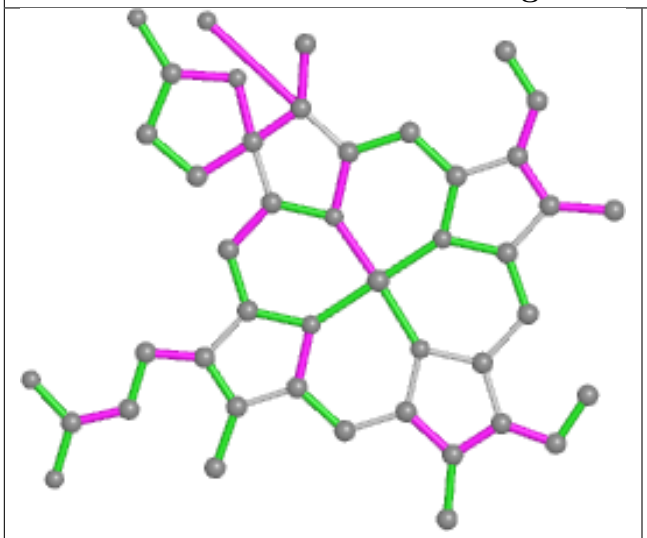


Torsions

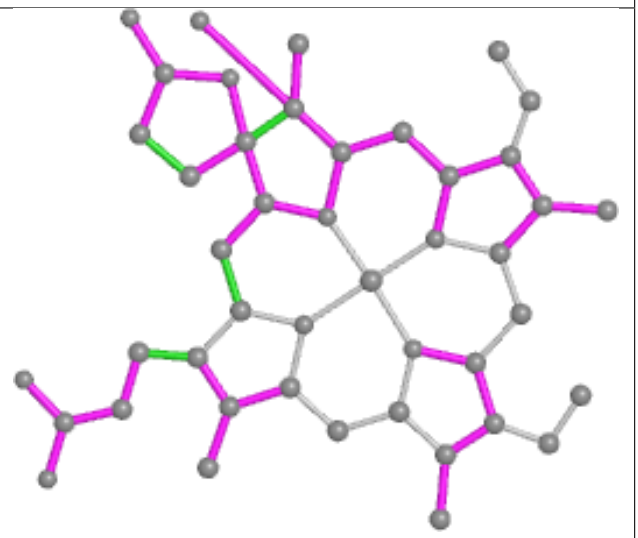


Rings

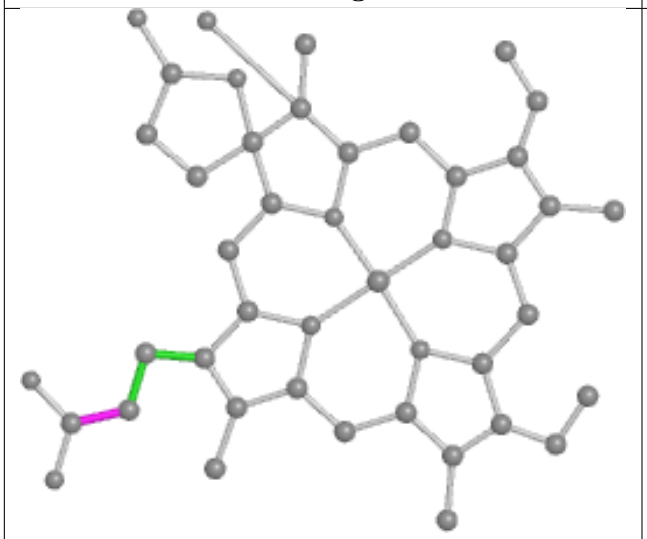
Ligand HDD B 760



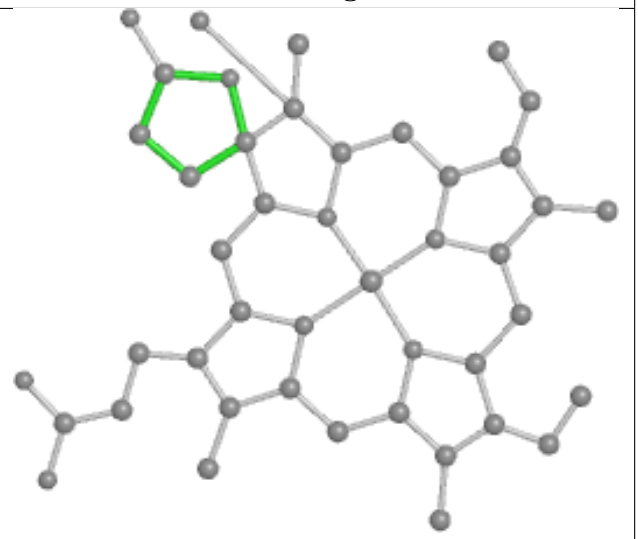
Bond lengths



Bond angles

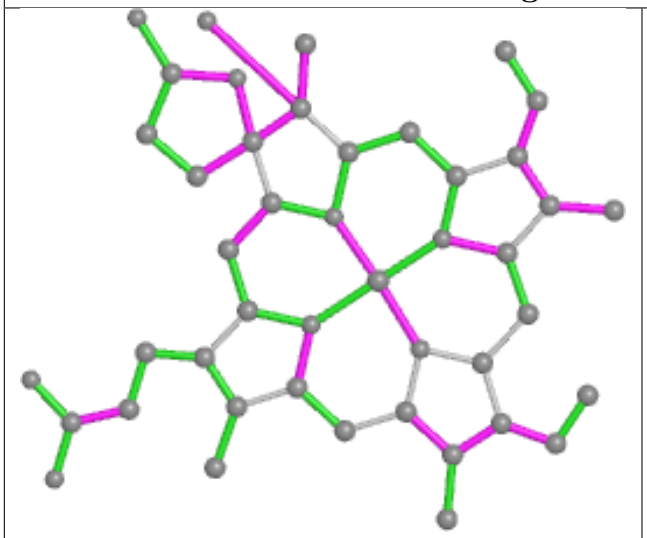


Torsions

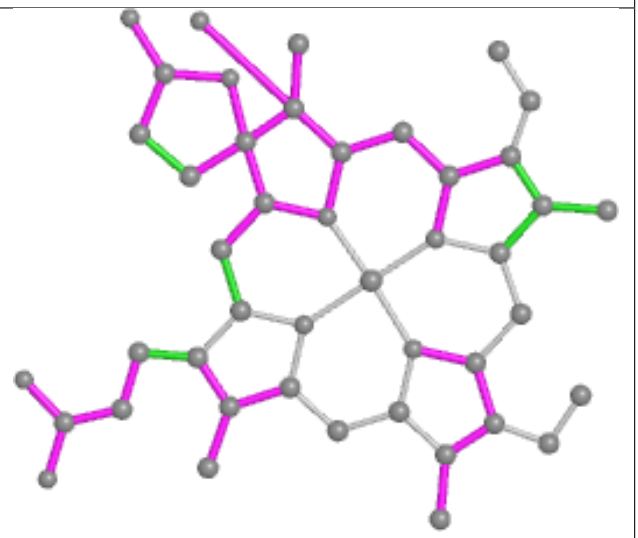


Rings

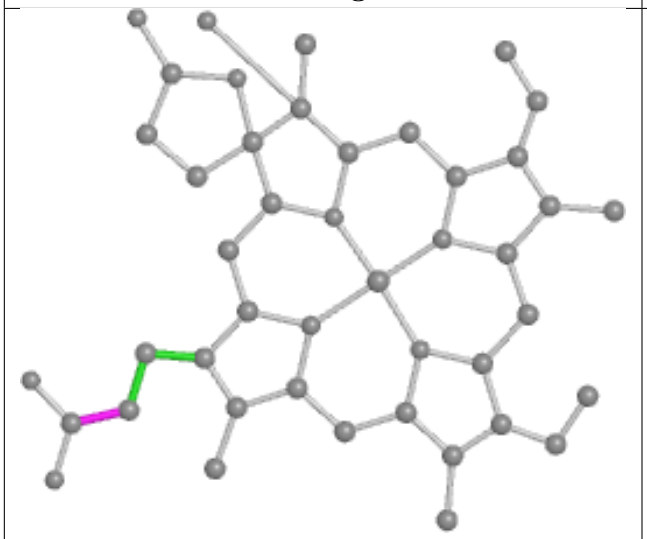
Ligand HDD C 760



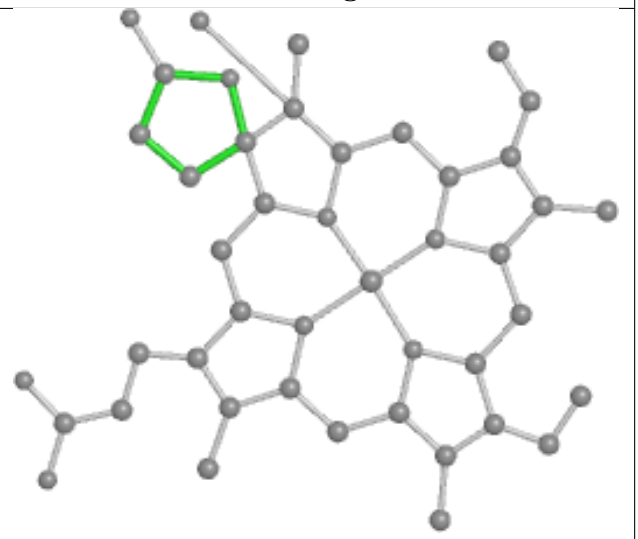
Bond lengths



Bond angles

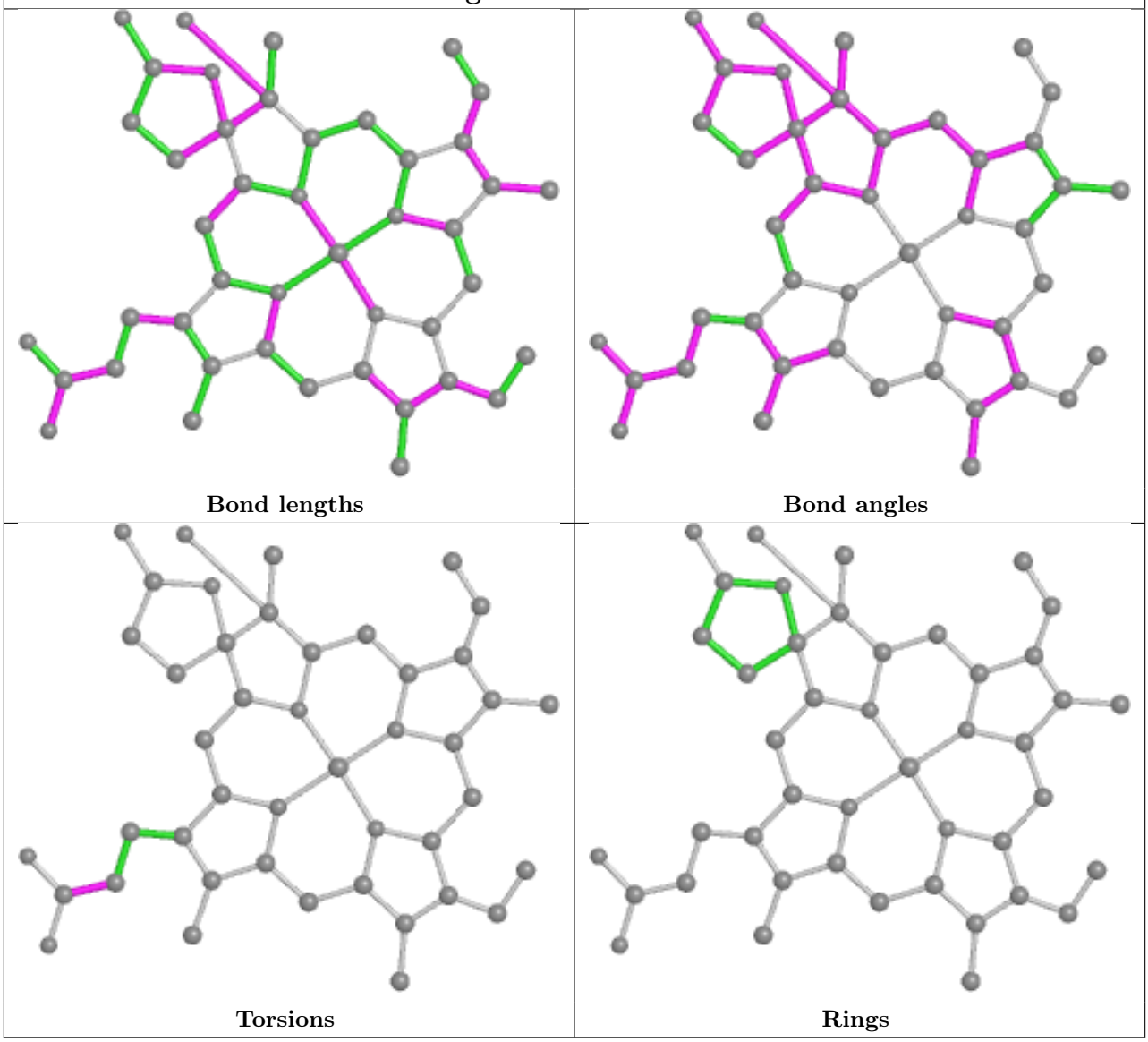


Torsions



Rings

Ligand HDD A 760



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	727/753 (96%)	-0.45	22 (3%)	50	44	7, 13, 30, 55	1 (0%)
1	B	727/753 (96%)	-0.33	23 (3%)	47	42	7, 15, 36, 50	1 (0%)
1	C	727/753 (96%)	-0.35	17 (2%)	60	56	8, 15, 34, 47	1 (0%)
1	D	727/753 (96%)	-0.42	26 (3%)	42	37	7, 14, 32, 48	1 (0%)
All	All	2908/3012 (96%)	-0.39	88 (3%)	50	44	7, 14, 34, 55	4 (0%)

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	ASP	10.5
1	C	28	SER	9.4
1	A	28	SER	9.4
1	C	27	ASP	8.4
1	A	711	ALA	8.2
1	B	28	SER	7.5
1	D	28	SER	7.0
1	D	27	ASP	6.8
1	B	27	ASP	6.2
1	B	32	GLU	5.7
1	D	29	LEU	5.3
1	A	29	LEU	4.8
1	A	32	GLU	4.7
1	D	33	ASP	4.6
1	B	34	GLY	4.5
1	D	35	SER	4.5
1	D	32	GLU	4.3
1	A	710	ILE	4.2
1	D	34	GLY	4.2
1	C	32	GLU	4.2
1	B	726	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	37	ARG	4.2
1	A	712	ASP	4.0
1	D	39	ALA	3.9
1	A	37	ARG	3.9
1	D	47	ALA	3.9
1	C	34	GLY	3.9
1	B	29	LEU	3.8
1	B	30	ALA	3.8
1	A	34	GLY	3.7
1	A	35	SER	3.7
1	B	713	GLN	3.6
1	C	726	GLY	3.6
1	D	750	LYS	3.6
1	B	37	ARG	3.5
1	D	38	PRO	3.5
1	B	33	ASP	3.3
1	C	594	PRO	3.3
1	D	749	ASP	3.2
1	D	41	GLU	3.2
1	C	29	LEU	3.2
1	B	40	ALA	3.2
1	D	31	PRO	3.2
1	B	612	ARG	3.1
1	A	749	ASP	3.1
1	A	713	GLN	3.1
1	B	38	PRO	3.1
1	B	39	ALA	3.0
1	A	709	LYS	2.9
1	D	60	THR	2.9
1	D	36	HIS	2.9
1	D	59	ASP	2.8
1	C	37	ARG	2.8
1	C	750	LYS	2.8
1	C	617	LEU	2.7
1	D	30	ALA	2.7
1	B	710	ILE	2.6
1	B	750	LYS	2.6
1	B	712	ASP	2.6
1	B	677	ASP	2.6
1	A	750	LYS	2.6
1	A	594	PRO	2.6
1	B	749	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	568	ASP	2.5
1	A	33	ASP	2.5
1	D	712	ASP	2.5
1	A	31	PRO	2.5
1	C	583	LYS	2.4
1	A	41	GLU	2.4
1	A	38	PRO	2.4
1	D	48	GLN	2.4
1	D	751	ILE	2.3
1	C	47	ALA	2.3
1	D	711	ALA	2.3
1	C	33	ASP	2.3
1	D	40	ALA	2.2
1	B	572	ASN	2.1
1	C	749	ASP	2.1
1	B	725	ASP	2.1
1	C	568	ASP	2.1
1	C	595	ASP	2.1
1	D	42	PRO	2.1
1	A	39	ALA	2.1
1	C	35	SER	2.1
1	A	30	ALA	2.0
1	D	713	GLN	2.0
1	B	36	HIS	2.0
1	A	716	GLU	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)

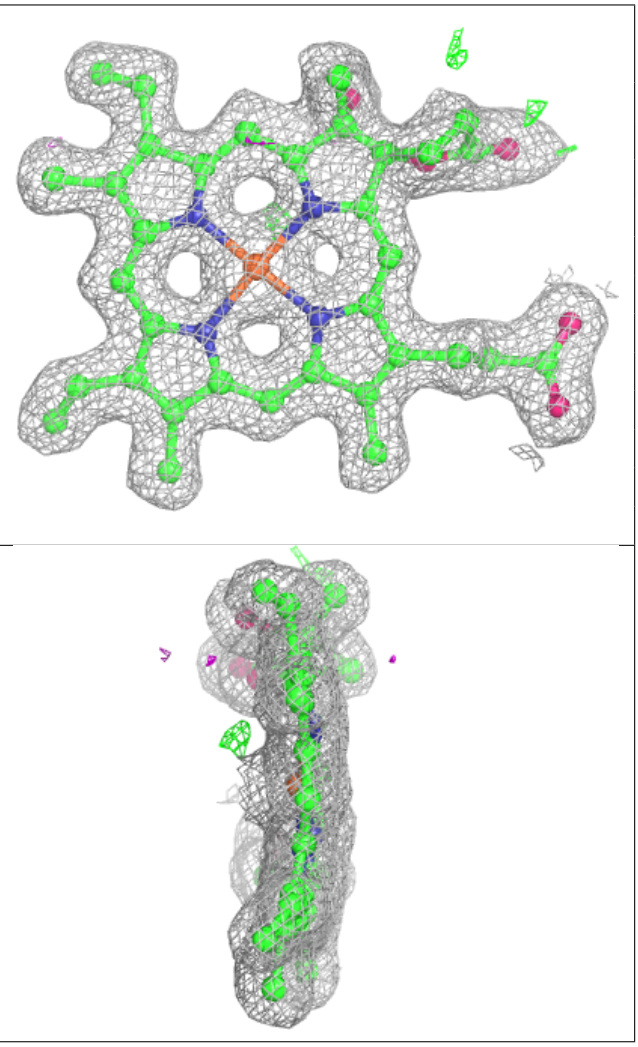
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	760	44/44	0.98	0.06	7,9,14,17	0
2	HDD	B	760	44/44	0.98	0.07	7,10,15,18	0
2	HDD	C	760	44/44	0.98	0.07	8,11,15,16	0
2	HDD	D	760	44/44	0.98	0.07	7,9,15,16	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.

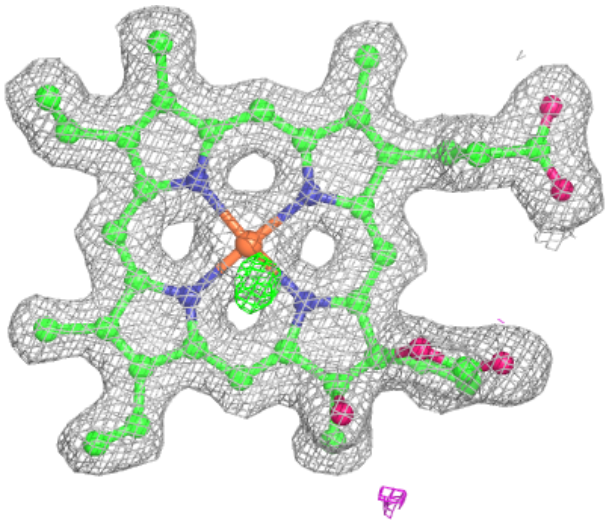
Electron density around HDD A 760:

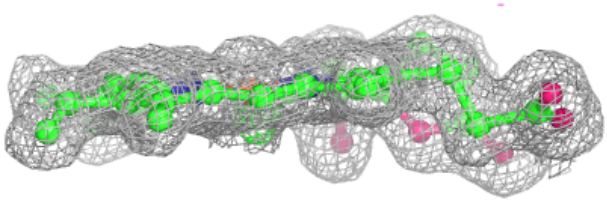
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

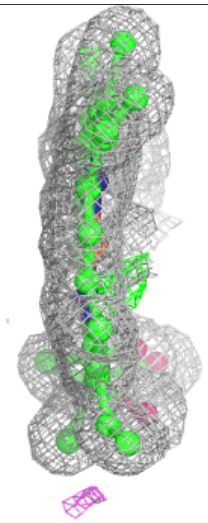


Electron density around HDD B 760:

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

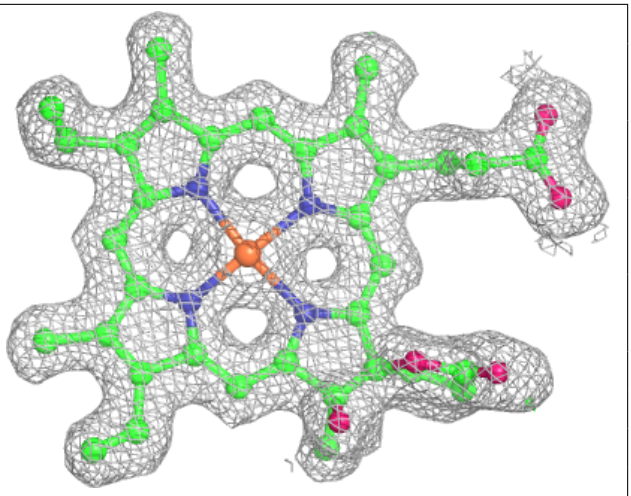


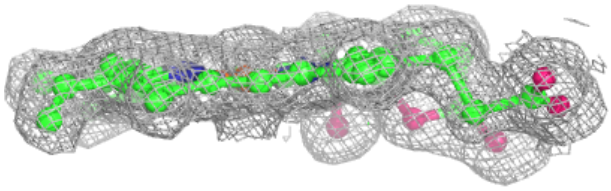


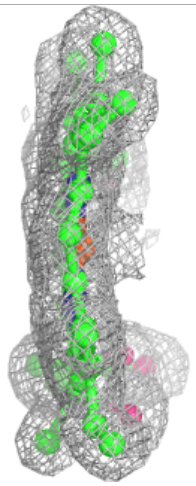


Electron density around HDD C 760:

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

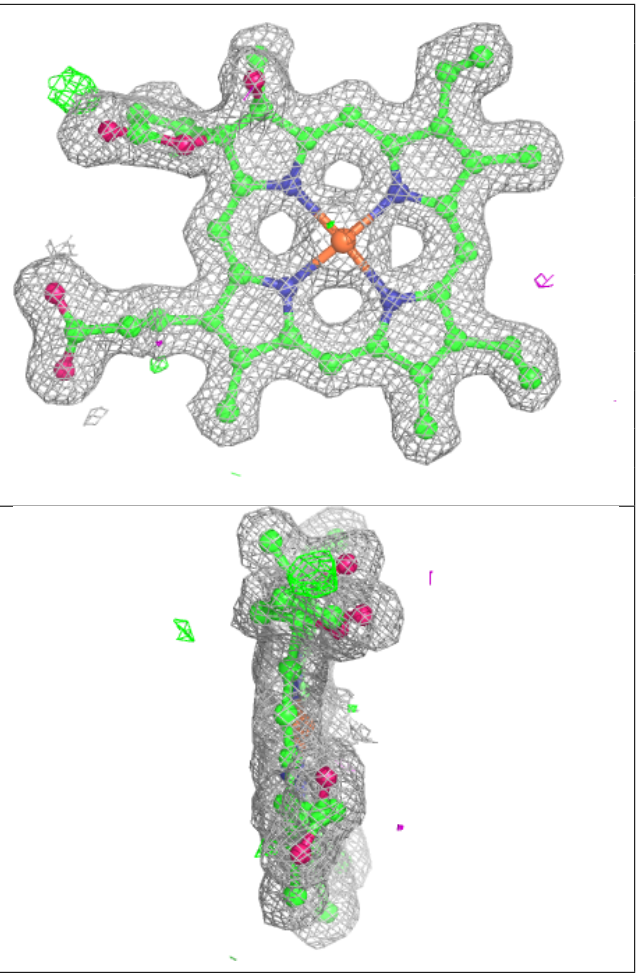






Electron density around HDD D 760:

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.