



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:33 PM UTC

PDB ID : 4ENU / pdb_00004enu
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

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

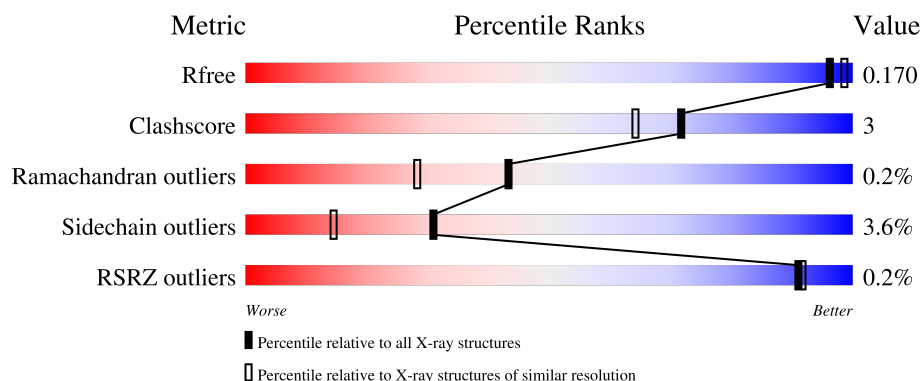
1 Overall quality at a glance

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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	753	 87% 9% . .
1	B	753	 84% 11% . .
1	C	753	 83% 12% . .
1	D	753	 83% 12% . .

2 Entry composition

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.

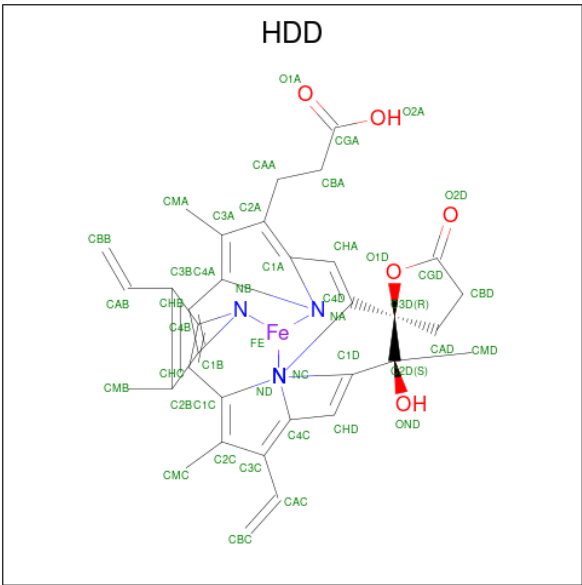
- Molecule 1 is a protein called Catalase HP11.

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

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 (CCD ID: HDD) (formula: C₃₄H₃₂FeN₄O₅).



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		

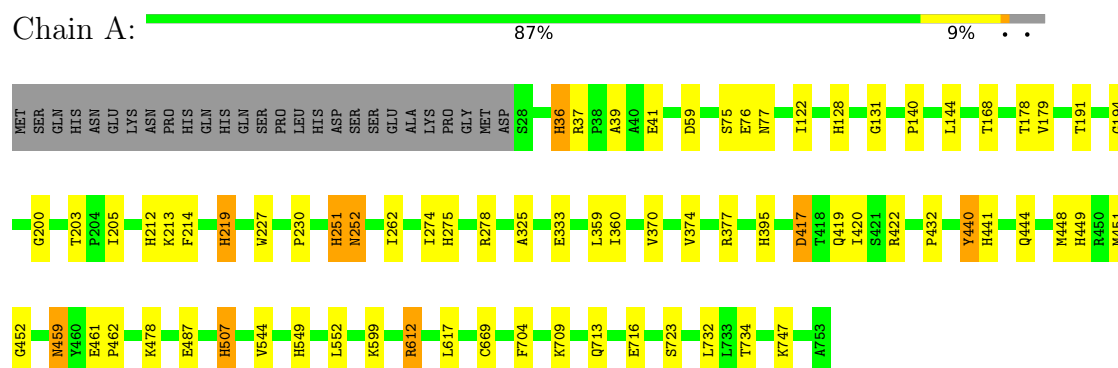
- Molecule 3 is water.

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		

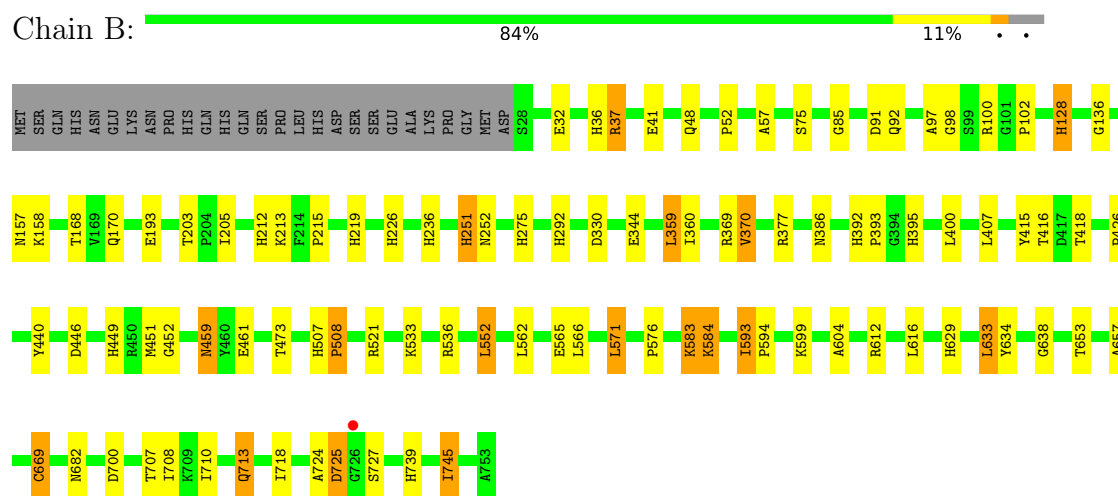
3 Residue-property plots [i](#)

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.

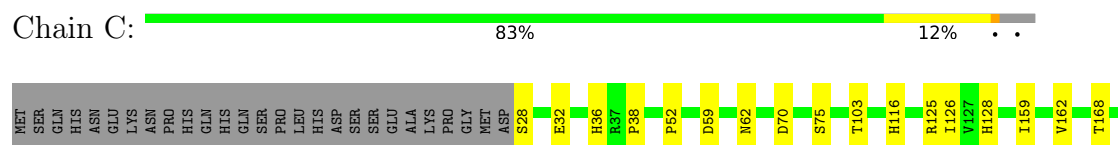
• Molecule 1: Catalase HP11

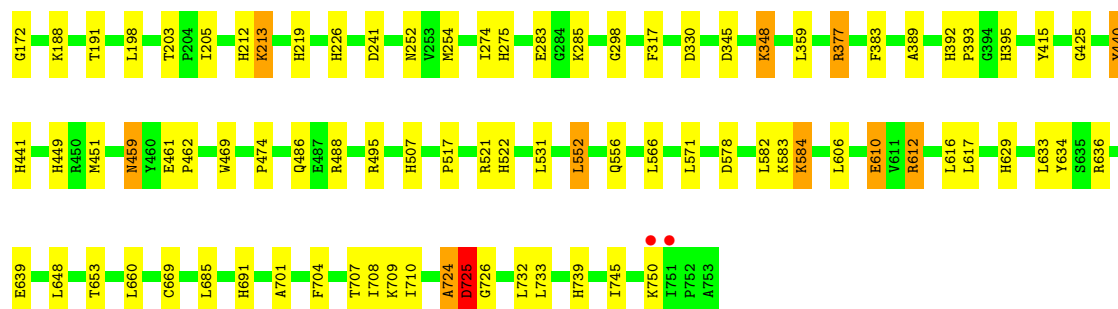


• Molecule 1: Catalase HP11



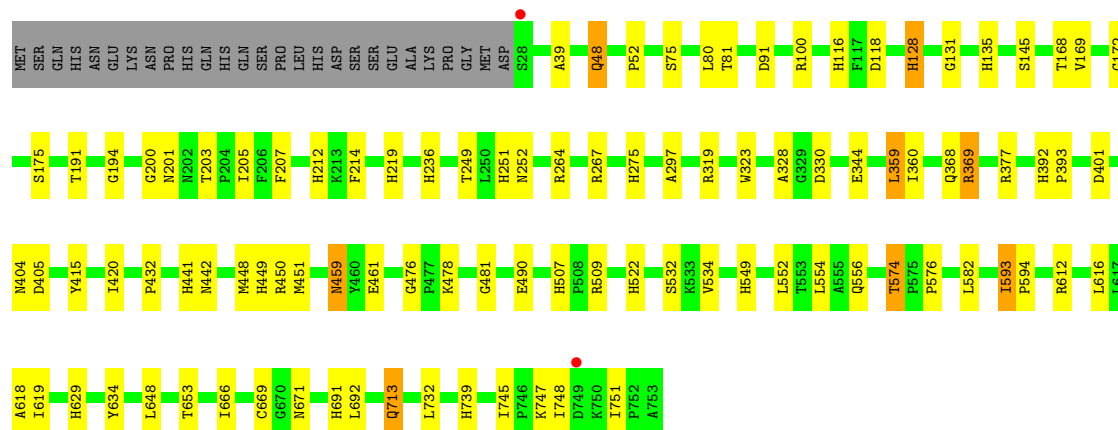
• Molecule 1: Catalase HP11





● Molecule 1: Catalase HP11

Chain D: 83% 12%



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.57	29/5920 (0.5%)	1.30	6/8047 (0.1%)
1	B	1.51	39/5914 (0.7%)	1.29	18/8039 (0.2%)
1	C	1.51	34/5937 (0.6%)	1.25	7/8069 (0.1%)
1	D	1.58	44/5925 (0.7%)	1.31	15/8054 (0.2%)
All	All	1.54	146/23696 (0.6%)	1.29	46/32209 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2

All (146) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	236	HIS	ND1-CE1	9.01	1.41	1.32
1	A	200	GLY	N-CA	8.40	1.52	1.44
1	D	691	HIS	CE1-NE2	8.16	1.40	1.32
1	A	275	HIS	ND1-CE1	8.16	1.40	1.32
1	D	442	ASN	C-O	8.03	1.31	1.24
1	C	522	HIS	ND1-CE1	7.98	1.40	1.32
1	D	200	GLY	N-CA	7.92	1.52	1.44
1	D	392	HIS	ND1-CE1	7.90	1.40	1.32
1	A	420	ILE	CA-CB	7.77	1.64	1.54
1	A	131	GLY	N-CA	7.67	1.53	1.45
1	A	178	THR	N-CA	7.57	1.55	1.46
1	C	226	HIS	CE1-NE2	7.47	1.40	1.32
1	D	203	THR	N-CA	7.30	1.52	1.45
1	A	395	HIS	ND1-CE1	7.28	1.39	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	226	HIS	CG-CD2	7.15	1.43	1.35
1	C	392	HIS	ND1-CE1	7.12	1.39	1.32
1	B	251	HIS	ND1-CE1	7.09	1.39	1.32
1	C	425	GLY	N-CA	7.05	1.54	1.44
1	B	275	HIS	ND1-CE1	7.05	1.39	1.32
1	B	473	THR	C-N	7.02	1.39	1.33
1	C	474	PRO	CA-C	6.98	1.55	1.51
1	B	203	THR	C-O	6.95	1.30	1.24
1	C	441	HIS	ND1-CE1	6.87	1.39	1.32
1	A	212	HIS	ND1-CE1	6.78	1.39	1.32
1	C	389	ALA	N-CA	6.54	1.54	1.46
1	D	275	HIS	CE1-NE2	6.54	1.39	1.32
1	D	135	HIS	ND1-CE1	6.49	1.39	1.32
1	A	704	PHE	N-CA	6.47	1.54	1.46
1	D	360	ILE	N-CA	6.46	1.51	1.46
1	B	236	HIS	CG-CD2	6.45	1.43	1.35
1	B	212	HIS	ND1-CE1	6.38	1.39	1.32
1	A	441	HIS	ND1-CE1	6.38	1.39	1.32
1	B	219	HIS	CE1-NE2	6.37	1.39	1.32
1	D	275	HIS	ND1-CE1	6.35	1.39	1.32
1	C	172	GLY	N-CA	6.33	1.53	1.45
1	C	739	HIS	CG-CD2	6.27	1.42	1.35
1	A	214	PHE	C-O	-6.24	1.18	1.24
1	D	212	HIS	ND1-CE1	6.24	1.38	1.32
1	B	98	GLY	N-CA	6.24	1.51	1.45
1	D	236	HIS	CE1-NE2	6.21	1.38	1.32
1	B	251	HIS	CG-CD2	6.16	1.42	1.35
1	D	131	GLY	N-CA	6.12	1.51	1.45
1	C	203	THR	CA-C	6.11	1.58	1.52
1	A	275	HIS	CE1-NE2	6.09	1.38	1.32
1	B	360	ILE	N-CA	6.04	1.51	1.46
1	C	522	HIS	CG-CD2	6.02	1.42	1.35
1	C	125	ARG	N-CA	5.99	1.53	1.46
1	D	666	ILE	N-CA	5.97	1.53	1.46
1	D	522	HIS	CG-CD2	5.94	1.42	1.35
1	B	400	LEU	N-CA	5.91	1.53	1.45
1	B	193	GLU	N-CA	5.89	1.52	1.46
1	D	420	ILE	CA-CB	5.88	1.61	1.54
1	C	298	GLY	N-CA	5.82	1.51	1.45
1	A	549	HIS	ND1-CE1	5.81	1.38	1.32
1	D	522	HIS	ND1-CE1	5.81	1.38	1.32
1	B	57	ALA	N-CA	5.80	1.53	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	39	ALA	N-CA	-5.75	1.39	1.46
1	D	194	GLY	N-CA	5.74	1.51	1.45
1	C	495	ARG	CZ-NH2	5.71	1.40	1.33
1	B	275	HIS	CE1-NE2	5.71	1.38	1.32
1	A	203	THR	C-N	5.71	1.38	1.33
1	B	359	LEU	N-CA	5.70	1.52	1.45
1	C	383	PHE	C-O	5.68	1.30	1.24
1	D	739	HIS	ND1-CE1	5.68	1.38	1.32
1	D	236	HIS	CG-CD2	5.67	1.42	1.35
1	D	172	GLY	N-CA	5.66	1.52	1.45
1	A	179	VAL	N-CA	5.66	1.53	1.46
1	D	251	HIS	CG-CD2	5.65	1.42	1.35
1	B	452	GLY	N-CA	5.65	1.51	1.45
1	B	576	PRO	CA-C	5.65	1.57	1.52
1	D	214	PHE	CA-C	5.65	1.59	1.52
1	B	41	GLU	CA-C	5.64	1.58	1.52
1	C	116	HIS	ND1-CE1	5.64	1.38	1.32
1	D	128	HIS	ND1-CE1	5.64	1.38	1.32
1	C	691	HIS	CE1-NE2	5.62	1.38	1.32
1	D	251	HIS	ND1-CE1	5.62	1.38	1.32
1	A	219	HIS	CG-CD2	5.59	1.42	1.35
1	C	36	HIS	CE1-NE2	5.58	1.38	1.32
1	A	360	ILE	N-CA	5.58	1.50	1.46
1	D	441	HIS	CG-ND1	-5.58	1.32	1.38
1	B	739	HIS	CG-CD2	5.57	1.42	1.35
1	C	275	HIS	CE1-NE2	5.56	1.38	1.32
1	B	85	GLY	N-CA	5.56	1.53	1.45
1	A	417	ASP	CA-C	5.53	1.60	1.52
1	B	407	LEU	C-O	-5.53	1.17	1.24
1	C	739	HIS	CE1-NE2	5.51	1.38	1.32
1	A	452	GLY	N-CA	5.50	1.52	1.45
1	A	544	VAL	N-CA	5.46	1.53	1.46
1	D	328	ALA	N-CA	5.46	1.53	1.46
1	A	440	TYR	CE1-CZ	5.46	1.51	1.38
1	A	36	HIS	ND1-CE1	5.45	1.38	1.32
1	B	392	HIS	ND1-CE1	5.45	1.38	1.32
1	C	377	ARG	CZ-NH1	5.44	1.40	1.32
1	A	251	HIS	ND1-CE1	5.42	1.38	1.32
1	C	469	TRP	CD2-CE2	5.41	1.50	1.41
1	D	175	SER	N-CA	5.38	1.52	1.45
1	C	283	GLU	N-CA	5.37	1.53	1.46
1	D	441	HIS	ND1-CE1	5.35	1.38	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	450	ARG	CZ-NH1	5.35	1.40	1.32
1	B	219	HIS	CG-CD2	5.34	1.41	1.35
1	C	38	PRO	C-O	5.33	1.29	1.23
1	A	734	THR	C-O	5.31	1.30	1.24
1	B	418	THR	N-CA	5.27	1.52	1.46
1	C	691	HIS	CG-CD2	5.27	1.41	1.35
1	B	102	PRO	C-O	5.27	1.29	1.23
1	A	140	PRO	CA-C	5.26	1.58	1.52
1	D	81	THR	C-O	5.26	1.30	1.23
1	D	619	ILE	N-CA	5.25	1.52	1.46
1	C	395	HIS	CE1-NE2	5.25	1.37	1.32
1	D	692	LEU	CA-CB	5.24	1.61	1.53
1	B	446	ASP	N-CA	5.24	1.54	1.47
1	C	701	ALA	N-CA	5.24	1.53	1.46
1	D	236	HIS	CG-ND1	-5.24	1.32	1.38
1	B	52	PRO	C-O	5.23	1.30	1.23
1	B	292	HIS	CG-CD2	5.23	1.41	1.35
1	D	80	LEU	N-CA	5.23	1.52	1.46
1	C	212	HIS	ND1-CE1	5.20	1.37	1.32
1	B	36	HIS	CG-CD2	5.20	1.41	1.35
1	D	377	ARG	CZ-NH2	5.20	1.40	1.33
1	B	449[A]	HIS	ND1-CE1	5.19	1.37	1.32
1	B	449[B]	HIS	ND1-CE1	5.19	1.37	1.32
1	A	251	HIS	CG-CD2	5.17	1.41	1.35
1	D	359	LEU	N-CA	5.16	1.51	1.45
1	B	36	HIS	CE1-NE2	5.14	1.37	1.32
1	A	194	GLY	N-CA	5.14	1.50	1.45
1	C	103	THR	N-CA	5.13	1.52	1.46
1	C	392	HIS	CE1-NE2	5.13	1.37	1.32
1	C	395	HIS	ND1-CE1	5.11	1.37	1.32
1	D	549	HIS	CG-CD2	5.10	1.41	1.35
1	B	395	HIS	ND1-CE1	5.09	1.37	1.32
1	A	507	HIS	CE1-NE2	5.07	1.37	1.32
1	D	401	ASP	N-CA	5.07	1.51	1.46
1	B	136	GLY	N-CA	5.07	1.51	1.45
1	C	59	ASP	CB-CG	5.07	1.64	1.52
1	B	226	HIS	CG-CD2	5.05	1.41	1.35
1	B	157	ASN	CB-CG	5.05	1.64	1.52
1	B	215	PRO	CA-CB	-5.04	1.46	1.53
1	D	145	SER	N-CA	5.04	1.52	1.46
1	D	264	ARG	CD-NE	5.04	1.53	1.46
1	A	122	ILE	N-CA	5.03	1.50	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	323	TRP	NE1-CE2	5.03	1.43	1.37
1	A	444	GLN	N-CA	5.03	1.52	1.46
1	D	481	GLY	N-CA	5.03	1.51	1.45
1	B	97	ALA	N-CA	5.01	1.52	1.46
1	C	441	HIS	CE1-NE2	5.01	1.37	1.32
1	B	128	HIS	ND1-CE1	5.00	1.37	1.32

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	745	ILE	CA-C-N	-7.90	111.58	119.56
1	B	745	ILE	C-N-CA	-7.90	111.58	119.56
1	D	574	THR	CA-C-N	7.77	125.33	119.66
1	D	574	THR	C-N-CA	7.77	125.33	119.66
1	D	377	ARG	CG-CD-NE	-7.58	95.32	112.00
1	C	745	ILE	CA-C-N	-7.50	111.91	119.56
1	C	745	ILE	C-N-CA	-7.50	111.91	119.56
1	D	745	ILE	CA-C-N	-7.39	112.09	119.56
1	D	745	ILE	C-N-CA	-7.39	112.09	119.56
1	D	574	THR	CB-CA-C	7.04	119.61	109.26
1	D	377	ARG	NE-CZ-NH1	-7.00	114.50	121.50
1	D	377	ARG	NH1-CZ-NH2	6.77	128.10	119.30
1	C	377	ARG	NE-CZ-NH1	-6.35	115.15	121.50
1	A	377	ARG	CG-CD-NE	-6.25	98.26	112.00
1	D	593	ILE	CA-C-N	6.18	127.56	119.84
1	D	593	ILE	C-N-CA	6.18	127.56	119.84
1	B	370	VAL	N-CA-CB	-6.15	103.82	112.12
1	B	536	ARG	CA-C-N	-6.07	112.76	119.19
1	B	536	ARG	C-N-CA	-6.07	112.76	119.19
1	B	593	ILE	CA-C-N	6.02	127.36	119.84
1	B	593	ILE	C-N-CA	6.02	127.36	119.84
1	B	657	ALA	CA-C-N	5.95	126.29	119.92
1	B	657	ALA	C-N-CA	5.95	126.29	119.92
1	B	745	ILE	N-CA-CB	5.93	114.23	110.50
1	C	126	ILE	CB-CA-C	-5.86	104.23	112.14
1	A	213	LYS	CA-CB-CG	-5.77	102.55	114.10
1	B	377	ARG	CA-CB-CG	-5.72	102.66	114.10
1	C	348	LYS	CA-CB-CG	-5.57	102.97	114.10
1	B	100	ARG	CB-CA-C	-5.50	102.58	111.28
1	C	241	ASP	N-CA-C	-5.49	105.20	111.07
1	B	638	GLY	O-C-N	-5.47	119.53	123.08
1	B	377	ARG	CG-CD-NE	-5.42	100.08	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	ALA	N-CA-C	-5.35	105.53	111.36
1	A	262	ILE	CA-C-N	-5.33	114.76	120.03
1	A	262	ILE	C-N-CA	-5.33	114.76	120.03
1	D	745	ILE	O-C-N	5.24	123.77	120.42
1	D	618	ALA	N-CA-C	-5.22	105.67	111.36
1	B	370	VAL	CB-CA-C	5.22	115.76	110.65
1	B	48	GLN	CA-C-N	-5.21	114.59	119.85
1	B	48	GLN	C-N-CA	-5.21	114.59	119.85
1	D	297	ALA	N-CA-C	-5.20	106.91	113.20
1	C	317	PHE	N-CA-C	5.12	116.86	111.28
1	D	100	ARG	CB-CA-C	-5.11	103.21	111.28
1	A	360	ILE	N-CA-C	-5.08	102.52	107.55
1	B	416	THR	N-CA-C	-5.07	105.46	111.69
1	D	534	VAL	N-CA-C	-5.03	100.54	108.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5761	0	5593	32	1
1	B	5758	0	5589	47	1
1	C	5773	0	5612	41	0
1	D	5765	0	5598	42	0
2	A	44	0	31	1	0
2	B	44	0	31	0	0
2	C	44	0	31	3	0
2	D	44	0	31	1	0
3	A	802	0	0	10	1
3	B	708	0	0	9	0
3	C	727	0	0	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	816	0	0	10	1
All	All	26286	0	22516	151	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 (151) 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:D:451:MET:SD	3:D:1638:HOH:O	2.05	1.14
1:B:451:MET:HE2	1:D:451:MET:HE2	1.14	1.13
1:B:533:LYS:HE3	3:C:1500:HOH:O	1.47	1.12
1:A:451:MET:HE2	1:C:451:MET:HE2	1.33	1.05
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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:LEU:H	1:B:507:HIS:HD2	1.49	0.58
1:B:451:MET:HE2	1:D:451:MET:CE	2.09	0.58
1:B:533:LYS:CE	3:C:1500:HOH:O	2.26	0.57
1:A:274:ILE:HD12	2:A:801:HDD:HMB3	1.87	0.56
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
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:B:451:MET:CE	1:D:451:MET:HE2	2.10	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
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.19	0.51
1:B:369:ARG:HG2	3:B:1305:HOH:O	2.11	0.50
1:B:599:LYS:NZ	3:B:1450:HOH:O	2.45	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:D:201:ASN:CG	2:D:801:HDD:HMB2	2.41	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:732:LEU:C	1:D:732:LEU:HD13	2.42	0.45
1:A:461:GLU:HA	1:A:462:PRO:C	2.42	0.44
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:359:LEU:C	1:A:359:LEU:HD12	2.42	0.44
1:C:461:GLU:HA	1:C:462:PRO:C	2.42	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:D:404:ASN:O	1:D:405:ASP:C	2.60	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:716:GLU:CD	3:A:1646:HOH:O	2.57	0.42
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:B:713:GLN:H	1:B:713:GLN:CD	2.28	0.42
1:B:359:LEU:HD12	1:B:359:LEU:C	2.44	0.42
1:C:725:ASP:HB3	1:C:726:GLY:H	1.73	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: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:B:386:ASN:OD1	1:B:386:ASN:C	2.63	0.40
1:B:521:ARG:NH2	1:B:745:ILE:CD1	2.68	0.40
1:C:62:ASN:OD1	1:C:62:ASN:C	2.64	0.40
1:C:254:MET:HE3	1:C:254:MET:HB3	1.99	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%)	48	31
1	B	726/753 (96%)	706 (97%)	17 (2%)	3 (0%)	30	16
1	C	729/753 (97%)	710 (97%)	17 (2%)	2 (0%)	36	22
1	D	727/753 (96%)	713 (98%)	13 (2%)	1 (0%)	48	31
All	All	2909/3012 (97%)	2841 (98%)	61 (2%)	7 (0%)	43	28

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%)	600 (98%)	14 (2%)	44	27
1	B	613/635 (96%)	592 (97%)	21 (3%)	32	16
1	C	616/635 (97%)	582 (94%)	34 (6%)	19	6
1	D	614/635 (97%)	595 (97%)	19 (3%)	35	18
All	All	2457/2540 (97%)	2369 (96%)	88 (4%)	31	14

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	191	THR
1	A	205	ILE
1	A	252	ASN
1	A	432	PRO
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	612	ARG
1	A	617	LEU
1	A	709	LYS
1	A	713	GLN
1	A	732	LEU
1	A	747	LYS
1	B	32	GLU
1	B	37	ARG
1	B	158	LYS
1	B	205	ILE
1	B	213	LYS
1	B	252	ASN
1	B	344	GLU
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	584	LYS
1	B	616	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	633	LEU
1	B	713	GLN
1	C	32	GLU
1	C	159[A]	ILE
1	C	159[B]	ILE
1	C	191	THR
1	C	198	LEU
1	C	205	ILE
1	C	213	LYS
1	C	252	ASN
1	C	285	LYS
1	C	377	ARG
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	610	GLU
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	191	THR
1	D	205	ILE
1	D	252	ASN
1	D	344	GLU
1	D	369	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	432	PRO
1	D	459	ASN
1	D	478	LYS
1	D	490	GLU
1	D	552	LEU
1	D	554	LEU
1	D	574	THR
1	D	582	LEU
1	D	612	ARG
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 (28) 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	713	GLN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	B	713	GLN
1	C	77	ASN
1	C	252	ASN
1	C	419	GLN
1	C	459	ASN
1	C	486	GLN
1	C	507	HIS
1	C	546	GLN
1	C	629	HIS
1	C	671	ASN
1	C	682	ASN
1	D	48	GLN
1	D	252	ASN
1	D	459	ASN
1	D	507	HIS
1	D	546	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	556	GLN
1	D	629	HIS
1	D	671	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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(°)	Ideal(°)
1	B	669	OCS	OD1-SG-CB	5.52	115.00	106.76
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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	801	1	46,52,52	1.83	9 (19%)	62,89,89	3.89	24 (38%)
2	HDD	B	801	3,1	46,52,52	1.94	15 (32%)	62,89,89	3.47	24 (38%)
2	HDD	C	801	3,1	46,52,52	2.01	12 (26%)	62,89,89	3.05	27 (43%)
2	HDD	A	801	1	46,52,52	1.99	12 (26%)	62,89,89	3.94	23 (37%)

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

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	A	801	HDD	CHB-C1B	4.76	1.47	1.38
2	A	801	HDD	OND-C2D	4.48	1.51	1.42
2	C	801	HDD	C4C-NC	-4.47	1.31	1.39
2	B	801	HDD	CHC-C4B	4.40	1.47	1.38
2	C	801	HDD	CHC-C4B	4.10	1.46	1.38
2	D	801	HDD	CHB-C1B	4.05	1.46	1.38
2	B	801	HDD	C4C-NC	-3.82	1.32	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HDD	C4D-ND	3.76	1.44	1.37
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	C	801	HDD	CHB-C4A	3.32	1.46	1.39
2	D	801	HDD	C3B-C2B	3.28	1.43	1.37
2	D	801	HDD	C1A-NA	-3.22	1.33	1.39
2	A	801	HDD	O1D-CGD	3.18	1.40	1.35
2	A	801	HDD	CHA-C1A	3.17	1.46	1.39
2	A	801	HDD	C3B-C2B	3.16	1.43	1.37
2	B	801	HDD	C3B-C2B	3.13	1.43	1.37
2	C	801	HDD	CHA-C1A	3.13	1.46	1.39
2	A	801	HDD	CHC-C4B	3.13	1.44	1.38
2	B	801	HDD	O1D-C3D	3.10	1.51	1.46
2	C	801	HDD	CHB-C1B	3.10	1.44	1.38
2	B	801	HDD	C1B-NB	-2.96	1.34	1.39
2	A	801	HDD	C2A-C3A	2.93	1.46	1.38
2	D	801	HDD	CMD-C2D	2.88	1.57	1.53
2	B	801	HDD	CMA-C3A	2.83	1.56	1.50
2	B	801	HDD	O1D-CGD	2.82	1.40	1.35
2	B	801	HDD	CHB-C4A	2.74	1.45	1.39
2	B	801	HDD	C1C-NC	-2.73	1.34	1.39
2	A	801	HDD	C4A-C3A	2.70	1.49	1.43
2	A	801	HDD	CAD-C3D	-2.67	1.48	1.53
2	D	801	HDD	CHA-C1A	2.65	1.45	1.39
2	B	801	HDD	CHB-C1B	2.57	1.43	1.38
2	C	801	HDD	CHC-C1C	2.45	1.44	1.39
2	D	801	HDD	C3B-C4B	2.43	1.50	1.46
2	C	801	HDD	CBD-CGD	2.42	1.54	1.50
2	C	801	HDD	O1D-CGD	2.35	1.39	1.35
2	A	801	HDD	O2D-CGD	2.32	1.29	1.22
2	A	801	HDD	C4C-NC	-2.32	1.35	1.39
2	C	801	HDD	C4A-C3A	2.25	1.48	1.43
2	C	801	HDD	C2A-C3A	2.24	1.44	1.38
2	B	801	HDD	CHD-C4C	2.23	1.44	1.39
2	B	801	HDD	O1A-CGA	2.18	1.29	1.22
2	B	801	HDD	C4A-C3A	2.11	1.48	1.43
2	D	801	HDD	C4B-NB	-2.10	1.35	1.39
2	B	801	HDD	CHA-C1A	2.05	1.44	1.39

All (98) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	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	CMC-C2C-C1C	6.22	134.88	125.42
2	B	801	HDD	C4A-C3A-C2A	-5.48	100.54	106.82
2	D	801	HDD	C3B-C2B-C1B	-5.20	102.12	107.05
2	D	801	HDD	C3C-C2C-C1C	-5.16	101.08	107.17
2	A	801	HDD	C3B-C2B-C1B	-5.06	102.26	107.05
2	A	801	HDD	CAA-CBA-CGA	-4.84	100.82	113.67
2	C	801	HDD	CBD-CAD-C3D	4.83	110.86	103.98
2	D	801	HDD	CAA-CBA-CGA	-4.77	101.02	113.67
2	D	801	HDD	O1D-C3D-CAD	-4.75	94.28	103.06
2	C	801	HDD	C3C-C2C-C1C	-4.58	101.77	107.17
2	A	801	HDD	C3C-C2C-C1C	-4.52	101.84	107.17
2	A	801	HDD	CBD-CAD-C3D	4.47	110.36	103.98
2	D	801	HDD	C2C-C1C-NC	4.35	117.11	110.14
2	D	801	HDD	CBD-CAD-C3D	4.12	109.86	103.98
2	B	801	HDD	C3C-C2C-C1C	-4.08	102.36	107.17
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	B	801	HDD	CAD-CBD-CGD	3.76	110.06	104.48
2	B	801	HDD	CMD-C2D-C1D	3.63	118.83	112.68
2	C	801	HDD	CAA-CBA-CGA	-3.58	104.17	113.67
2	B	801	HDD	CBD-CAD-C3D	3.43	108.88	103.98
2	A	801	HDD	CAA-C2A-C1A	3.42	131.61	124.94
2	D	801	HDD	C3C-C4C-NC	3.38	112.65	109.80
2	B	801	HDD	C3B-C2B-C1B	-3.34	103.89	107.05
2	C	801	HDD	CMC-C2C-C1C	3.21	130.30	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HDD	C2A-C1A-NA	3.06	113.55	110.15
2	B	801	HDD	C3D-C4D-CHA	-3.06	115.26	124.14
2	B	801	HDD	CHB-C4A-C3A	-3.03	118.62	127.43
2	A	801	HDD	C2C-C1C-NC	3.02	114.98	110.14
2	D	801	HDD	C4A-C3A-C2A	-2.99	103.39	106.82
2	C	801	HDD	C3D-C4D-CHA	-2.98	115.50	124.14
2	C	801	HDD	CHC-C1C-C2C	-2.97	118.81	127.43
2	C	801	HDD	CHC-C4B-C3B	-2.90	120.32	125.21
2	B	801	HDD	CHC-C1C-C2C	-2.84	119.19	127.43
2	D	801	HDD	C2B-C1B-NB	2.80	114.82	109.64
2	C	801	HDD	CHB-C4A-NA	2.76	128.86	123.86
2	C	801	HDD	CAA-C2A-C1A	2.76	130.32	124.94
2	B	801	HDD	C3A-C4A-NA	2.74	114.54	110.14
2	B	801	HDD	CAA-CBA-CGA	-2.73	106.43	113.67
2	B	801	HDD	C2C-C1C-NC	2.73	114.52	110.14
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	C	801	HDD	C4B-C3B-C2B	-2.71	104.47	106.81
2	C	801	HDD	CHB-C4A-C3A	-2.70	119.59	127.43
2	B	801	HDD	C2B-C1B-NB	2.70	114.62	109.64
2	C	801	HDD	C2C-C1C-NC	2.69	114.45	110.14
2	A	801	HDD	CMC-C2C-C1C	2.68	129.51	125.42
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	C1A-CHA-C4D	-2.54	120.87	125.81
2	D	801	HDD	CBC-CAC-C3C	-2.51	114.97	127.53
2	A	801	HDD	C4C-CHD-C1D	-2.50	120.95	125.81
2	C	801	HDD	C4A-C3A-C2A	-2.48	103.98	106.82
2	C	801	HDD	C1A-CHA-C4D	-2.47	121.01	125.81
2	D	801	HDD	CHB-C4A-C3A	-2.47	120.26	127.43
2	D	801	HDD	OND-C2D-C3D	-2.47	104.67	110.46
2	C	801	HDD	C2D-C1D-CHD	-2.45	120.46	124.27
2	A	801	HDD	CHC-C1C-C2C	-2.45	120.31	127.43
2	D	801	HDD	O2A-CGA-CBA	2.45	121.73	114.00
2	B	801	HDD	CMA-C3A-C2A	2.41	130.74	125.62
2	C	801	HDD	CHD-C4C-NC	2.37	128.16	123.86
2	A	801	HDD	C2B-C1B-NB	2.37	114.02	109.64
2	D	801	HDD	CHB-C4A-NA	2.34	128.10	123.86
2	A	801	HDD	CHB-C4A-C3A	-2.31	120.72	127.43
2	C	801	HDD	CMD-C2D-C1D	2.30	116.57	112.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	HDD	C4C-NC-C1C	-2.29	102.08	105.82
2	C	801	HDD	CAD-CBD-CGD	2.24	107.80	104.48
2	A	801	HDD	CHD-C4C-NC	2.22	127.89	123.86
2	A	801	HDD	CHC-C4B-NB	2.22	126.87	124.45
2	A	801	HDD	CBC-CAC-C3C	-2.20	116.54	127.53
2	B	801	HDD	CHB-C1B-NB	-2.18	122.08	124.45
2	C	801	HDD	CBB-CAB-C3B	-2.16	116.74	127.53
2	B	801	HDD	CMA-C3A-C4A	2.15	128.69	125.42
2	A	801	HDD	CMB-C2B-C3B	2.13	133.59	128.43
2	D	801	HDD	CAD-CBD-CGD	2.12	107.62	104.48
2	D	801	HDD	CHC-C1C-C2C	-2.10	121.34	127.43
2	C	801	HDD	CHA-C4D-ND	2.06	127.12	124.28
2	C	801	HDD	CHC-C4B-NB	2.05	126.69	124.45
2	C	801	HDD	C4C-CHD-C1D	-2.03	121.87	125.81
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

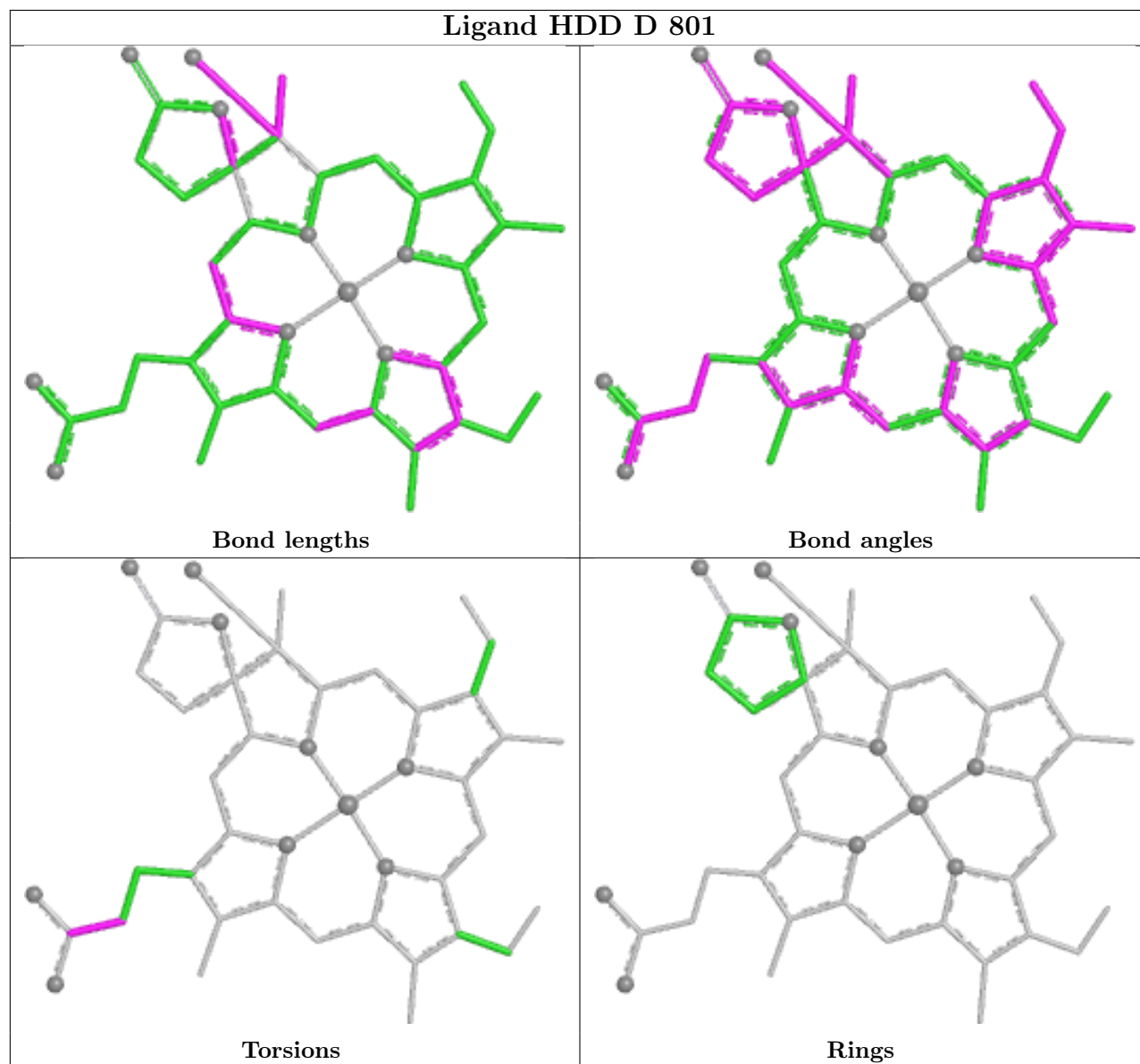
There are no ring outliers.

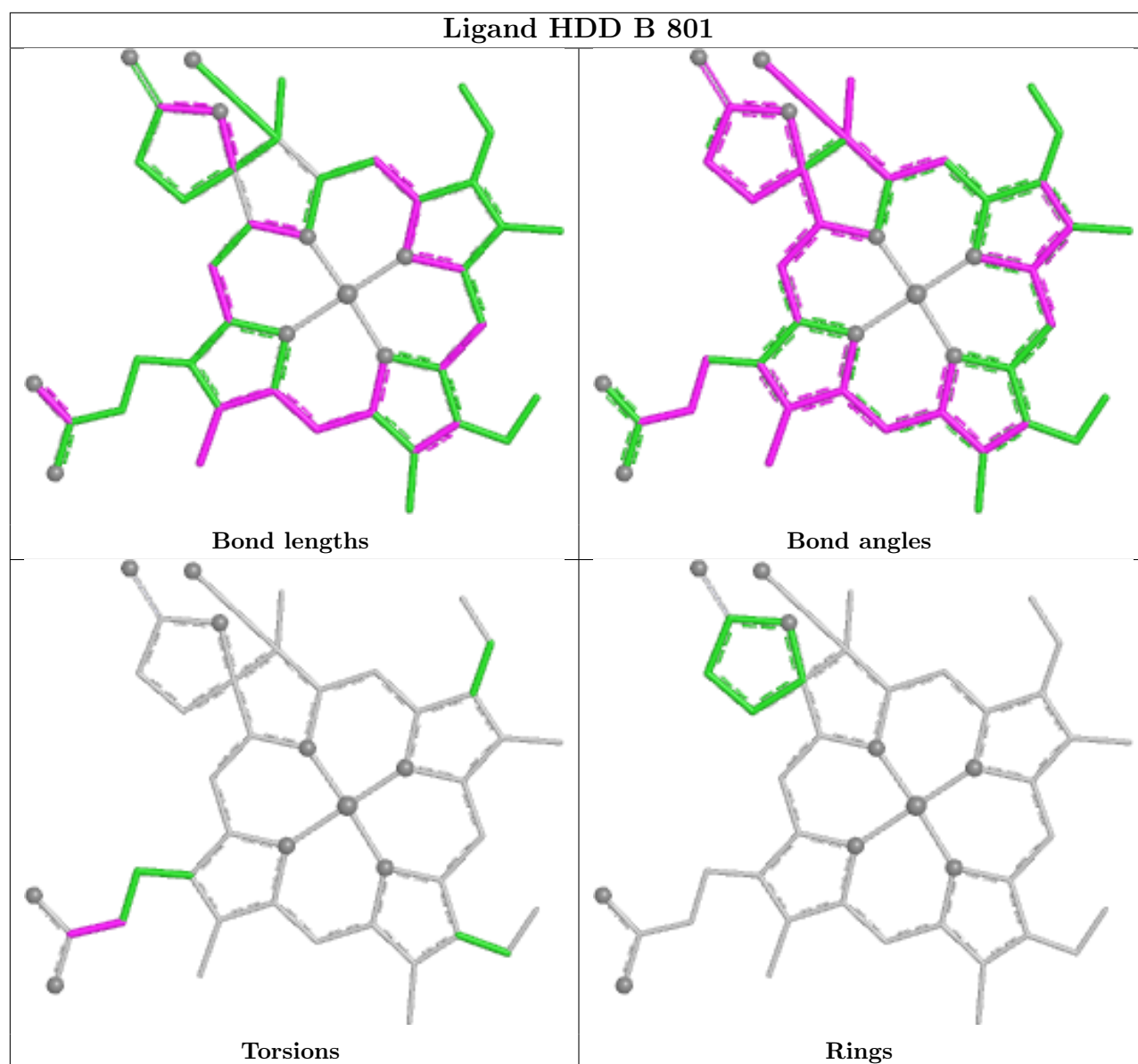
3 monomers are involved in 5 short contacts:

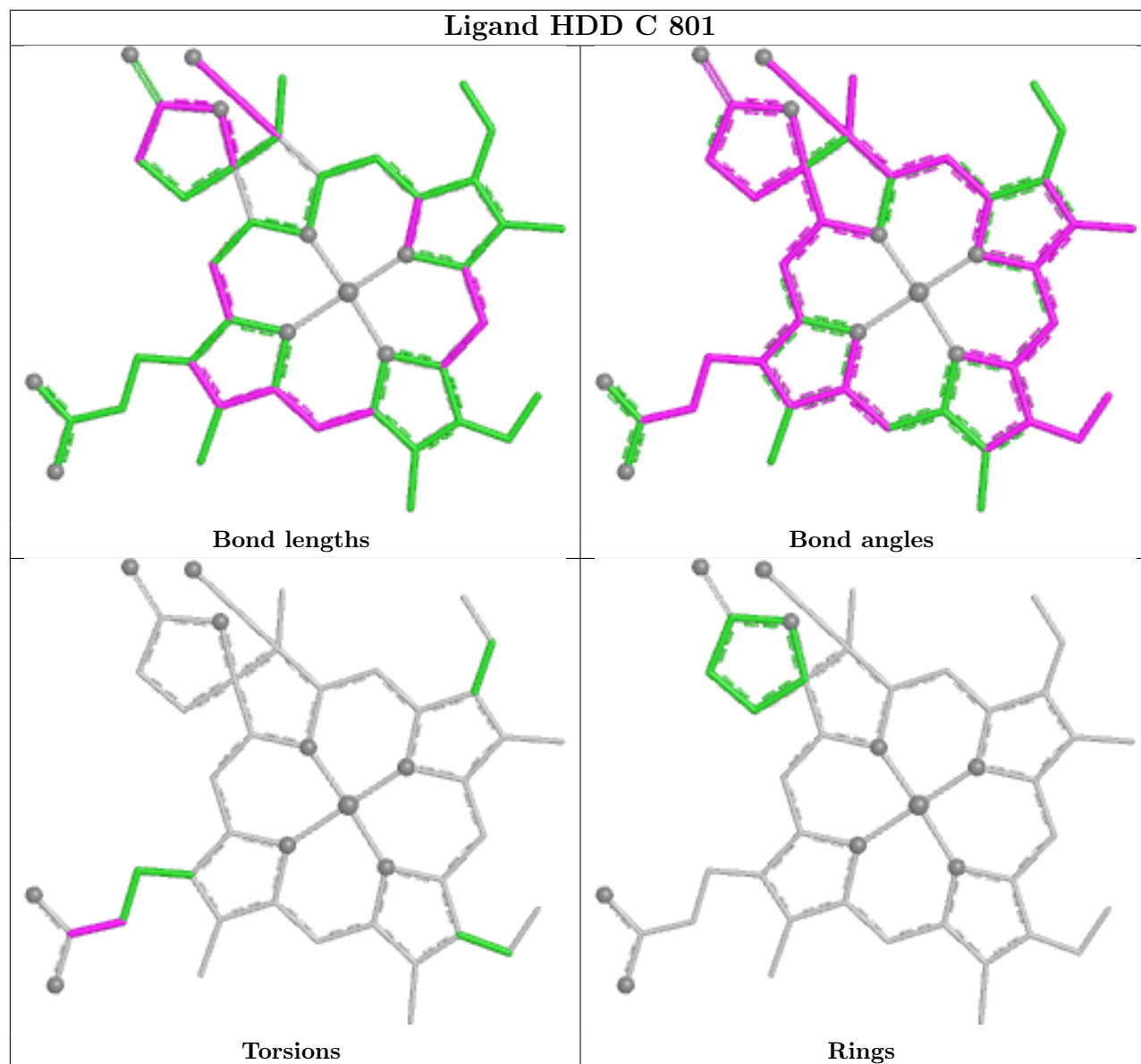
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	801	HDD	1	0
2	C	801	HDD	3	0
2	A	801	HDD	1	0

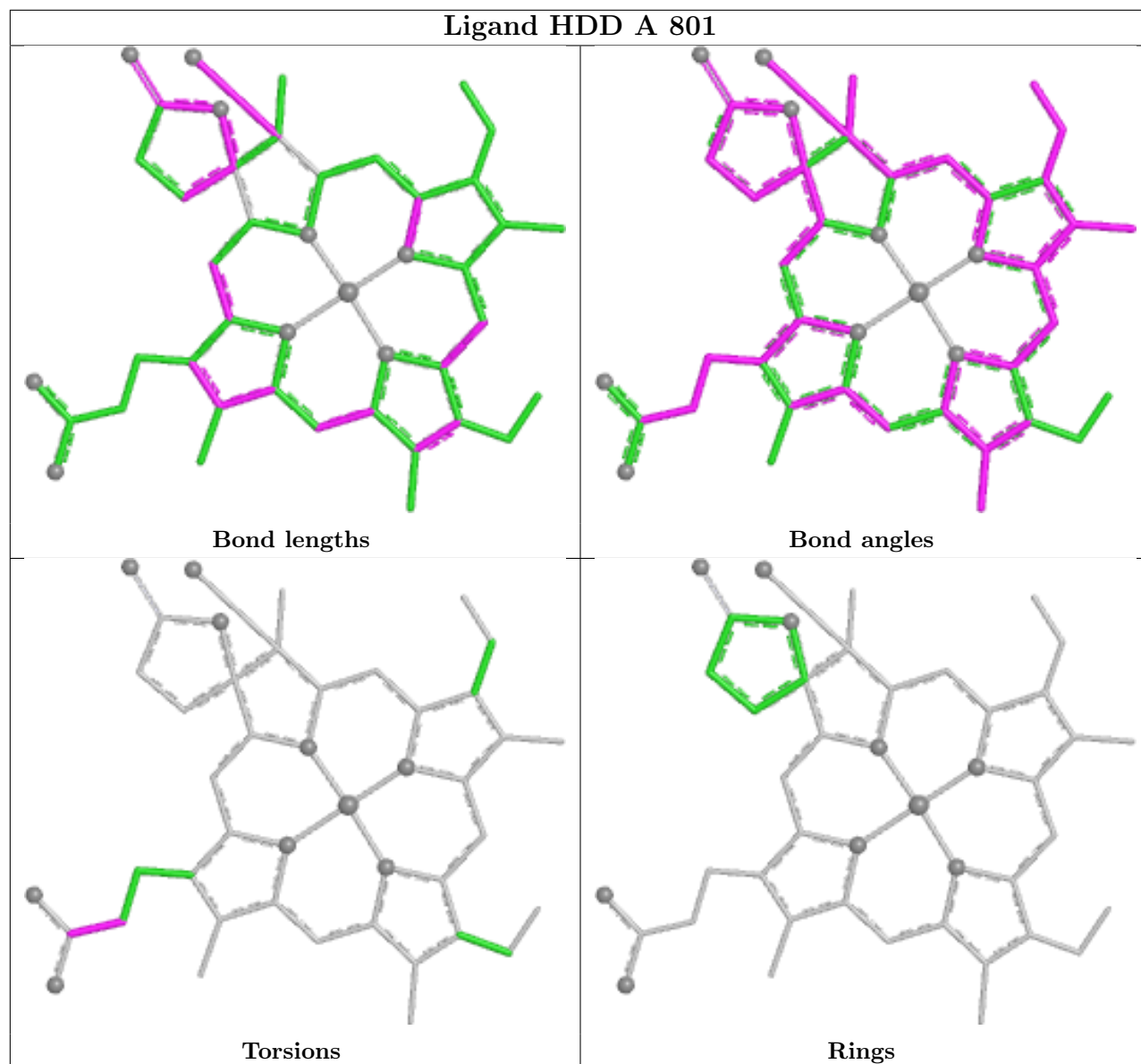
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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%)	-0.80	0	100 100	5, 11, 26, 54	5 (0%)
1	B	725/753 (96%)	-0.64	1 (0%)	92 92	5, 13, 36, 58	4 (0%)
1	C	725/753 (96%)	-0.68	2 (0%)	90 91	4, 12, 35, 54	7 (0%)
1	D	725/753 (96%)	-0.76	2 (0%)	90 91	5, 11, 28, 56	5 (0%)
All	All	2900/3012 (96%)	-0.72	5 (0%)	91 92	4, 12, 32, 58	21 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	28	SER	3.1
1	C	751	ILE	2.9
1	D	749	ASP	2.5
1	C	750	LYS	2.2
1	B	726	GLY	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	C	669	9/10	0.92	0.10	27,31,41,44	0
1	OCS	B	669	9/10	0.93	0.09	29,31,40,46	0
1	OCS	D	669	9/10	0.93	0.10	19,23,28,38	0
1	OCS	A	669	9/10	0.94	0.09	16,20,31,38	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

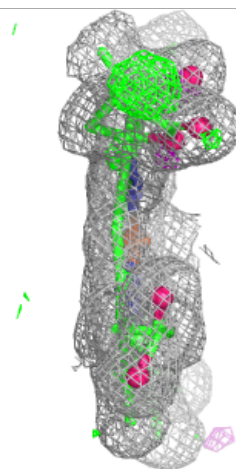
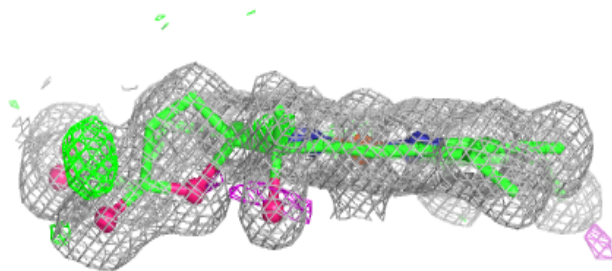
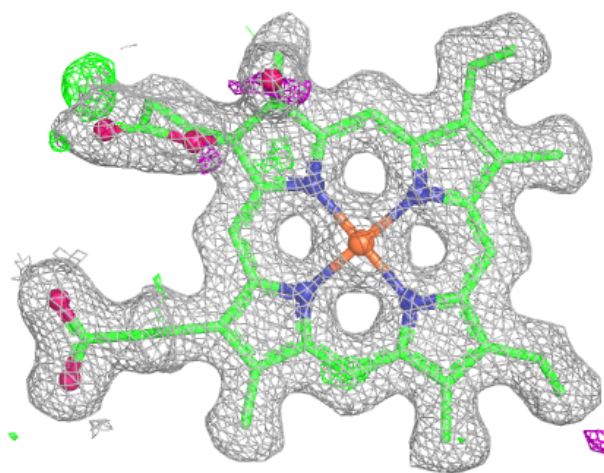
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HDD	A	801	44/44	0.99	0.04	5,6,13,16	0
2	HDD	B	801	44/44	0.99	0.04	6,7,13,17	0
2	HDD	C	801	44/44	0.99	0.04	6,7,15,18	0
2	HDD	D	801	44/44	0.99	0.04	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.

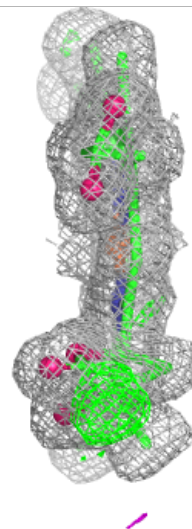
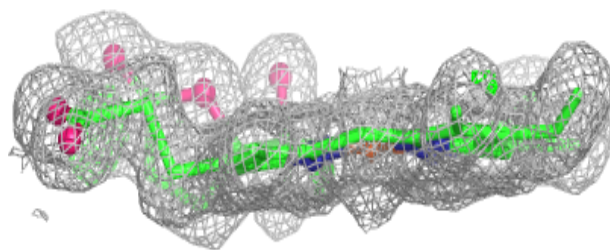
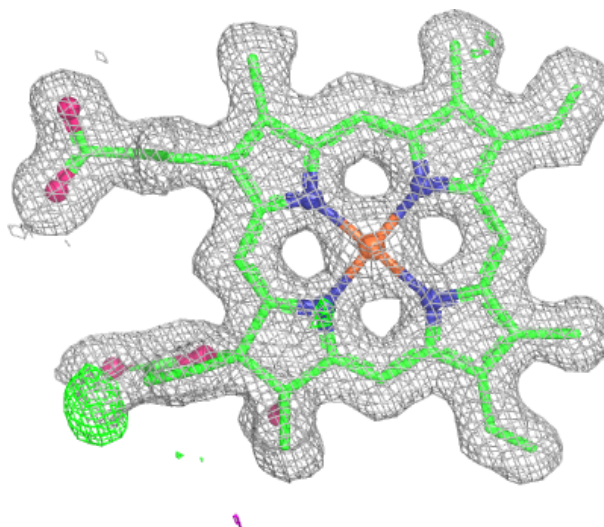
Electron density around HDD A 801:

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



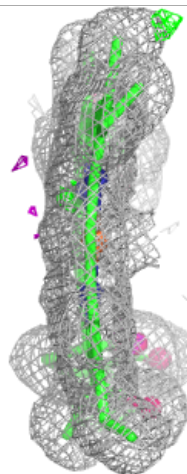
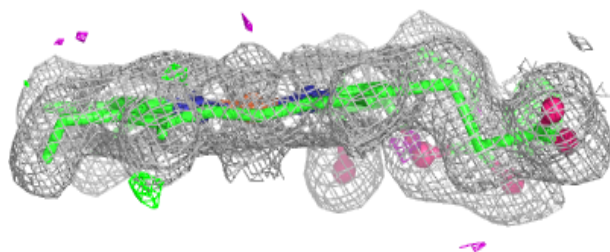
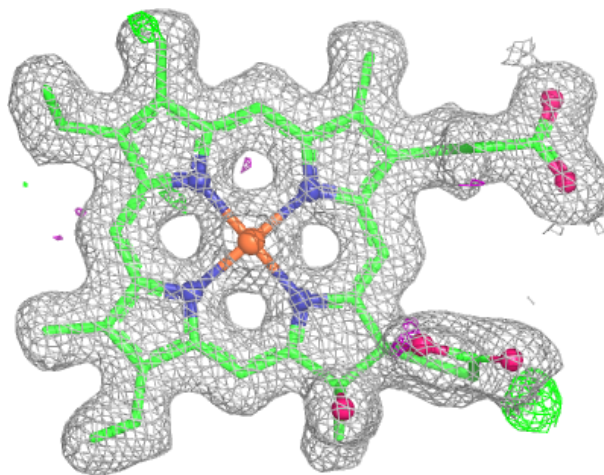
Electron density around HDD B 801:

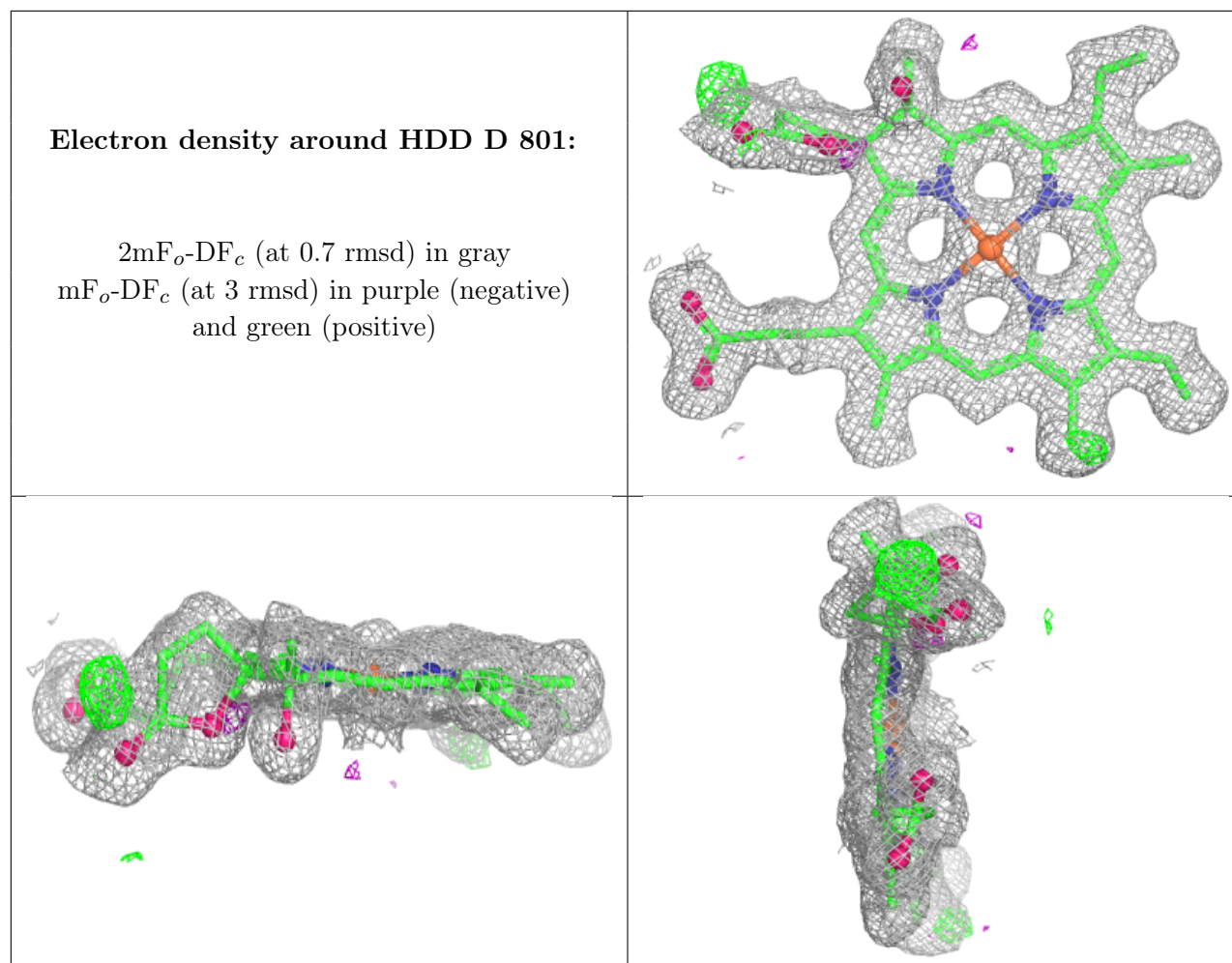
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.