Full wwPDB X-ray Structure Validation Report (i)

Jun 19, 2024 – 07:12 AM EDT

PDB ID	:	4ENU
Title	:	Structure of the S234D variant of E. coli KatE
Authors	:	Loewen, P.C.; Jha, V.
Deposited on	:	2012-04-13
Resolution	:	1.70 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:

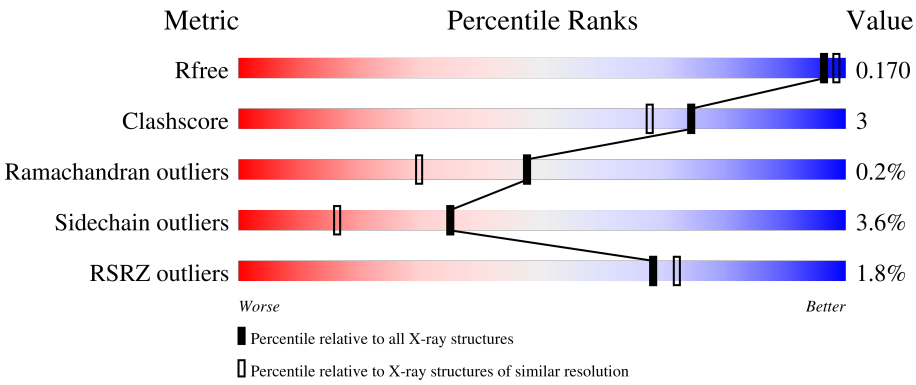
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	% 86% 10% • •
1	B	753	3% 86% 8% • •
1	C	753	3% 84% 10% • •
1	D	753	% 86% 10% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 26286 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.

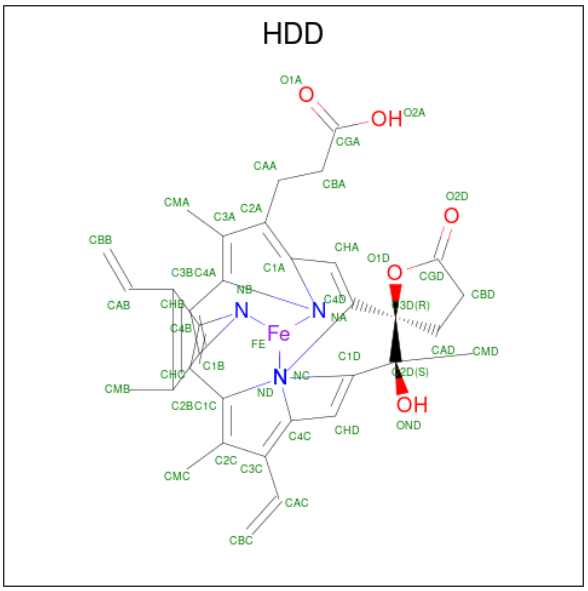
- Molecule 1 is a protein called Catalase HPII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	726	5761	3656	1006	1087	12	0	4	0
1	B	726	5758	3654	1006	1086	12	0	3	0
1	C	726	5773	3665	1008	1088	12	0	6	0
1	D	726	5765	3661	1006	1086	12	0	4	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	234	ASP	SER	ENGINEERED MUTATION	UNP P21179
B	234	ASP	SER	ENGINEERED MUTATION	UNP P21179
C	234	ASP	SER	ENGINEERED MUTATION	UNP P21179
D	234	ASP	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.

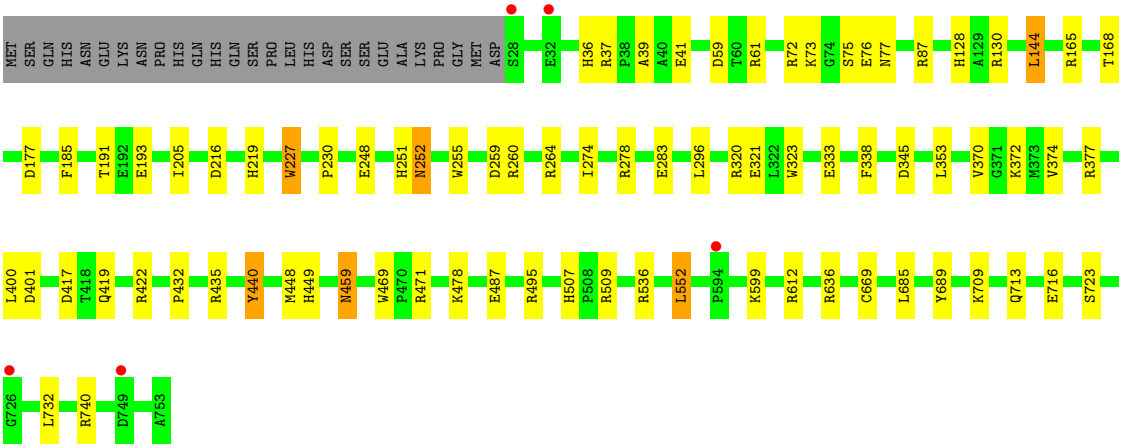
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	802	Total	O	0	0
			802	802		
3	B	708	Total	O	0	0
			708	708		
3	C	727	Total	O	0	0
			727	727		
3	D	816	Total	O	0	0
			816	816		

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.

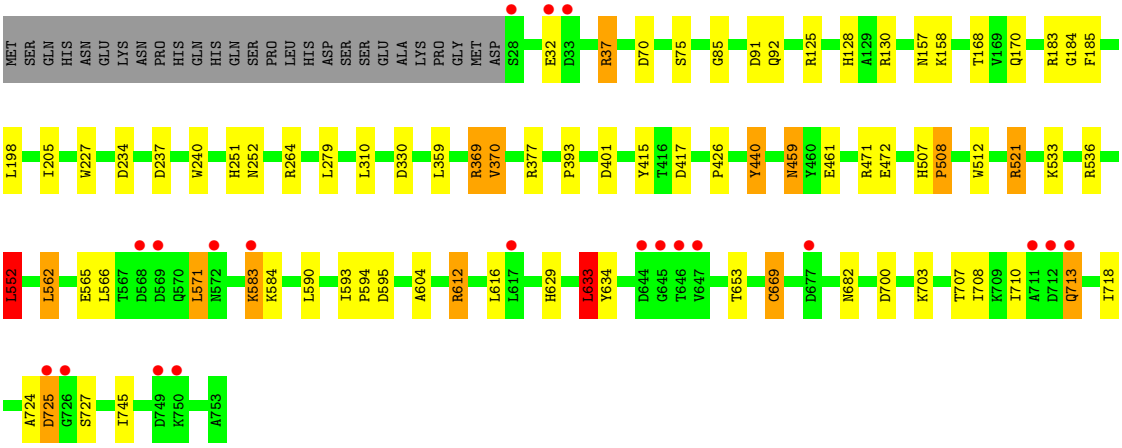
• Molecule 1: Catalase HPII

Chain A:



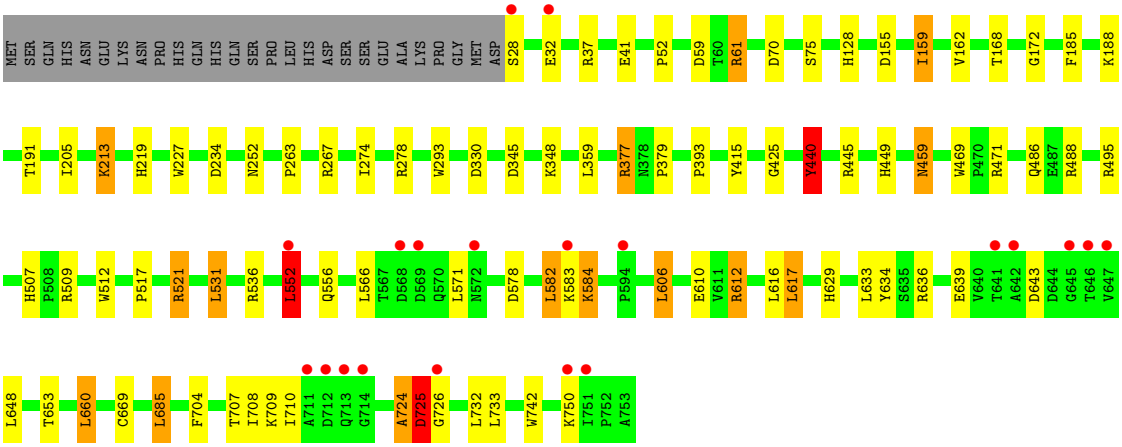
• Molecule 1: Catalase HPII

Chain B:



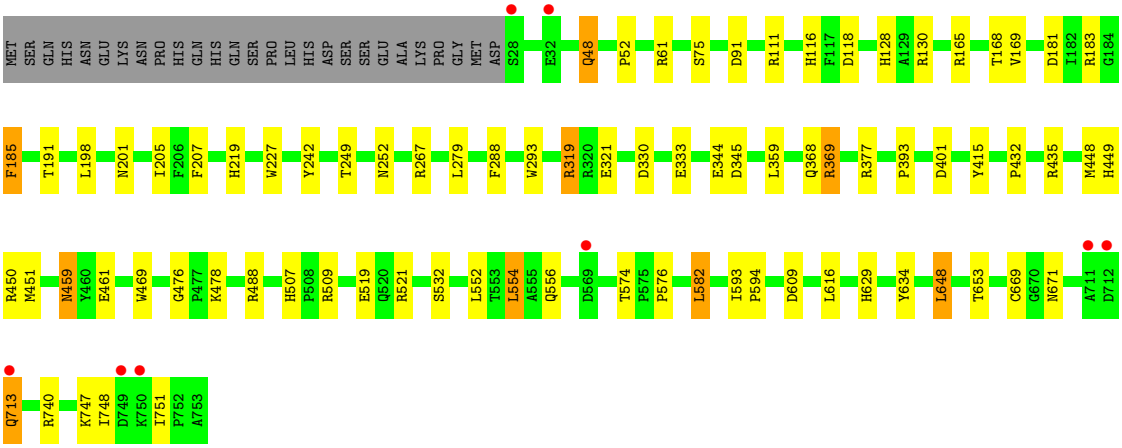
• Molecule 1: Catalase HPII

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	93.56Å 132.61Å 122.81Å 90.00° 109.28° 90.00°	Depositor
Resolution (Å)	32.11 – 1.70 32.11 – 1.70	Depositor EDS
% Data completeness (in resolution range)	91.7 (32.11-1.70) 91.7 (32.11-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	4.10 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.134 , 0.170 0.134 , 0.170	Depositor DCC
R_{free} test set	14327 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	12.2	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	26286	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 3.47% 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: OCS, 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	1.25	9/5920 (0.2%)	1.18	32/8047 (0.4%)
1	B	1.18	6/5914 (0.1%)	1.15	28/8039 (0.3%)
1	C	1.20	11/5937 (0.2%)	1.13	25/8069 (0.3%)
1	D	1.24	9/5925 (0.2%)	1.16	26/8054 (0.3%)
All	All	1.22	35/23696 (0.1%)	1.16	111/32209 (0.3%)

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 (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	440	TYR	CE1-CZ	9.84	1.51	1.38
1	D	333	GLU	CD-OE2	-7.73	1.17	1.25
1	C	469	TRP	CD2-CE2	7.67	1.50	1.41
1	A	321	GLU	CD-OE1	6.50	1.32	1.25
1	B	440	TYR	CE2-CZ	6.31	1.46	1.38
1	C	59	ASP	CB-CG	6.17	1.64	1.51
1	A	255	TRP	CD2-CE2	6.12	1.48	1.41
1	A	469	TRP	CD2-CE2	6.11	1.48	1.41
1	B	512	TRP	CD2-CE2	6.05	1.48	1.41
1	C	495	ARG	CZ-NH2	6.02	1.40	1.33
1	B	157	ASN	CB-CG	5.92	1.64	1.51
1	C	512	TRP	CD2-CE2	5.88	1.48	1.41
1	B	472	GLU	CD-OE2	5.86	1.32	1.25
1	A	323	TRP	CD2-CE2	5.76	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	41	GLU	CD-OE2	-5.68	1.19	1.25
1	C	742	TRP	CD2-CE2	5.65	1.48	1.41
1	A	283	GLU	CD-OE1	5.62	1.31	1.25
1	C	377	ARG	CZ-NH1	5.62	1.40	1.33
1	D	293	TRP	CG-CD1	5.55	1.44	1.36
1	C	425	GLY	N-CA	5.55	1.54	1.46
1	C	41	GLU	CD-OE1	-5.54	1.19	1.25
1	D	450	ARG	CZ-NH1	5.53	1.40	1.33
1	D	377	ARG	CZ-NH2	5.50	1.40	1.33
1	A	193	GLU	CD-OE1	5.46	1.31	1.25
1	D	344	GLU	CD-OE2	5.34	1.31	1.25
1	D	288	PHE	CG-CD2	5.32	1.46	1.38
1	A	320	ARG	CZ-NH2	5.26	1.39	1.33
1	D	469	TRP	CD2-CE2	5.22	1.47	1.41
1	B	240	TRP	CD2-CE2	5.21	1.47	1.41
1	D	321	GLU	CD-OE1	5.21	1.31	1.25
1	C	172	GLY	N-CA	5.18	1.53	1.46
1	C	293	TRP	CD2-CE2	5.16	1.47	1.41
1	A	689	TYR	CG-CD1	5.15	1.45	1.39
1	D	519	GLU	CD-OE1	5.15	1.31	1.25
1	B	85	GLY	N-CA	5.07	1.53	1.46

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	377	ARG	NE-CZ-NH1	-11.59	114.50	120.30
1	C	377	ARG	NE-CZ-NH1	-10.30	115.15	120.30
1	B	521	ARG	NE-CZ-NH1	9.82	125.21	120.30
1	D	521	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	A	552	LEU	CB-CG-CD1	8.54	125.51	111.00
1	D	377	ARG	NH1-CZ-NH2	7.91	128.10	119.40
1	D	377	ARG	CG-CD-NE	-7.85	95.32	111.80
1	A	740	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	D	554	LEU	CB-CG-CD2	7.64	123.98	111.00
1	D	648	LEU	CB-CG-CD2	7.63	123.98	111.00
1	B	552	LEU	CA-CB-CG	7.61	132.81	115.30
1	C	267	ARG	NE-CZ-NH1	-7.59	116.51	120.30
1	C	660	LEU	CB-CG-CD1	7.41	123.60	111.00
1	B	377	ARG	NE-CZ-NH1	-7.14	116.73	120.30
1	A	264	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	D	130	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	C	445	ARG	NE-CZ-NH1	6.91	123.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	521	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	A	377	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	C	531	LEU	CB-CG-CD1	6.75	122.47	111.00
1	C	159[A]	ILE	CB-CG1-CD1	-6.73	95.06	113.90
1	C	159[B]	ILE	CB-CG1-CD1	-6.73	95.06	113.90
1	B	370	VAL	CG1-CB-CG2	6.72	121.65	110.90
1	A	177	ASP	CB-CG-OD1	-6.69	112.28	118.30
1	A	401	ASP	CB-CG-OD2	6.68	124.31	118.30
1	C	37	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	C	685	LEU	CB-CG-CD1	6.56	122.16	111.00
1	D	609	ASP	CB-CG-OD2	6.56	124.21	118.30
1	A	377	ARG	CG-CD-NE	-6.45	98.26	111.80
1	C	536	ARG	NE-CZ-NH1	-6.44	117.08	120.30
1	D	345	ASP	CB-CG-OD2	-6.44	112.51	118.30
1	A	165	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	C	234	ASP	CB-CG-OD1	6.42	124.08	118.30
1	C	509	ARG	NE-CZ-NH2	6.41	123.51	120.30
1	D	435	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	C	59	ASP	CB-CG-OD1	6.34	124.01	118.30
1	A	509	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	D	198	LEU	CB-CG-CD2	-6.29	100.31	111.00
1	A	636	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	B	125	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	130	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	353	LEU	CB-CG-CD1	-6.16	100.53	111.00
1	B	130	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	D	740	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	369	ARG	NE-CZ-NH2	6.07	123.34	120.30
1	A	73	LYS	CD-CE-NZ	-6.03	97.83	111.70
1	A	471	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	B	310	LEU	CB-CG-CD2	-6.00	100.81	111.00
1	D	111	ARG	NE-CZ-NH1	-5.99	117.31	120.30
1	B	562	LEU	CB-CG-CD1	5.98	121.17	111.00
1	B	471	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	C	552	LEU	CB-CG-CD1	5.95	121.11	111.00
1	A	372	LYS	CD-CE-NZ	-5.92	98.08	111.70
1	B	595	ASP	CB-CG-OD1	5.91	123.62	118.30
1	B	369	ARG	NE-CZ-NH1	-5.91	117.35	120.30
1	A	72	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	D	582	LEU	CB-CG-CD1	5.87	120.97	111.00
1	A	435	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	C	471	ARG	NE-CZ-NH2	-5.83	117.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	183	ARG	NE-CZ-NH1	-5.83	117.39	120.30
1	B	401	ASP	CB-CG-OD2	5.83	123.54	118.30
1	D	377	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	B	552	LEU	CB-CG-CD1	5.79	120.84	111.00
1	D	369	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	C	61	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	C	552	LEU	CA-CB-CG	5.72	128.45	115.30
1	D	185	PHE	CB-CG-CD2	-5.72	116.80	120.80
1	A	495	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	D	165	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	D	242	TYR	CB-CG-CD2	-5.61	117.63	121.00
1	B	130	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	B	377	ARG	CG-CD-NE	-5.58	100.08	111.80
1	B	198	LEU	CB-CG-CD2	-5.58	101.52	111.00
1	A	216	ASP	CB-CG-OD1	-5.55	113.30	118.30
1	A	259	ASP	CB-CG-OD1	-5.55	113.30	118.30
1	D	61	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	A	248	GLU	OE1-CD-OE2	-5.53	116.67	123.30
1	B	633	LEU	CB-CG-CD1	5.52	120.39	111.00
1	C	440	TYR	CB-CG-CD2	5.51	124.31	121.00
1	A	345	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	B	70	ASP	CB-CG-OD1	5.47	123.23	118.30
1	A	87	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	A	536	ARG	NE-CZ-NH2	5.45	123.03	120.30
1	D	488	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	536	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	234	ASP	CB-CG-OD1	5.42	123.17	118.30
1	A	61	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	685	LEU	CB-CG-CD1	-5.38	101.86	111.00
1	D	183	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	D	279	LEU	CB-CG-CD2	-5.31	101.98	111.00
1	B	279	LEU	CB-CG-CD1	-5.30	101.99	111.00
1	C	582	LEU	CB-CG-CD1	-5.30	101.99	111.00
1	C	440	TYR	CB-CG-CD1	-5.29	117.83	121.00
1	D	319	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	C	617	LEU	CA-CB-CG	5.26	127.41	115.30
1	A	296	LEU	CB-CG-CD1	-5.26	102.06	111.00
1	C	643	ASP	CB-CG-OD1	5.26	123.04	118.30
1	B	417	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	C	155	ASP	CB-CG-OD1	-5.18	113.63	118.30
1	D	181	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	125	ARG	NE-CZ-NH2	-5.14	117.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	606	LEU	CB-CG-CD1	5.14	119.74	111.00
1	B	590	LEU	CB-CG-CD2	-5.14	102.26	111.00
1	A	509	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	260	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	338	PHE	CB-CG-CD1	-5.12	117.22	120.80
1	B	264	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	D	401	ASP	CB-CG-OD2	5.06	122.86	118.30
1	A	144	LEU	CB-CG-CD1	-5.04	102.42	111.00
1	A	400	LEU	CB-CG-CD1	-5.03	102.45	111.00
1	C	278	ARG	NE-CZ-NH1	-5.03	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts (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	5761	0	5593	28	1
1	B	5758	0	5589	41	1
1	C	5773	0	5612	41	0
1	D	5765	0	5598	37	0
2	A	44	0	31	2	0
2	B	44	0	31	1	0
2	C	44	0	31	4	0
2	D	44	0	31	3	0
3	A	802	0	0	9	1
3	B	708	0	0	8	0
3	C	727	0	0	9	0
3	D	816	0	0	10	1
All	All	26286	0	22516	144	2

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 3.

All (144) 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:449[A]:HIS:CE1	3:A:1701:HOH:O	1.85	1.26
1:B:521:ARG:HD3	3:B:1548:HOH:O	1.37	1.21
1:C:521:ARG:HH11	1:C:521:ARG:CG	1.46	1.19
1:D:451:MET:SD	3:D:1638:HOH:O	2.05	1.14
1:C:521:ARG:HG2	1:C:521:ARG:NH1	1.18	1.14
1:B:533:LYS:HE3	3:C:1500:HOH:O	1.47	1.12
1:D:267:ARG:HG3	3:D:1377:HOH:O	1.61	0.99
1:B:521:ARG:NH2	1:B:745:ILE:HD13	1.80	0.97
1:C:612:ARG:HH11	1:C:612:ARG:HB2	1.33	0.91
1:C:612:ARG:HB2	1:C:612:ARG:NH1	1.89	0.86
1:C:521:ARG:CG	1:C:521:ARG:NH1	2.11	0.83
1:D:368:GLN:OE1	3:D:1565:HOH:O	2.01	0.79
1:D:748:ILE:O	1:D:751:ILE:HG22	1.84	0.77
1:C:636:ARG:NH1	3:C:1516:HOH:O	2.21	0.74
1:C:70:ASP:OD1	3:C:1483:HOH:O	2.04	0.73
1:C:578[A]:ASP:HB2	1:C:582:LEU:O	1.87	0.73
1:B:583:LYS:H	1:B:583:LYS:NZ	1.87	0.72
1:A:716:GLU:OE1	3:A:1646:HOH:O	2.08	0.72
1:A:612:ARG:HH22	1:A:723:SER:HB2	1.53	0.72
1:B:521:ARG:HH22	1:B:745:ILE:HD13	1.54	0.72
1:B:708:ILE:HD12	1:B:710:ILE:HD11	1.72	0.69
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.78	0.66
1:C:486:GLN:OE1	3:C:1542:HOH:O	2.13	0.66
1:A:448:MET:O	1:A:449[B]:HIS:HB2	1.97	0.65
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.80	0.64
1:B:710:ILE:HD13	1:B:718:ILE:HG13	1.80	0.63
1:C:610:GLU:O	1:C:610:GLU:HG3	1.98	0.63
1:A:612:ARG:HG3	3:A:1566:HOH:O	2.00	0.62
1:D:532[A]:SER:OG	3:D:1704:HOH:O	2.15	0.62
2:D:801:HDD:HBC1	2:D:801:HDD:HMC1	1.82	0.60
1:C:552:LEU:HD22	1:C:556:GLN:HG3	1.82	0.60
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.85	0.59
3:B:1140:HOH:O	1:D:449[B]:HIS:HD2	1.86	0.59
1:D:369:ARG:NH1	1:D:369:ARG:HB2	2.17	0.59
1:B:359:LEU:H	1:B:507:HIS:HD2	1.49	0.58
1:B:533:LYS:CE	3:C:1500:HOH:O	2.26	0.57
1:D:359:LEU:H	1:D:507:HIS:HD2	1.54	0.56
1:C:629:HIS:HD2	3:C:1210:HOH:O	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:HIS:CD2	1:A:36:HIS:H	2.24	0.55
1:A:459:ASN:HD22	1:A:459:ASN:H	1.53	0.55
1:D:369:ARG:HB2	1:D:369:ARG:HH11	1.72	0.55
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.89	0.55
1:C:556:GLN:HG2	1:C:566:LEU:HD12	1.87	0.55
1:B:629:HIS:HD2	3:B:1159:HOH:O	1.90	0.54
1:C:724:ALA:O	1:C:725:ASP:HB2	2.07	0.54
1:B:634:TYR:O	1:B:653:THR:HA	2.07	0.54
1:B:583:LYS:H	1:B:583:LYS:HZ2	1.53	0.54
1:C:359:LEU:H	1:C:507:HIS:HD2	1.56	0.54
1:D:629:HIS:HD2	3:D:1258:HOH:O	1.90	0.54
1:D:448:MET:O	1:D:449[A]:HIS:HB2	2.09	0.53
1:A:449[A]:HIS:NE2	3:A:1701:HOH:O	2.13	0.53
3:A:1335:HOH:O	1:C:449[B]:HIS:HE1	1.91	0.53
1:C:440:TYR:HD2	3:C:1372:HOH:O	1.91	0.53
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.91	0.52
1:D:713:GLN:O	1:D:713:GLN:HG2	2.09	0.52
1:C:583:LYS:O	1:C:584:LYS:HB3	2.10	0.51
1:C:612:ARG:HH11	1:C:612:ARG:CB	2.14	0.51
1:B:359:LEU:H	1:B:507:HIS:CD2	2.26	0.51
1:B:37:ARG:HD2	3:B:1523:HOH:O	2.10	0.51
2:C:801:HDD:HMC1	2:C:801:HDD:HBC1	1.92	0.51
1:B:369:ARG:HG2	3:B:1305:HOH:O	2.11	0.50
1:B:583:LYS:O	1:B:584:LYS:HB3	2.12	0.50
1:B:521:ARG:HH22	1:B:745:ILE:CD1	2.24	0.49
1:A:274:ILE:HD12	2:A:801:HDD:HMB1	1.95	0.49
2:D:801:HDD:HMC1	2:D:801:HDD:CBC	2.42	0.49
3:B:1341:HOH:O	1:D:449[A]:HIS:HE1	1.96	0.49
1:C:634:TYR:O	1:C:653:THR:HA	2.13	0.49
1:B:708:ILE:HD12	1:B:710:ILE:CD1	2.42	0.48
1:C:345:ASP:HA	1:C:348:LYS:HG3	1.96	0.48
1:B:604:ALA:HB1	1:B:633:LEU:HD22	1.95	0.48
2:C:801:HDD:HBB1	2:C:801:HDD:HMB1	1.95	0.48
1:A:419:GLN:HE22	1:A:422:ARG:HH11	1.62	0.47
1:D:128:HIS:CE1	1:D:169:VAL:HG22	2.50	0.47
1:A:478:LYS:HG2	3:A:1370:HOH:O	2.14	0.47
1:C:359:LEU:H	1:C:507:HIS:CD2	2.33	0.47
1:C:521:ARG:HH11	1:C:521:ARG:CB	2.20	0.46
1:B:393:PRO:HD2	1:B:415:TYR:CG	2.51	0.46
1:D:593:ILE:HA	1:D:594:PRO:HD2	1.64	0.46
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:583:LYS:H	1:B:583:LYS:HZ3	1.62	0.46
1:D:556:GLN:NE2	3:D:1578:HOH:O	2.49	0.46
1:B:724:ALA:O	1:B:725:ASP:O	2.33	0.46
1:A:612:ARG:HH22	1:A:723:SER:CB	2.24	0.45
1:D:207:PHE:O	1:D:249:THR:HA	2.16	0.45
1:A:144:LEU:HD11	1:A:370:VAL:HG13	1.97	0.45
1:D:128:HIS:HA	1:D:168:THR:O	2.16	0.45
3:A:1047:HOH:O	1:C:52:PRO:HG3	2.17	0.45
1:B:92:GLN:HA	1:C:213:LYS:HD2	1.97	0.45
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.52	0.45
1:B:725:ASP:OD2	1:B:727:SER:N	2.50	0.45
1:C:162:VAL:HA	1:C:188:LYS:O	2.16	0.45
1:D:671:ASN:ND2	3:D:1460:HOH:O	2.48	0.45
1:A:36:HIS:HE1	3:A:1350:HOH:O	2.00	0.45
1:B:128:HIS:HA	1:B:168:THR:O	2.17	0.45
1:D:359:LEU:H	1:D:507:HIS:CD2	2.31	0.45
1:D:593:ILE:HD12	3:D:1664:HOH:O	2.17	0.45
1:A:39:ALA:HB1	1:A:41:GLU:HG2	1.98	0.45
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.32	0.45
1:C:128:HIS:HA	1:C:168:THR:O	2.16	0.45
1:C:578[B]:ASP:OD2	1:C:583:LYS:HG3	2.17	0.45
1:B:669:OCS:OD1	1:B:700:ASP:HB2	2.17	0.45
1:A:448:MET:O	1:A:449[B]:HIS:CB	2.64	0.45
1:D:393:PRO:HD2	1:D:415:TYR:CG	2.52	0.44
1:B:713:GLN:NE2	1:B:713:GLN:H	2.16	0.44
1:A:128:HIS:HA	1:A:168:THR:O	2.18	0.44
1:A:230:PRO:HB3	3:D:1714:HOH:O	2.17	0.44
1:B:459:ASN:H	1:B:459:ASN:HD22	1.66	0.43
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.33	0.43
1:C:724:ALA:O	1:C:725:ASP:CB	2.64	0.43
1:D:634:TYR:O	1:D:653:THR:HA	2.17	0.43
3:B:1090:HOH:O	1:D:52:PRO:HG3	2.18	0.43
1:B:170:GLN:HB2	3:B:1592:HOH:O	2.18	0.43
2:C:801:HDD:HBD2	3:C:1090:HOH:O	2.18	0.43
1:D:476:GLY:HA3	3:D:1009:HOH:O	2.17	0.43
1:A:459:ASN:HD22	1:A:459:ASN:N	2.12	0.43
1:C:28:SER:HA	3:C:1609:HOH:O	2.19	0.43
1:D:459:ASN:HD22	1:D:459:ASN:H	1.67	0.43
1:D:509:ARG:HD2	1:D:576:PRO:HD2	2.01	0.42
1:A:333:GLU:HG2	1:A:374:VAL:HG22	2.01	0.42
1:C:556:GLN:HG2	1:C:566:LEU:CD1	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:GLU:OE1	1:D:91:ASP:OD1	2.37	0.42
1:A:227:TRP:O	1:D:319:ARG:HD3	2.20	0.42
1:A:76:GLU:O	1:A:77:ASN:HB2	2.19	0.42
1:C:725:ASP:HB3	1:C:726:GLY:H	1.73	0.42
2:A:801:HDD:HBC1	2:A:801:HDD:HMC1	2.02	0.42
1:C:610:GLU:O	1:C:610:GLU:CG	2.68	0.42
1:B:91:ASP:OD1	1:D:461:GLU:OE1	2.38	0.41
1:C:704:PHE:O	1:C:707:THR:HG22	2.20	0.41
1:D:48:GLN:HE21	1:D:48:GLN:HB3	1.66	0.41
1:B:552:LEU:HD21	1:B:571:LEU:HD12	2.03	0.41
1:C:274:ILE:HD12	2:C:801:HDD:HMB1	2.03	0.41
1:A:417:ASP:OD2	1:D:118:ASP:OD1	2.38	0.41
1:B:251:HIS:HA	1:B:508:PRO:HG3	2.03	0.41
1:B:426:PRO:HB2	1:D:116:HIS:CD2	2.56	0.41
1:B:593:ILE:HA	1:B:594:PRO:HD2	1.89	0.41
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.36	0.41
1:C:393:PRO:HD2	1:C:415:TYR:CG	2.55	0.41
1:A:252:ASN:HD22	1:A:252:ASN:HA	1.73	0.40
1:B:184:GLY:HA3	2:B:801:HDD:HMA2	2.03	0.40
1:A:251:HIS:CE1	1:A:507:HIS:HB3	2.56	0.40
1:A:599:LYS:HD3	3:A:1391:HOH:O	2.21	0.40
1:C:556:GLN:CG	1:C:566:LEU:HD12	2.51	0.40
1:D:201:ASN:CG	2:D:801:HDD:HMB2	2.41	0.40
1:B:521:ARG:NH2	1:B:745:ILE:CD1	2.68	0.40

All (2) 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:1596:HOH:O	3:D:1512:HOH:O[1_455]	1.99	0.21
1:A:59:ASP:OD1	1:B:369:ARG:NH1[2_545]	2.10	0.10

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	727/753 (96%)	712 (98%)	14 (2%)	1 (0%)	51	33
1	B	726/753 (96%)	706 (97%)	17 (2%)	3 (0%)	34	18
1	C	729/753 (97%)	710 (97%)	17 (2%)	2 (0%)	41	24
1	D	727/753 (96%)	713 (98%)	13 (2%)	1 (0%)	51	33
All	All	2909/3012 (97%)	2841 (98%)	61 (2%)	7 (0%)	47	30

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	725	ASP
1	B	75	SER
1	A	75	SER
1	C	75	SER
1	C	725	ASP
1	B	612	ARG
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	614/635 (97%)	601 (98%)	13 (2%)	53	36
1	B	613/635 (96%)	590 (96%)	23 (4%)	33	14
1	C	616/635 (97%)	580 (94%)	36 (6%)	20	6
1	D	614/635 (97%)	597 (97%)	17 (3%)	43	25
All	All	2457/2540 (97%)	2368 (96%)	89 (4%)	35	16

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG

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Mol	Chain	Res	Type
1	A	185	PHE
1	A	191	THR
1	A	205	ILE
1	A	227	TRP
1	A	252	ASN
1	A	432	PRO
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	709	LYS
1	A	713	GLN
1	A	732	LEU
1	B	32	GLU
1	B	37	ARG
1	B	158	LYS
1	B	185	PHE
1	B	205	ILE
1	B	227	TRP
1	B	237	ASP
1	B	252	ASN
1	B	370	VAL
1	B	440	TYR
1	B	459	ASN
1	B	508	PRO
1	B	552	LEU
1	B	562	LEU
1	B	565	GLU
1	B	566	LEU
1	B	571	LEU
1	B	583	LYS
1	B	612	ARG
1	B	616	LEU
1	B	633	LEU
1	B	703	LYS
1	B	713	GLN
1	C	32	GLU
1	C	61	ARG
1	C	159[A]	ILE
1	C	159[B]	ILE
1	C	185	PHE
1	C	191	THR
1	C	205	ILE

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Mol	Chain	Res	Type
1	C	213	LYS
1	C	227	TRP
1	C	252	ASN
1	C	263	PRO
1	C	377	ARG
1	C	379	PRO
1	C	440	TYR
1	C	459	ASN
1	C	488	ARG
1	C	517	PRO
1	C	521	ARG
1	C	531	LEU
1	C	552	LEU
1	C	571	LEU
1	C	584	LYS
1	C	606	LEU
1	C	612	ARG
1	C	616	LEU
1	C	617	LEU
1	C	633	LEU
1	C	639	GLU
1	C	648	LEU
1	C	660	LEU
1	C	685	LEU
1	C	709	LYS
1	C	725	ASP
1	C	732	LEU
1	C	733	LEU
1	C	750	LYS
1	D	48	GLN
1	D	185	PHE
1	D	191	THR
1	D	205	ILE
1	D	227	TRP
1	D	252	ASN
1	D	432	PRO
1	D	459	ASN
1	D	478	LYS
1	D	552	LEU
1	D	554	LEU
1	D	574	THR
1	D	582	LEU

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Mol	Chain	Res	Type
1	D	616	LEU
1	D	648	LEU
1	D	713	GLN
1	D	747	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) 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	459	ASN
1	B	507	HIS
1	B	629	HIS
1	B	713	GLN
1	C	252	ASN
1	C	419	GLN
1	C	459	ASN
1	C	486	GLN
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	459	ASN
1	D	507	HIS
1	D	546	GLN
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)

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	OCS	C	669	1	6,8,9	1.75	1 (16%)	7,11,13	1.60	1 (14%)
1	OCS	D	669	1	6,8,9	2.34	2 (33%)	7,11,13	1.93	3 (42%)
1	OCS	B	669	1	6,8,9	2.18	1 (16%)	7,11,13	2.34	1 (14%)
1	OCS	A	669	1	6,8,9	2.71	2 (33%)	7,11,13	2.35	2 (28%)

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
1	OCS	C	669	1	-	1/4/7/9	-
1	OCS	D	669	1	-	1/4/7/9	-
1	OCS	B	669	1	-	1/4/7/9	-
1	OCS	A	669	1	-	4/4/7/9	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	669	OCS	OD2-SG	4.97	1.65	1.47
1	B	669	OCS	OD2-SG	4.87	1.65	1.47
1	A	669	OCS	CB-CA	3.90	1.56	1.53
1	D	669	OCS	CB-CA	3.89	1.56	1.53
1	C	669	OCS	OD2-SG	3.82	1.61	1.47
1	D	669	OCS	OD2-SG	3.63	1.60	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	669	OCS	OD1-SG-CB	5.52	115.00	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	669	OCS	OD1-SG-CB	3.87	112.53	106.76
1	A	669	OCS	OD2-SG-CB	3.86	113.44	105.97
1	C	669	OCS	OD2-SG-CB	3.61	112.95	105.97
1	D	669	OCS	OD3-SG-CB	-2.91	102.42	106.76
1	D	669	OCS	OD2-SG-CB	-2.57	101.01	105.97
1	D	669	OCS	OD2-SG-OD1	2.38	117.36	111.40

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	669	OCS	N-CA-CB-SG
1	A	669	OCS	CA-CB-SG-OD2
1	B	669	OCS	N-CA-CB-SG
1	C	669	OCS	N-CA-CB-SG
1	D	669	OCS	N-CA-CB-SG
1	A	669	OCS	CA-CB-SG-OD3
1	A	669	OCS	CA-CB-SG-OD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	669	OCS	1	0

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	C	801	1,3	41,52,52	1.85	9 (21%)	34,89,89	3.90	17 (50%)
2	HDD	B	801	1,3	41,52,52	1.66	7 (17%)	34,89,89	4.72	20 (58%)
2	HDD	A	801	1	41,52,52	1.95	11 (26%)	34,89,89	5.08	16 (47%)
2	HDD	D	801	1	41,52,52	1.97	7 (17%)	34,89,89	4.94	18 (52%)

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

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	HDD	C3B-C4B	6.02	1.50	1.41
2	C	801	HDD	O1D-C3D	5.75	1.55	1.46
2	D	801	HDD	O1D-C3D	5.01	1.54	1.46
2	A	801	HDD	O1D-C3D	5.01	1.54	1.46
2	B	801	HDD	C3B-C4B	4.53	1.48	1.41
2	A	801	HDD	OND-C2D	4.48	1.51	1.42
2	A	801	HDD	CHD-C1D	4.41	1.43	1.35
2	D	801	HDD	CHD-C1D	4.18	1.43	1.35
2	C	801	HDD	C3B-C4B	4.05	1.47	1.41
2	B	801	HDD	C4D-ND	3.76	1.44	1.37
2	A	801	HDD	C3B-C4B	3.74	1.46	1.41
2	C	801	HDD	OND-C2D	3.54	1.49	1.42
2	D	801	HDD	OND-C2D	3.46	1.49	1.42
2	A	801	HDD	O1D-CGD	3.18	1.40	1.35
2	D	801	HDD	C4A-NA	3.11	1.42	1.36
2	B	801	HDD	O1D-C3D	3.10	1.51	1.46
2	A	801	HDD	C2A-C3A	3.00	1.46	1.37
2	D	801	HDD	CMD-C2D	2.88	1.57	1.53
2	B	801	HDD	O1D-CGD	2.82	1.40	1.35
2	A	801	HDD	CAD-C3D	-2.67	1.48	1.53
2	A	801	HDD	C2B-C1B	2.57	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	HDD	C3B-C2B	2.54	1.43	1.40
2	C	801	HDD	C4C-NC	-2.53	1.31	1.36
2	B	801	HDD	CMA-C3A	2.48	1.56	1.51
2	C	801	HDD	CBD-CGD	2.42	1.54	1.50
2	C	801	HDD	C2A-C3A	2.39	1.44	1.37
2	A	801	HDD	C3B-C2B	2.37	1.43	1.40
2	C	801	HDD	O1D-CGD	2.35	1.39	1.35
2	B	801	HDD	C3B-C2B	2.33	1.43	1.40
2	A	801	HDD	O2D-CGD	2.32	1.29	1.22
2	A	801	HDD	CHA-C4D	2.31	1.39	1.35
2	C	801	HDD	CHD-C1D	2.28	1.39	1.35
2	B	801	HDD	O1A-CGA	2.18	1.29	1.22
2	C	801	HDD	C4A-CHB	2.11	1.46	1.41

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	801	HDD	O1D-CGD-O2D	17.43	135.50	120.81
2	A	801	HDD	O1D-CGD-CBD	-15.60	95.94	110.17
2	A	801	HDD	O1D-CGD-O2D	15.09	133.52	120.81
2	B	801	HDD	O1D-CGD-O2D	13.90	132.52	120.81
2	A	801	HDD	C3D-O1D-CGD	13.76	123.97	111.14
2	C	801	HDD	O1D-CGD-O2D	12.43	131.28	120.81
2	D	801	HDD	O1D-CGD-CBD	-12.15	99.09	110.17
2	D	801	HDD	C3D-O1D-CGD	11.88	122.22	111.14
2	B	801	HDD	C3D-O1D-CGD	11.27	121.65	111.14
2	B	801	HDD	O1D-CGD-CBD	-10.91	100.22	110.17
2	B	801	HDD	C4A-C3A-C2A	-9.28	100.54	107.00
2	C	801	HDD	O1D-CGD-CBD	-8.80	102.15	110.17
2	C	801	HDD	C3D-O1D-CGD	7.76	118.38	111.14
2	B	801	HDD	OND-C2D-CMD	-7.75	94.47	109.45
2	C	801	HDD	OND-C2D-CMD	-7.16	95.60	109.45
2	A	801	HDD	O1D-C3D-CAD	-6.58	90.88	103.06
2	D	801	HDD	OND-C2D-CMD	-6.29	97.29	109.45
2	D	801	HDD	C4A-C3A-C2A	-5.18	103.39	107.00
2	A	801	HDD	CAA-CBA-CGA	-4.83	100.82	113.83
2	C	801	HDD	CBD-CAD-C3D	4.83	110.86	103.98
2	B	801	HDD	C1A-CHA-C4D	-4.81	120.87	130.04
2	A	801	HDD	C4C-CHD-C1D	-4.76	120.95	130.04
2	D	801	HDD	CAA-CBA-CGA	-4.75	101.02	113.83
2	D	801	HDD	O1D-C3D-CAD	-4.75	94.28	103.06
2	C	801	HDD	C1A-CHA-C4D	-4.74	121.01	130.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	HDD	CBD-CAD-C3D	4.47	110.36	103.98
2	A	801	HDD	CMB-C2B-C3B	4.46	133.59	124.68
2	D	801	HDD	CMC-C2C-C1C	4.39	134.88	128.46
2	C	801	HDD	C4A-C3A-C2A	-4.34	103.98	107.00
2	C	801	HDD	C4C-CHD-C1D	-4.28	121.87	130.04
2	D	801	HDD	CBD-CAD-C3D	4.12	109.86	103.98
2	A	801	HDD	OND-C2D-CMD	-4.05	101.61	109.45
2	B	801	HDD	CHA-C4D-ND	3.99	129.79	124.28
2	D	801	HDD	CMB-C2B-C3B	3.92	132.52	124.68
2	B	801	HDD	CAD-CBD-CGD	3.76	110.06	104.48
2	B	801	HDD	CMB-C2B-C3B	3.70	132.08	124.68
2	B	801	HDD	CMD-C2D-C1D	3.63	118.83	112.68
2	C	801	HDD	CAA-CBA-CGA	-3.58	104.17	113.83
2	C	801	HDD	C2B-C3B-C4B	-3.48	104.47	106.90
2	B	801	HDD	CBD-CAD-C3D	3.43	108.88	103.98
2	A	801	HDD	C1A-CHA-C4D	-3.40	123.55	130.04
2	D	801	HDD	C4C-CHD-C1D	-3.30	123.74	130.04
2	B	801	HDD	CMA-C3A-C2A	3.07	130.74	124.94
2	B	801	HDD	C3D-C4D-CHA	-3.06	115.26	124.14
2	C	801	HDD	CMB-C2B-C3B	3.02	130.72	124.68
2	C	801	HDD	C3D-C4D-CHA	-2.98	115.50	124.14
2	B	801	HDD	CMC-C2C-C3C	2.97	130.61	124.68
2	A	801	HDD	C4A-C3A-C2A	-2.77	105.07	107.00
2	D	801	HDD	C1A-CHA-C4D	-2.77	124.75	130.04
2	B	801	HDD	CAA-CBA-CGA	-2.75	106.43	113.83
2	D	801	HDD	CMD-C2D-C1D	2.72	117.29	112.68
2	A	801	HDD	C3D-C4D-CHA	-2.72	116.25	124.14
2	D	801	HDD	C3C-C4C-NC	2.66	112.65	109.21
2	A	801	HDD	C2D-C1D-CHD	-2.61	120.21	124.27
2	C	801	HDD	O1D-C3D-CAD	-2.60	98.26	103.06
2	B	801	HDD	C2D-C1D-CHD	-2.59	120.24	124.27
2	B	801	HDD	O1D-C3D-CAD	-2.54	98.36	103.06
2	B	801	HDD	C4C-CHD-C1D	-2.53	125.22	130.04
2	A	801	HDD	CBA-CAA-C2A	-2.51	108.31	112.54
2	D	801	HDD	OND-C2D-C3D	-2.47	104.67	110.46
2	B	801	HDD	C2B-C3B-C4B	-2.47	105.18	106.90
2	C	801	HDD	C2D-C1D-CHD	-2.45	120.46	124.27
2	D	801	HDD	O2A-CGA-CBA	2.45	121.73	114.00
2	A	801	HDD	CMA-C3A-C2A	2.44	129.54	124.94
2	B	801	HDD	CBA-CAA-C2A	-2.37	108.56	112.54
2	C	801	HDD	CMD-C2D-C1D	2.30	116.57	112.68
2	C	801	HDD	CAD-CBD-CGD	2.24	107.80	104.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	HDD	CMA-C3A-C4A	-2.18	125.26	128.46
2	D	801	HDD	CAD-CBD-CGD	2.12	107.62	104.48
2	C	801	HDD	CHA-C4D-ND	2.06	127.12	124.28
2	D	801	HDD	CMD-C2D-C3D	2.02	120.41	115.11

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

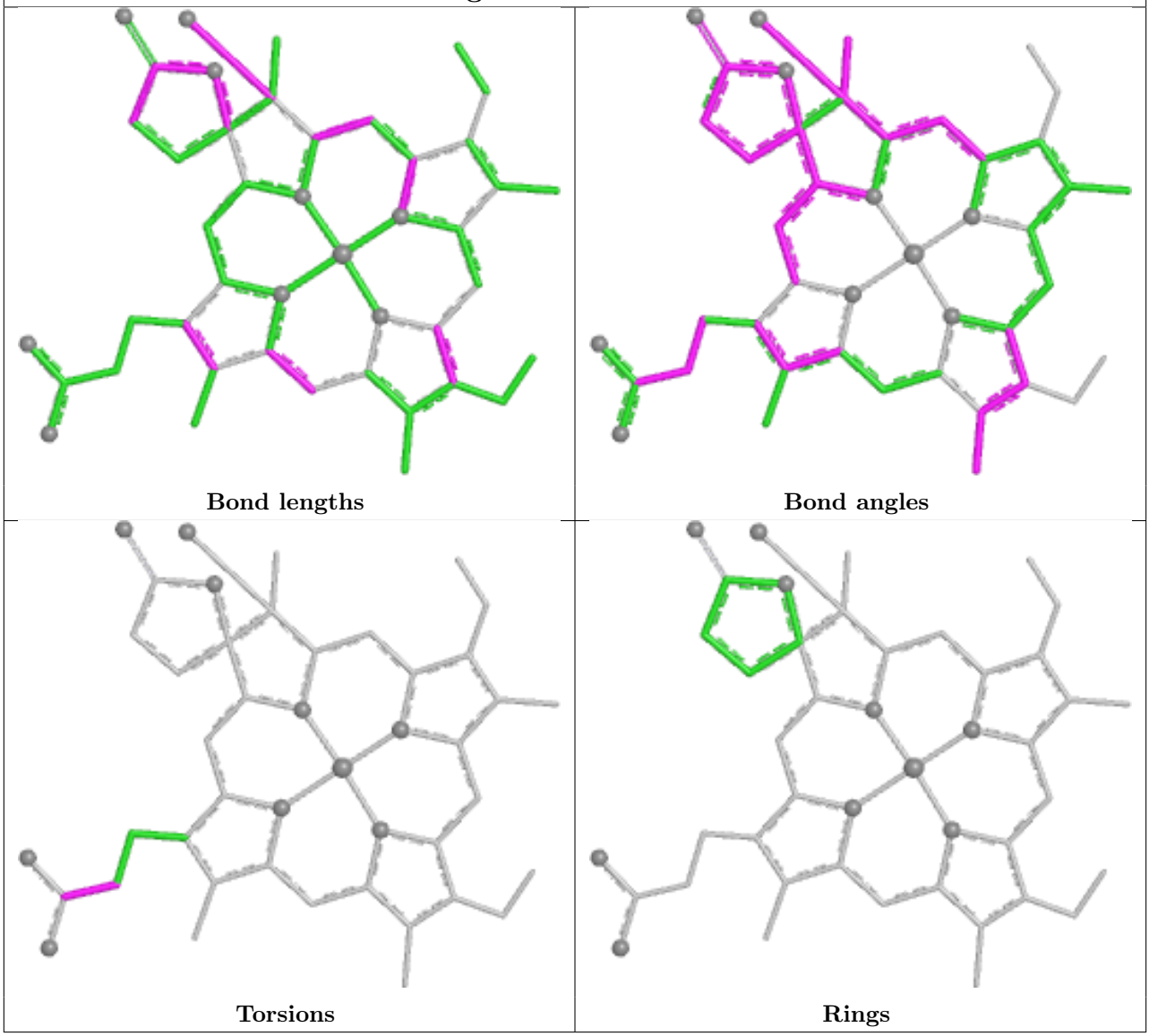
There are no ring outliers.

4 monomers are involved in 10 short contacts:

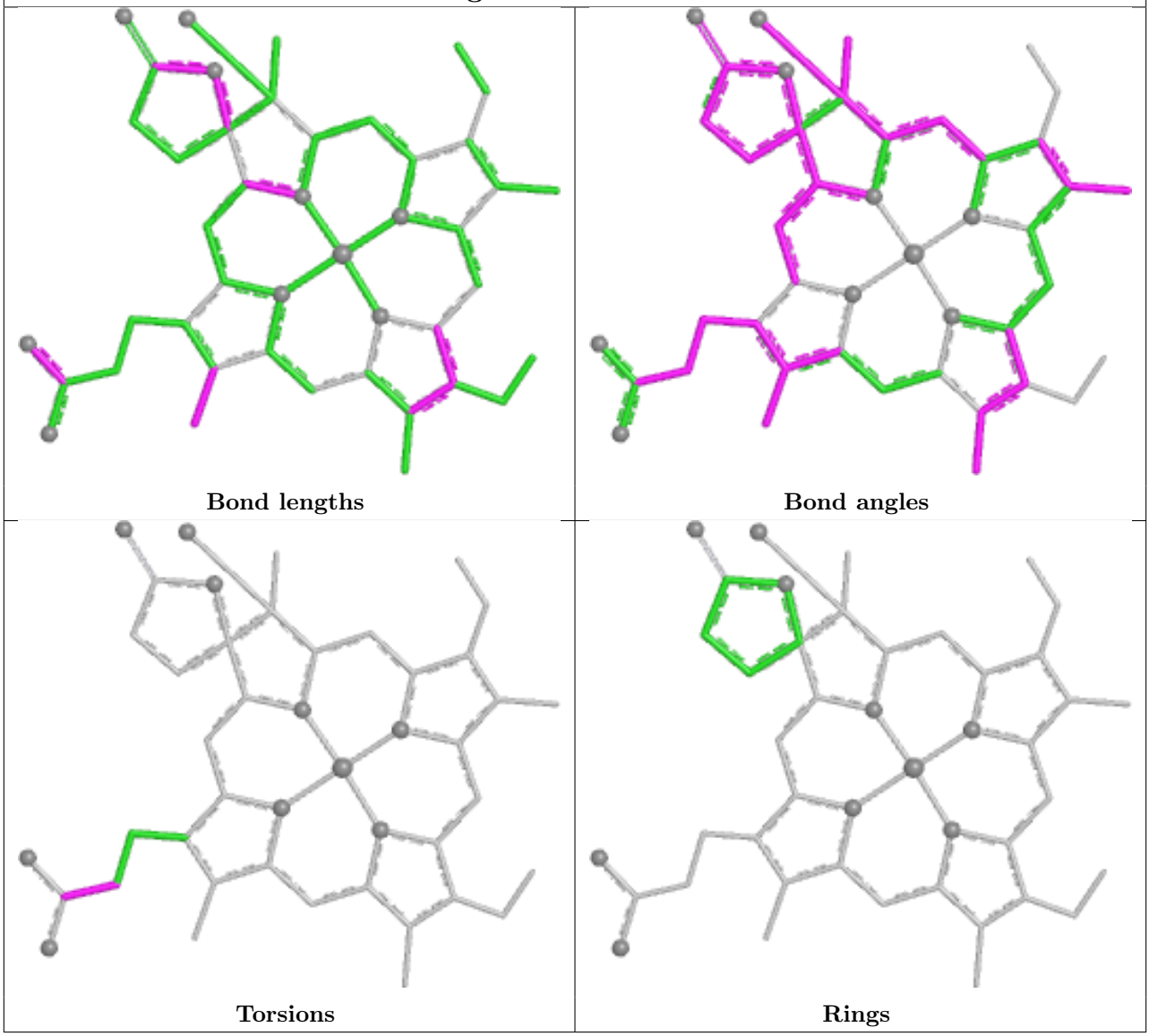
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	801	HDD	4	0
2	B	801	HDD	1	0
2	A	801	HDD	2	0
2	D	801	HDD	3	0

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 C 801



Ligand HDD B 801



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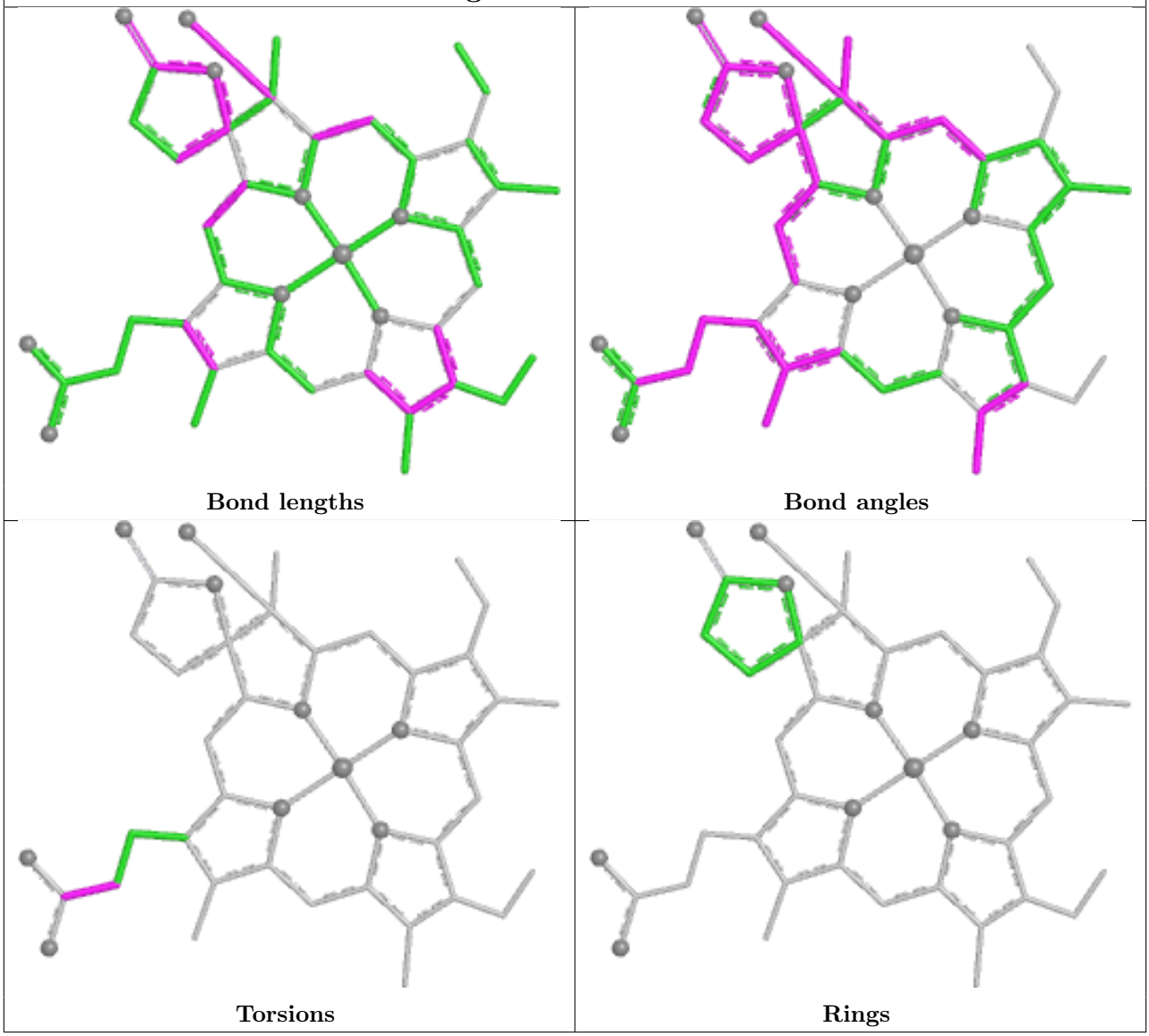
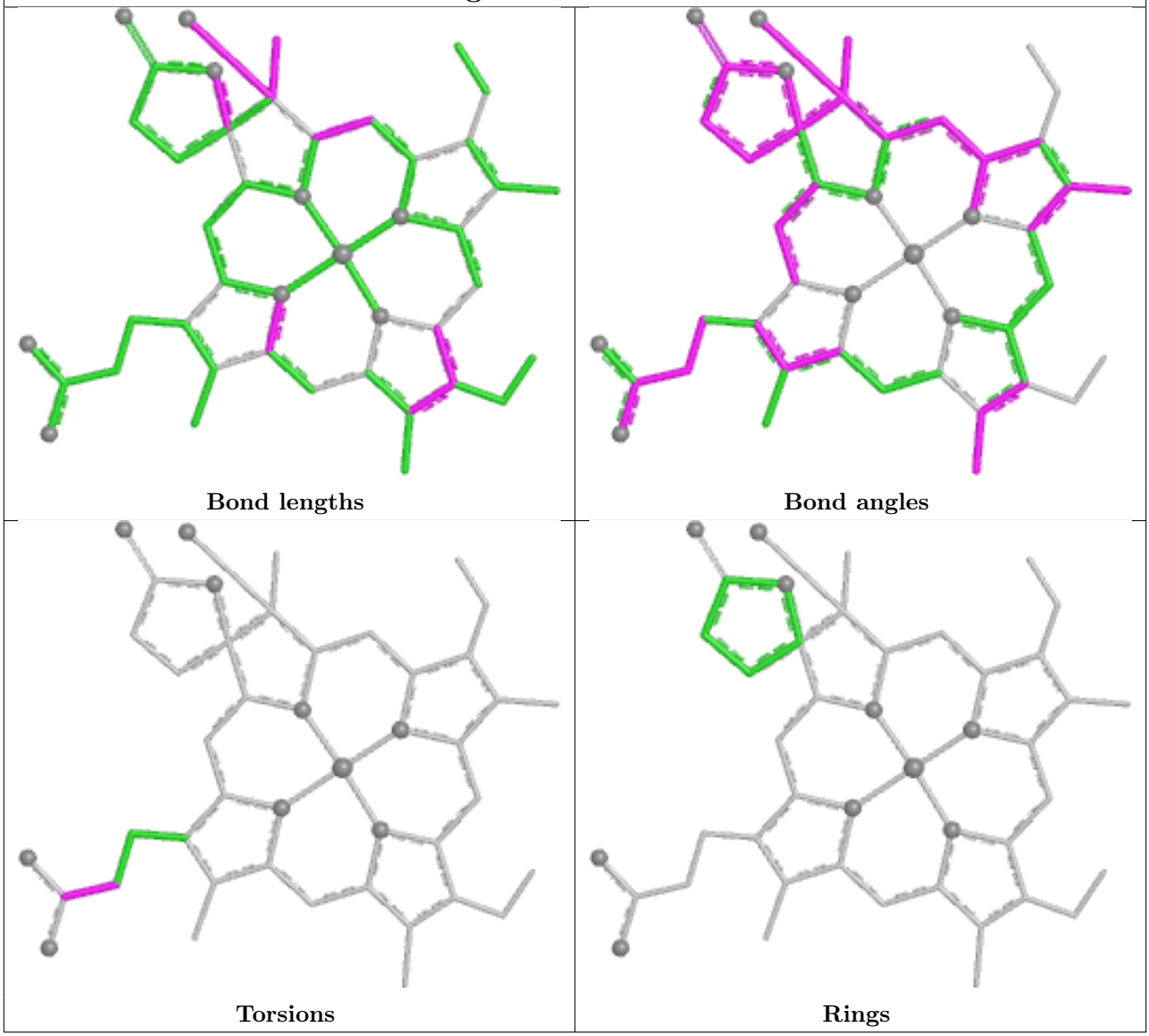


Ligand HDD D 801



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	725/753 (96%)	-0.50	5 (0%)	87	90	5, 11, 26, 54	1 (0%)
1	B	725/753 (96%)	-0.37	20 (2%)	53	57	5, 13, 36, 58	1 (0%)
1	C	725/753 (96%)	-0.40	20 (2%)	53	57	5, 12, 35, 54	1 (0%)
1	D	725/753 (96%)	-0.48	8 (1%)	80	83	5, 11, 28, 56	1 (0%)
All	All	2900/3012 (96%)	-0.44	53 (1%)	68	72	5, 12, 32, 58	4 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	726	GLY	5.0
1	B	28	SER	4.6
1	C	711	ALA	4.5
1	B	32	GLU	4.0
1	B	713	GLN	3.5
1	D	750	LYS	3.4
1	A	28	SER	3.4
1	B	712	ASP	3.4
1	B	750	LYS	3.2
1	C	726	GLY	3.1
1	A	32	GLU	3.1
1	C	712	ASP	3.0
1	D	28	SER	3.0
1	D	713	GLN	3.0
1	B	647	VAL	2.9
1	B	677	ASP	2.8
1	B	568	ASP	2.8
1	B	572	ASN	2.8
1	C	713	GLN	2.8
1	D	749	ASP	2.8
1	C	750	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	28	SER	2.7
1	C	552	LEU	2.7
1	B	646	THR	2.7
1	C	641	THR	2.7
1	C	647	VAL	2.7
1	C	646	THR	2.6
1	D	32	GLU	2.6
1	B	583	LYS	2.6
1	C	32	GLU	2.5
1	A	749	ASP	2.4
1	A	726	GLY	2.4
1	B	644	ASP	2.4
1	B	617	LEU	2.4
1	C	569	ASP	2.4
1	C	594	PRO	2.4
1	D	712	ASP	2.4
1	B	711	ALA	2.4
1	C	568	ASP	2.3
1	C	751	ILE	2.3
1	B	33	ASP	2.3
1	B	645	GLY	2.2
1	C	583	LYS	2.2
1	C	645	GLY	2.2
1	C	642	ALA	2.2
1	D	569	ASP	2.1
1	B	569	ASP	2.1
1	C	714	GLY	2.1
1	D	711	ALA	2.0
1	B	725	ASP	2.0
1	B	749	ASP	2.0
1	A	594	PRO	2.0
1	C	572	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	OCS	A	669	9/10	0.91	0.12	16,20,31,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	OCS	B	669	9/10	0.92	0.15	29,31,40,46	0
1	OCS	C	669	9/10	0.93	0.16	27,31,41,44	0
1	OCS	D	669	9/10	0.94	0.13	19,23,28,38	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

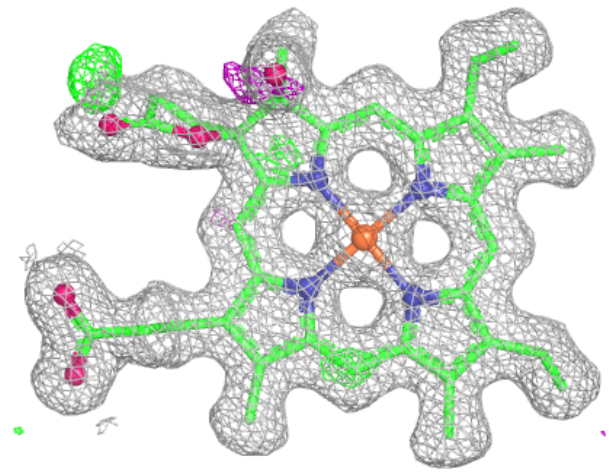
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

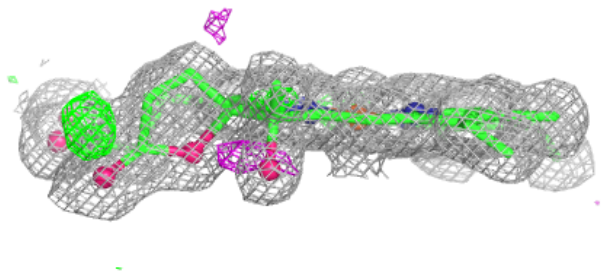
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HDD	A	801	44/44	0.99	0.07	5,6,13,16	0
2	HDD	B	801	44/44	0.99	0.07	6,7,13,17	0
2	HDD	C	801	44/44	0.99	0.07	6,7,15,18	0
2	HDD	D	801	44/44	0.99	0.07	5,6,12,16	0

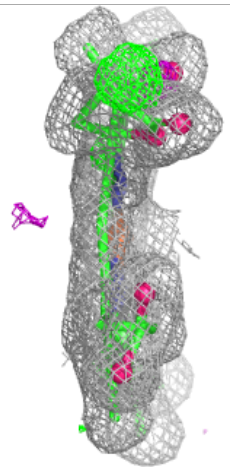
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HDD A 801:

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

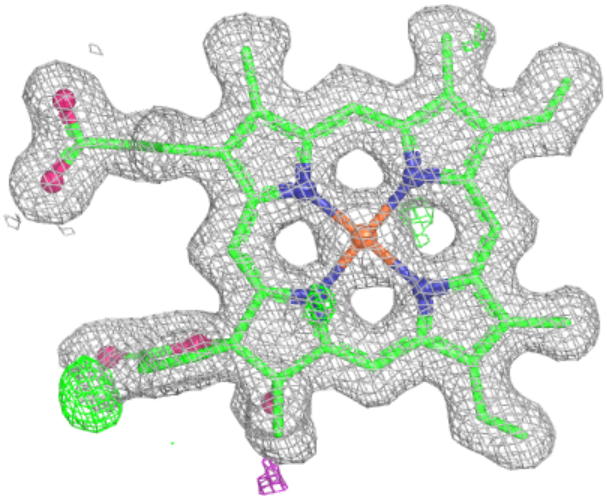


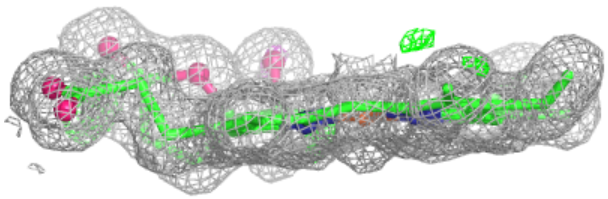


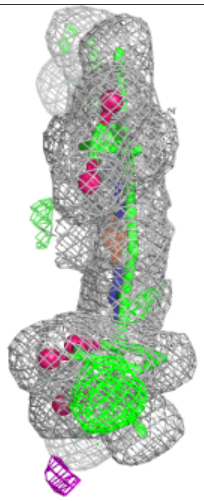


Electron density around HDD B 801:

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

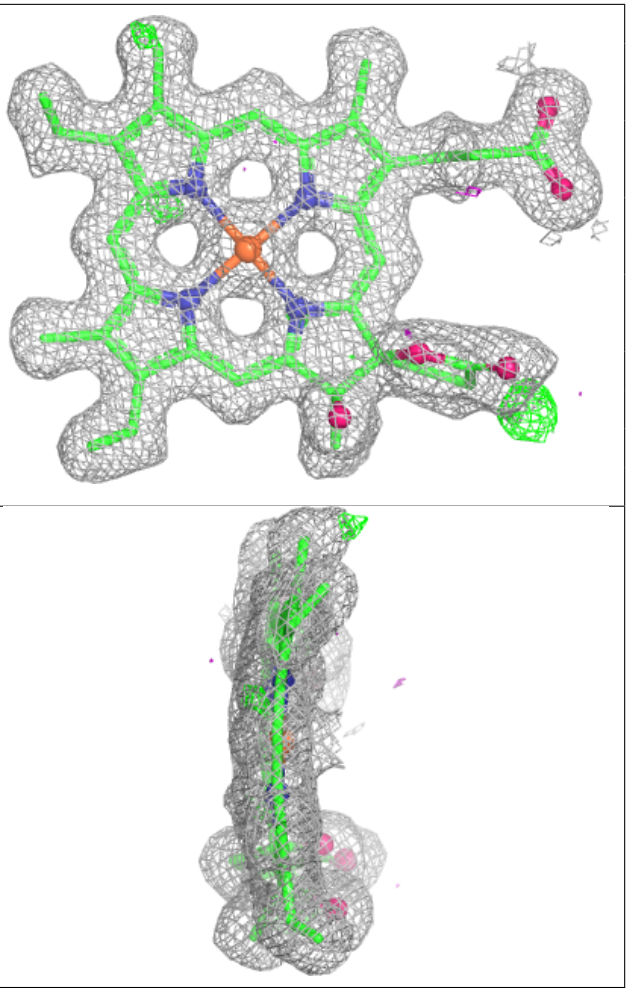






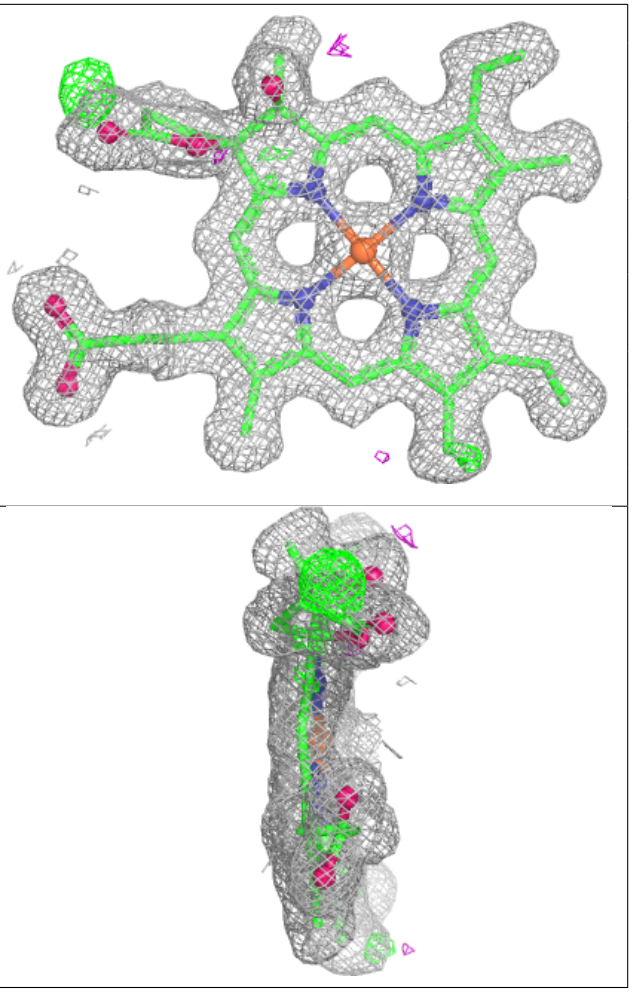
Electron density around HDD C 801:

$2mF_o$-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.