



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:44 PM UTC

PDB ID : 4ENW / pdb_00004enw
Title : Structure of the S234N variant of E. coli KatE
Authors : Loewen, P.C.; Jha, V.
Deposited on : 2012-04-13
Resolution : 1.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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

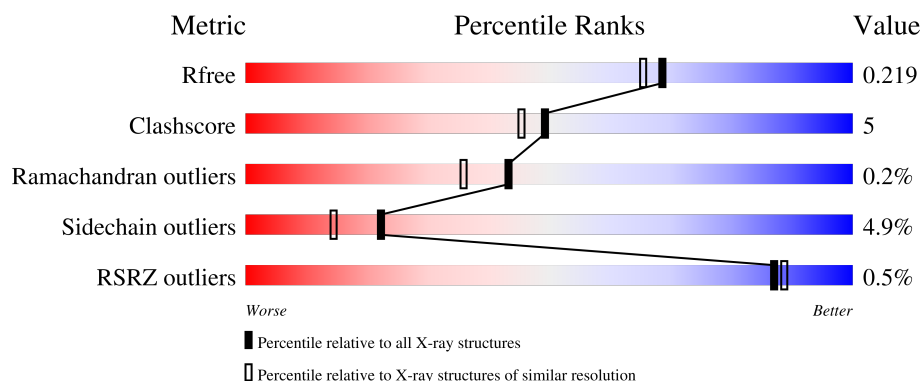
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	% 85% 10% ...
1	B	753	% 82% 12% ...
1	C	753	% 81% 14% ...
1	D	753	% 81% 13% ...

2 Entry composition

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

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

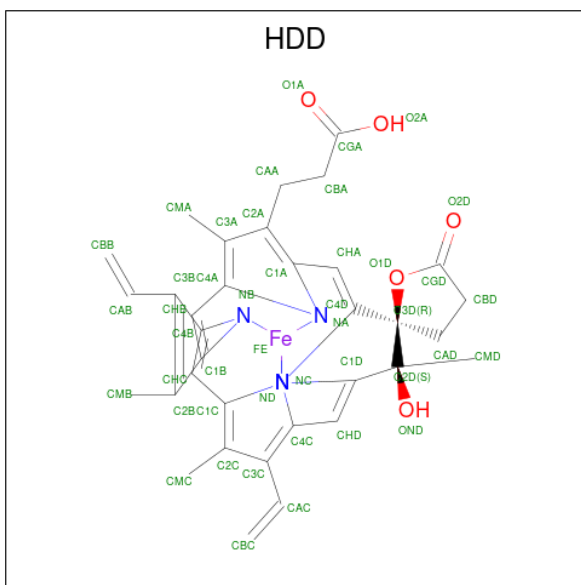
- Molecule 1 is a protein called Catalase HP11.

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (CCD ID: HDD) (formula: C₃₄H₃₂FeN₄O₅).



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

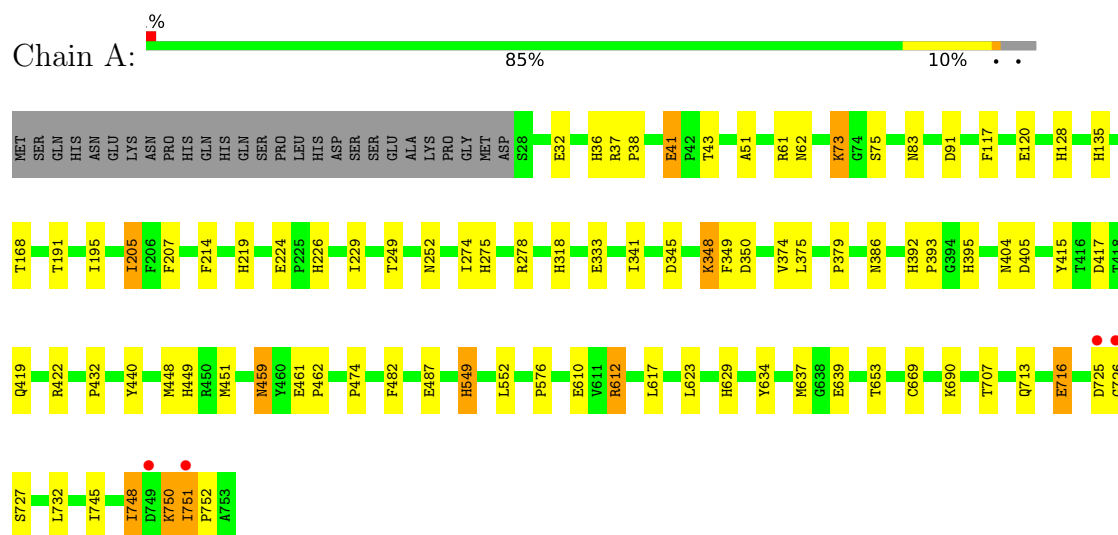
- Molecule 3 is water.

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

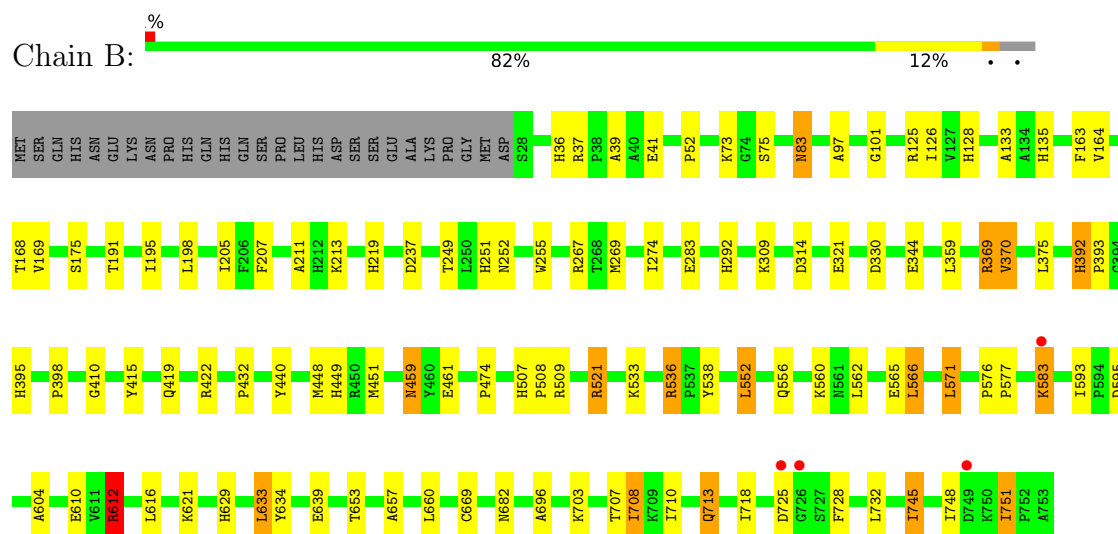
3 Residue-property plots

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.

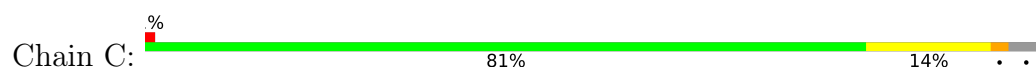
• Molecule 1: Catalase HP1I

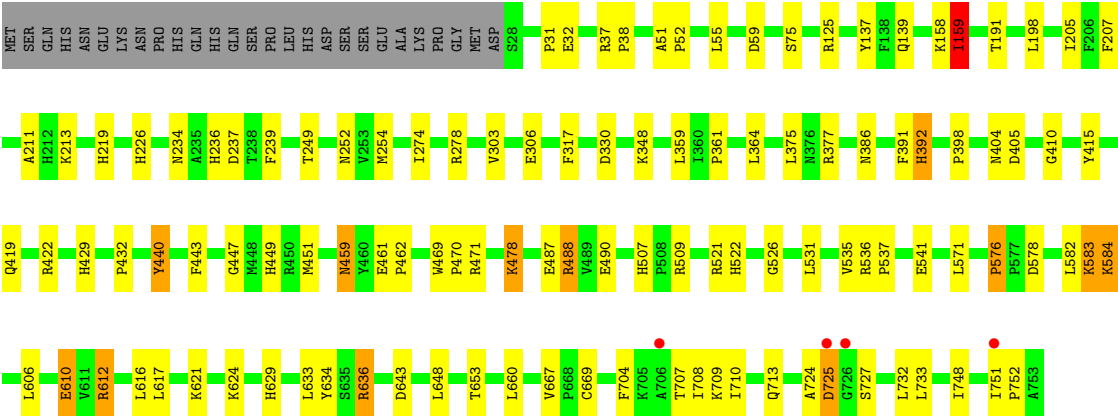


• Molecule 1: Catalase HP1I

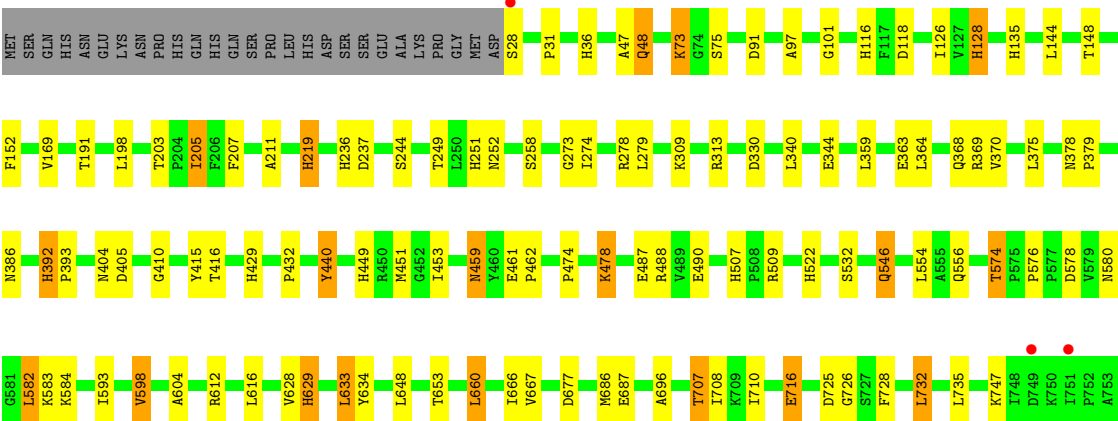
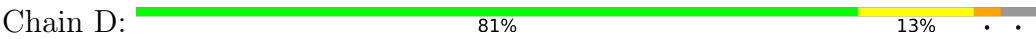


• Molecule 1: Catalase HP1I





● Molecule 1: Catalase HP11



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.39Å 132.57Å 122.57Å 90.00° 109.23° 90.00°	Depositor
Resolution (Å)	35.13 – 1.90 35.13 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.4 (35.13-1.90) 93.4 (35.13-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.66 (at 1.89Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.175 , 0.221 0.174 , 0.219	Depositor DCC
R_{free} test set	10355 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	11.0	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25927	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

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

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: 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	1.28	16/5907 (0.3%)	1.17	12/8031 (0.1%)
1	B	1.25	10/5907 (0.2%)	1.17	19/8031 (0.2%)
1	C	1.24	7/5915 (0.1%)	1.15	13/8042 (0.2%)
1	D	1.31	16/5916 (0.3%)	1.17	15/8043 (0.2%)
All	All	1.27	49/23645 (0.2%)	1.17	59/32147 (0.2%)

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 (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	392	HIS	ND1-CE1	8.60	1.41	1.32
1	D	474	PRO	CA-C	8.36	1.56	1.51
1	B	474	PRO	CA-C	7.15	1.55	1.51
1	B	392	HIS	ND1-CE1	7.00	1.39	1.32
1	A	474	PRO	CA-C	6.77	1.55	1.51
1	D	128	HIS	CB-CG	6.71	1.59	1.50
1	A	214	PHE	C-O	-6.68	1.18	1.24
1	D	522	HIS	CG-CD2	6.45	1.43	1.35
1	D	274	ILE	N-CA	6.38	1.54	1.46
1	B	292	HIS	CE1-NE2	6.23	1.38	1.32
1	D	660	LEU	N-CA	6.09	1.54	1.46
1	D	135	HIS	ND1-CE1	5.85	1.38	1.32
1	D	416	THR	C-O	5.77	1.30	1.24
1	A	549	HIS	CG-CD2	5.76	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	522	HIS	ND1-CE1	5.74	1.38	1.32
1	A	135	HIS	CG-CD2	5.72	1.42	1.35
1	B	395	HIS	ND1-CE1	5.72	1.38	1.32
1	A	275	HIS	CE1-NE2	5.71	1.38	1.32
1	C	392	HIS	ND1-CE1	5.66	1.38	1.32
1	D	219	HIS	CD2-NE2	-5.63	1.31	1.37
1	A	482	PHE	C-O	-5.58	1.17	1.24
1	D	251	HIS	CG-CD2	5.53	1.42	1.35
1	B	269	MET	C-O	5.52	1.30	1.23
1	A	629	HIS	ND1-CE1	5.49	1.38	1.32
1	D	236	HIS	CG-CD2	5.46	1.41	1.35
1	B	135	HIS	ND1-CE1	5.44	1.38	1.32
1	D	203	THR	N-CA	5.43	1.50	1.45
1	D	379	PRO	N-CA	-5.43	1.40	1.47
1	A	229	ILE	CA-C	5.41	1.58	1.52
1	C	236	HIS	CE1-NE2	5.38	1.38	1.32
1	D	453	ILE	C-O	5.33	1.30	1.24
1	C	526	GLY	N-CA	5.29	1.52	1.45
1	B	255	TRP	CD2-CE2	5.26	1.50	1.41
1	A	318	HIS	CG-CD2	5.26	1.41	1.35
1	A	549	HIS	ND1-CE1	5.25	1.37	1.32
1	D	116	HIS	CG-ND1	-5.25	1.32	1.38
1	A	395	HIS	ND1-CE1	5.22	1.37	1.32
1	B	36	HIS	CE1-NE2	5.20	1.37	1.32
1	B	168	THR	N-CA	5.20	1.51	1.45
1	C	391	PHE	N-CA	5.19	1.52	1.45
1	B	83	ASN	N-CA	5.15	1.53	1.46
1	C	576	PRO	CA-C	5.14	1.56	1.52
1	C	522	HIS	CG-CD2	5.12	1.41	1.35
1	A	623	LEU	N-CA	5.07	1.52	1.46
1	A	117	PHE	C-O	5.05	1.30	1.24
1	A	226	HIS	ND1-CE1	5.05	1.37	1.32
1	C	226	HIS	N-CA	5.04	1.52	1.46
1	A	43	THR	CA-CB	5.03	1.61	1.54
1	A	379	PRO	CA-C	5.03	1.58	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	139	GLN	CA-C-N	-8.67	111.81	120.31
1	C	139	GLN	C-N-CA	-8.67	111.81	120.31
1	D	478	LYS	CD-CE-NZ	7.17	134.84	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	378	ASN	CA-C-N	6.95	127.36	119.92
1	D	378	ASN	C-N-CA	6.95	127.36	119.92
1	C	725	ASP	N-CA-C	6.91	125.51	110.80
1	D	574	THR	CB-CA-C	6.82	119.29	109.26
1	D	667	VAL	CA-C-N	-6.81	113.50	120.85
1	D	667	VAL	C-N-CA	-6.81	113.50	120.85
1	B	474	PRO	CA-C-N	-6.76	113.33	120.03
1	B	474	PRO	C-N-CA	-6.76	113.33	120.03
1	D	478	LYS	CB-CG-CD	6.60	126.47	111.30
1	B	745	ILE	CA-C-N	-6.52	112.28	119.19
1	B	745	ILE	C-N-CA	-6.52	112.28	119.19
1	B	657	ALA	CA-C-N	6.12	127.49	119.84
1	B	657	ALA	C-N-CA	6.12	127.49	119.84
1	B	560	LYS	N-CA-C	-6.07	104.58	111.14
1	C	667	VAL	CA-C-N	-6.02	114.56	120.52
1	C	667	VAL	C-N-CA	-6.02	114.56	120.52
1	B	370	VAL	CB-CA-C	6.00	116.53	110.65
1	D	629	HIS	N-CA-C	5.96	118.60	110.55
1	A	120	GLU	N-CA-C	5.87	118.46	111.71
1	B	370	VAL	N-CA-CB	-5.85	104.22	112.12
1	C	748	ILE	N-CA-C	5.84	119.27	111.44
1	A	349	PHE	CA-C-N	-5.83	113.32	122.65
1	A	349	PHE	C-N-CA	-5.83	113.32	122.65
1	D	273	GLY	N-CA-C	-5.79	107.74	115.32
1	D	152	PHE	N-CA-C	5.74	119.76	112.87
1	B	126	ILE	CB-CA-C	-5.74	104.40	112.14
1	D	735	LEU	N-CA-C	-5.73	105.11	111.36
1	C	348	LYS	CA-CB-CG	-5.67	102.75	114.10
1	A	745	ILE	CA-C-N	-5.61	113.11	119.28
1	A	745	ILE	C-N-CA	-5.61	113.11	119.28
1	C	159	ILE	CB-CG1-CD1	-5.51	102.22	113.80
1	A	751	ILE	N-CA-C	5.49	113.35	108.63
1	D	258	SER	N-CA-C	-5.42	102.88	110.35
1	C	317	PHE	N-CA-C	5.39	117.58	111.11
1	D	126	ILE	CB-CA-C	-5.35	104.92	112.14
1	D	237	ASP	N-CA-C	5.34	117.52	111.11
1	A	214	PHE	CA-C-N	-5.33	113.54	119.19
1	A	214	PHE	C-N-CA	-5.33	113.54	119.19
1	C	159	ILE	CB-CA-C	5.32	118.75	110.83
1	A	748	ILE	N-CA-C	5.25	119.80	112.50
1	A	350	ASP	CB-CA-C	5.21	119.37	110.56
1	C	447	GLY	N-CA-C	-5.18	106.15	112.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	37	ARG	CA-C-N	-5.16	114.64	119.85
1	B	37	ARG	C-N-CA	-5.16	114.64	119.85
1	B	593	ILE	CA-C-N	5.16	126.29	119.84
1	B	593	ILE	C-N-CA	5.16	126.29	119.84
1	B	314	ASP	CA-C-N	-5.15	114.52	119.87
1	B	314	ASP	C-N-CA	-5.15	114.52	119.87
1	A	41	GLU	CB-CA-C	-5.13	100.55	109.32
1	D	707	THR	CB-CA-C	-5.10	102.32	110.79
1	B	536	ARG	CA-C-N	-5.06	113.72	119.28
1	B	536	ARG	C-N-CA	-5.06	113.72	119.28
1	B	163	PHE	N-CA-C	-5.04	99.76	108.69
1	C	158	LYS	CA-C-N	-5.04	116.94	123.19
1	C	158	LYS	C-N-CA	-5.04	116.94	123.19
1	A	726	GLY	N-CA-C	-5.03	106.62	113.37

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	5747	0	5582	53	0
1	B	5747	0	5582	68	0
1	C	5752	0	5593	75	1
1	D	5753	0	5589	64	0
2	A	44	0	31	2	0
2	B	44	0	31	4	0
2	C	44	0	31	3	0
2	D	44	0	31	2	0
3	A	730	0	0	7	0
3	B	629	0	0	11	1
3	C	649	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	744	0	0	9	0
All	All	25927	0	22470	245	1

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

All (245) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:HIS:ND1	1:A:415:TYR:CB	1.71	1.54
1:D:392:HIS:ND1	1:D:415:TYR:CB	1.69	1.53
1:B:392:HIS:ND1	1:B:415:TYR:CB	1.72	1.49
1:C:392:HIS:ND1	1:C:415:TYR:CB	1.71	1.49
3:B:1463:HOH:O	1:D:73:LYS:HD3	1.33	1.27
1:D:392:HIS:CE1	1:D:415:TYR:HB2	1.78	1.17
1:A:392:HIS:CE1	1:A:415:TYR:HB2	1.80	1.17
1:C:392:HIS:CE1	1:C:415:TYR:HB2	1.79	1.17
1:B:392:HIS:CE1	1:B:415:TYR:HB2	1.83	1.13
1:B:451:MET:HE2	1:D:451:MET:HE2	1.12	1.11
1:C:392:HIS:ND1	1:C:415:TYR:HB2	0.77	1.09
1:B:392:HIS:ND1	1:B:415:TYR:HB2	0.77	1.09
1:B:369:ARG:HG2	3:B:1296:HOH:O	1.51	1.08
1:A:392:HIS:ND1	1:A:415:TYR:HB2	0.75	1.08
1:D:392:HIS:ND1	1:D:415:TYR:HB2	0.75	1.07
1:A:451:MET:HE2	1:C:451:MET:HE2	1.31	1.07
1:A:392:HIS:CG	1:A:415:TYR:HB2	1.95	1.00
1:C:440:TYR:HD1	3:C:1353:HOH:O	1.42	1.00
1:D:392:HIS:CG	1:D:415:TYR:HB2	1.98	0.97
1:A:716:GLU:HG2	3:A:1302:HOH:O	1.64	0.96
1:A:449[B]:HIS:CG	1:C:449[B]:HIS:CG	2.34	0.95
1:B:392:HIS:CG	1:B:415:TYR:HB2	2.01	0.94
1:C:392:HIS:CG	1:C:415:TYR:HB2	2.00	0.94
1:B:710:ILE:HD13	1:B:718:ILE:HG13	1.51	0.93
1:A:639:GLU:HG3	3:A:1479:HOH:O	1.70	0.92
1:A:716:GLU:CG	3:A:1302:HOH:O	2.18	0.89
1:B:708:ILE:HD12	1:B:710:ILE:HD11	1.52	0.89
1:B:708:ILE:HD12	1:B:710:ILE:CD1	2.03	0.88
1:B:583:LYS:NZ	1:B:583:LYS:H	1.73	0.86
1:A:449[B]:HIS:CG	1:C:449[B]:HIS:ND1	2.04	0.86
1:C:610:GLU:OE1	1:C:643:ASP:HA	1.76	0.86
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:612:ARG:HH11	1:C:612:ARG:HG3	1.45	0.81
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.63	0.79
1:A:449[B]:HIS:ND1	1:C:449[B]:HIS:CG	2.09	0.78
1:B:451:MET:CE	1:D:451:MET:HE2	2.06	0.78
1:A:274:ILE:HD12	2:A:801:HDD:HMB3	1.66	0.77
1:C:612:ARG:HH11	1:C:612:ARG:CG	1.98	0.74
1:D:629:HIS:HD2	3:D:1259:HOH:O	1.70	0.74
1:D:598:VAL:HG13	1:D:628:VAL:CG2	2.19	0.73
1:A:73:LYS:HE2	1:C:440:TYR:O	1.89	0.72
1:D:368:GLN:OE1	3:D:1555:HOH:O	2.07	0.71
1:C:274:ILE:HD12	2:C:801:HDD:HMB3	1.72	0.70
1:A:690:LYS:HG3	1:A:751:ILE:HD11	1.72	0.70
1:A:392:HIS:ND1	1:A:415:TYR:CG	2.58	0.70
1:A:751:ILE:HD12	1:A:751:ILE:O	1.92	0.69
1:B:419:GLN:HE22	1:B:422:ARG:HH21	1.41	0.68
1:B:583:LYS:H	1:B:583:LYS:HZ2	1.41	0.67
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.77	0.67
1:B:612:ARG:NH1	1:B:669:CYS:SG	2.68	0.67
1:C:488:ARG:HD3	3:C:1429:HOH:O	1.94	0.67
1:C:636:ARG:HD3	3:C:1478:HOH:O	1.93	0.66
1:C:583:LYS:O	1:C:584:LYS:HB3	1.96	0.66
1:C:751:ILE:HG13	1:C:752:PRO:HD2	1.79	0.65
1:B:556:GLN:HG2	1:B:566:LEU:HD23	1.78	0.65
1:B:552:LEU:CD2	1:B:571:LEU:HD12	2.27	0.63
1:C:629:HIS:HD2	3:C:1201:HOH:O	1.79	0.63
1:C:469:TRP:CE3	1:C:471:ARG:HG3	2.34	0.63
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.29	0.63
1:B:710:ILE:CD1	1:B:718:ILE:HG13	2.28	0.62
1:C:612:ARG:NH1	1:C:612:ARG:HB2	2.14	0.62
1:C:578:ASP:HB2	1:C:582:LEU:O	1.99	0.62
1:C:584:LYS:NZ	3:C:1286:HOH:O	2.25	0.61
1:B:583:LYS:H	1:B:583:LYS:HZ3	1.45	0.61
1:D:392:HIS:ND1	1:D:415:TYR:HB3	2.05	0.61
1:C:392:HIS:ND1	1:C:415:TYR:CG	2.64	0.61
1:D:598:VAL:HG13	1:D:628:VAL:HG22	1.83	0.60
1:B:708:ILE:HD12	1:B:710:ILE:HD12	1.83	0.60
1:C:125:ARG:HB3	2:C:801:HDD:HBD1	1.84	0.59
1:D:708:ILE:HG13	1:D:710:ILE:HG12	1.83	0.59
1:B:125:ARG:HB3	2:B:801:HDD:HBD1	1.85	0.58
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.12	0.58
1:B:629:HIS:HD2	3:B:1159:HOH:O	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ASP:HA	1:A:348:LYS:HG3	1.86	0.58
1:C:37:ARG:NH1	3:C:1345:HOH:O	2.33	0.58
1:C:727:SER:HA	3:C:1477:HOH:O	2.03	0.58
1:D:716:GLU:HG3	3:D:938:HOH:O	2.04	0.57
1:C:583:LYS:HG2	3:C:1501:HOH:O	2.04	0.57
1:B:274:ILE:HD12	2:B:801:HDD:HMB3	1.86	0.57
1:A:36:HIS:CD2	1:A:36:HIS:H	2.23	0.56
1:D:392:HIS:ND1	1:D:415:TYR:CG	2.66	0.56
1:D:509:ARG:HD2	1:D:576:PRO:HD2	1.86	0.56
1:C:704:PHE:O	1:C:707:THR:HG22	2.06	0.56
1:D:278:ARG:HH12	1:D:487:GLU:CD	2.15	0.55
3:B:1463:HOH:O	1:D:73:LYS:CD	2.16	0.55
1:D:392:HIS:CG	1:D:415:TYR:CB	2.75	0.54
1:C:38:PRO:HG2	1:C:51:ALA:HB2	1.88	0.54
1:B:211:ALA:CB	1:B:410:GLY:HA3	2.37	0.54
1:D:556:GLN:NE2	3:D:1572:HOH:O	2.39	0.54
1:B:509:ARG:HD2	1:B:576:PRO:HD2	1.90	0.54
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.91	0.54
1:A:725:ASP:OD1	1:A:727:SER:HB3	2.08	0.53
1:B:612:ARG:HB2	1:B:612:ARG:CZ	2.38	0.53
1:B:521:ARG:CB	1:B:521:ARG:HH21	2.20	0.53
1:C:359:LEU:H	1:C:507:HIS:HD2	1.57	0.53
1:B:448:MET:HG3	1:B:449[B]:HIS:CD2	2.43	0.53
1:C:541:GLU:HG2	3:C:1544:HOH:O	2.09	0.53
1:C:634:TYR:O	1:C:653:THR:HA	2.09	0.52
1:D:359:LEU:H	1:D:507:HIS:HD2	1.57	0.52
1:A:392:HIS:CG	1:A:415:TYR:CB	2.74	0.51
2:C:801:HDD:HBD2	3:C:1083:HOH:O	2.10	0.51
1:C:52:PRO:HG2	1:C:55:LEU:HD12	1.93	0.50
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.94	0.50
1:C:612:ARG:CG	1:C:612:ARG:NH1	2.67	0.50
1:B:459:ASN:HD22	1:B:459:ASN:H	1.59	0.50
1:C:612:ARG:HH11	1:C:612:ARG:CB	2.25	0.50
1:B:309:LYS:HD2	1:B:660:LEU:HD11	1.93	0.50
1:A:750:LYS:HE3	1:D:677:ASP:HB3	1.93	0.49
1:B:392:HIS:ND1	1:B:415:TYR:CA	2.68	0.49
1:D:205:ILE:H	1:D:205:ILE:HD13	1.78	0.49
1:A:610:GLU:HG3	3:A:1513:HOH:O	2.11	0.49
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.95	0.49
1:B:533:LYS:HD2	3:B:1456:HOH:O	2.12	0.49
1:A:91:ASP:OD1	1:C:461:GLU:OE1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:708:ILE:CD1	1:B:710:ILE:HD12	2.41	0.49
1:C:440:TYR:CD1	3:C:1353:HOH:O	2.31	0.49
1:D:578:ASP:OD1	1:D:583:LYS:HE3	2.12	0.49
1:B:52:PRO:HG3	3:D:1191:HOH:O	2.13	0.49
1:C:478:LYS:HB2	3:C:1532:HOH:O	2.13	0.49
1:B:359:LEU:H	1:B:507:HIS:HD2	1.60	0.49
1:B:39:ALA:HB1	1:B:41:GLU:HG2	1.95	0.48
1:B:552:LEU:C	1:B:552:LEU:HD13	2.38	0.48
1:C:392:HIS:CG	1:C:415:TYR:CB	2.78	0.48
1:A:448:MET:O	1:A:449[B]:HIS:HB2	2.14	0.48
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.29	0.48
1:B:392:HIS:CG	1:B:415:TYR:CB	2.79	0.48
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.43	0.48
1:C:361:PRO:HD2	1:C:364:LEU:HD12	1.96	0.48
1:C:207:PHE:O	1:C:249:THR:HA	2.12	0.47
1:D:440:TYR:C	1:D:440:TYR:CD2	2.92	0.47
1:D:386:ASN:OD1	1:D:386:ASN:C	2.57	0.47
1:D:459:ASN:HD22	1:D:459:ASN:H	1.62	0.47
1:A:461:GLU:HA	1:A:462:PRO:C	2.38	0.47
1:A:128:HIS:HA	1:A:168:THR:O	2.15	0.47
1:B:175:SER:HB2	3:B:1096:HOH:O	2.15	0.47
1:B:552:LEU:HD13	1:B:552:LEU:O	2.14	0.47
1:C:211:ALA:CB	1:C:410:GLY:HA3	2.45	0.47
1:C:359:LEU:H	1:C:507:HIS:CD2	2.33	0.47
1:D:478:LYS:HE3	3:D:1499:HOH:O	2.14	0.47
1:D:634:TYR:O	1:D:653:THR:HA	2.14	0.47
1:A:386:ASN:OD1	1:A:386:ASN:C	2.57	0.47
1:B:251:HIS:HA	1:B:508:PRO:HG3	1.96	0.47
1:D:363:GLU:HB2	1:D:582:LEU:HD21	1.97	0.47
1:B:128:HIS:CE1	1:B:169:VAL:HG22	2.49	0.47
1:C:612:ARG:NH2	1:C:669:CYS:SG	2.88	0.47
1:A:207:PHE:O	1:A:249:THR:HA	2.14	0.47
1:C:610:GLU:O	1:C:610:GLU:HG3	2.14	0.46
1:C:704:PHE:O	1:C:707:THR:CG2	2.63	0.46
1:A:419:GLN:HE22	1:A:422:ARG:HH11	1.63	0.46
1:B:696:ALA:HB1	1:B:728:PHE:CZ	2.50	0.46
1:C:461:GLU:HB2	1:C:462:PRO:HA	1.98	0.46
1:C:509:ARG:HD2	1:C:576:PRO:HD2	1.97	0.46
1:A:612:ARG:HH11	1:A:669:CYS:CB	2.29	0.46
1:B:392:HIS:ND1	1:B:415:TYR:CG	2.69	0.46
1:B:538:TYR:CD2	1:C:31:PRO:HG3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:ARG:HG3	1:D:660:LEU:HD12	1.98	0.46
1:A:61:ARG:HD2	3:A:1626:HOH:O	2.15	0.46
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.31	0.46
1:A:61:ARG:HG2	1:A:61:ARG:HH11	1.81	0.46
1:A:549:HIS:O	1:A:576:PRO:HD3	2.15	0.46
2:B:801:HDD:HMD3	2:B:801:HDD:HAD2	1.57	0.45
1:B:393:PRO:HD2	1:B:415:TYR:CD2	2.51	0.45
1:B:748:ILE:O	1:B:751:ILE:HG22	2.16	0.45
1:C:612:ARG:NH1	1:C:612:ARG:CB	2.79	0.45
1:D:309:LYS:HE2	1:D:687:GLU:OE2	2.16	0.45
1:A:83:ASN:HB3	1:C:429:HIS:CG	2.52	0.45
1:D:31:PRO:HD2	1:D:36:HIS:HB3	1.99	0.45
1:D:666:ILE:HD11	1:D:732:LEU:CD1	2.47	0.45
1:D:207:PHE:O	1:D:249:THR:HA	2.15	0.45
1:D:725:ASP:OD1	1:D:725:ASP:C	2.60	0.45
1:C:461:GLU:HA	1:C:462:PRO:C	2.42	0.44
1:A:637:MET:HG3	1:D:532:SER:HB2	1.97	0.44
1:C:237:ASP:OD2	1:C:536:ARG:HG3	2.17	0.44
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.32	0.44
1:C:330:ASP:OD1	1:C:629:HIS:CE1	2.66	0.44
1:B:448:MET:O	1:B:449[B]:HIS:HB2	2.18	0.44
2:B:801:HDD:HBD2	3:B:1039:HOH:O	2.18	0.44
1:C:419:GLN:HE22	1:C:422:ARG:HH11	1.65	0.44
1:C:459:ASN:H	1:C:459:ASN:HD22	1.66	0.44
1:D:364:LEU:HD11	1:D:580:ASN:HB2	2.01	0.43
1:D:393:PRO:HD2	1:D:415:TYR:CG	2.53	0.43
2:D:801:HDD:HBD2	3:D:1139:HOH:O	2.18	0.43
1:A:333:GLU:HG2	1:A:374:VAL:HG22	2.00	0.43
1:C:440:TYR:OH	3:C:1135:HOH:O	2.20	0.43
1:D:244:SER:HA	1:D:546[B]:GLN:OE1	2.19	0.43
1:C:386:ASN:OD1	1:C:386:ASN:C	2.61	0.43
1:C:443:PHE:CZ	1:C:470:PRO:HD2	2.54	0.43
1:B:73:LYS:NZ	3:B:1232:HOH:O	2.51	0.43
1:A:205:ILE:HD13	1:A:205:ILE:H	1.84	0.43
1:B:267:ARG:HD2	3:B:1132:HOH:O	2.19	0.43
1:B:745:ILE:O	1:B:748:ILE:HG12	2.19	0.43
1:C:137:TYR:HB2	1:C:159:ILE:HD12	2.01	0.43
1:C:490:GLU:OE1	1:D:488:ARG:NH2	2.45	0.43
1:A:459:ASN:HD22	1:A:459:ASN:H	1.65	0.42
1:A:634:TYR:O	1:A:653:THR:HA	2.18	0.42
1:B:133:ALA:HA	1:B:164:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:GLN:HE22	1:B:422:ARG:NH2	2.13	0.42
1:A:224:GLU:OE1	3:A:1024:HOH:O	2.22	0.42
1:A:751:ILE:HA	1:A:752:PRO:HD3	1.97	0.42
1:D:28:SER:N	3:D:1638:HOH:O	2.53	0.42
1:D:148:THR:HB	1:D:279:LEU:HB3	2.02	0.42
1:A:748:ILE:O	1:A:751:ILE:HG13	2.19	0.42
1:B:97:ALA:O	1:B:101:GLY:HA3	2.19	0.42
1:B:634:TYR:O	1:B:653:THR:HA	2.19	0.42
1:D:128:HIS:CE1	1:D:169:VAL:HG22	2.55	0.42
1:C:303:VAL:O	1:C:306:GLU:HB3	2.19	0.42
1:D:97:ALA:O	1:D:101:GLY:HA3	2.19	0.42
1:D:696:ALA:HB1	1:D:728:PHE:CZ	2.55	0.42
1:B:713:GLN:NE2	1:B:713:GLN:H	2.18	0.42
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.35	0.42
1:A:38:PRO:HG2	1:A:51:ALA:HB2	2.02	0.42
1:B:521:ARG:HH21	1:B:521:ARG:HB2	1.83	0.42
1:C:278:ARG:HH12	1:C:487:GLU:CD	2.28	0.42
1:D:686:MET:HG3	1:D:707:THR:HG22	2.00	0.42
1:A:62:ASN:OD1	1:A:62:ASN:C	2.62	0.42
1:A:393:PRO:HD2	1:A:415:TYR:CD2	2.55	0.41
1:A:751:ILE:HD12	1:A:751:ILE:C	2.43	0.41
1:B:461:GLU:OE1	1:D:91:ASP:OD1	2.38	0.41
1:C:404:ASN:O	1:C:405:ASP:C	2.61	0.41
2:D:801:HDD:HAD2	2:D:801:HDD:HMD3	1.60	0.41
1:C:234:ASN:HB3	1:C:239:PHE:CD2	2.56	0.41
2:A:801:HDD:HMC1	2:A:801:HDD:CBC	2.50	0.41
1:D:404:ASN:O	1:D:405:ASP:C	2.62	0.41
1:B:207:PHE:O	1:B:249:THR:HA	2.20	0.41
3:B:1330:HOH:O	1:D:449[A]:HIS:HE1	2.03	0.41
1:C:535:VAL:O	1:C:537:PRO:HD3	2.20	0.41
1:B:552:LEU:HD11	1:B:556:GLN:OE1	2.21	0.41
1:B:604:ALA:HB1	1:B:633:LEU:HD22	2.01	0.41
1:C:405:ASP:C	1:C:405:ASP:OD1	2.64	0.41
1:A:417:ASP:OD2	1:D:118:ASP:OD1	2.38	0.41
1:D:144:LEU:HD11	1:D:370:VAL:HG13	2.03	0.41
1:D:726:GLY:O	3:D:1500:HOH:O	2.22	0.41
1:B:577:PRO:HG2	3:B:1457:HOH:O	2.20	0.41
1:D:309:LYS:CE	1:D:687:GLU:OE2	2.69	0.41
1:C:624:LYS:HE2	3:C:1438:HOH:O	2.20	0.41
1:D:461:GLU:HA	1:D:462:PRO:C	2.45	0.41
1:D:359:LEU:H	1:D:507:HIS:CD2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ASN:HB3	1:D:429:HIS:CG	2.55	0.40
1:A:36:HIS:HE1	3:A:1350:HOH:O	2.04	0.40
1:A:637:MET:CG	1:D:532:SER:HB2	2.51	0.40
1:C:254:MET:HE3	1:C:254:MET:HB3	1.88	0.40
1:D:604:ALA:HB1	1:D:633:LEU:HD22	2.04	0.40
1:A:404:ASN:O	1:A:405:ASP:C	2.64	0.40
1:B:237:ASP:OD2	1:B:536:ARG:HG3	2.20	0.40
1:D:47:ALA:C	1:D:48:GLN:HG2	2.47	0.40

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

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	725/753 (96%)	706 (97%)	18 (2%)	1 (0%)	48	40
1	B	725/753 (96%)	702 (97%)	20 (3%)	3 (0%)	30	22
1	C	726/753 (96%)	710 (98%)	15 (2%)	1 (0%)	48	40
1	D	726/753 (96%)	704 (97%)	21 (3%)	1 (0%)	48	40
All	All	2902/3012 (96%)	2822 (97%)	74 (2%)	6 (0%)	43	36

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	725	ASP
1	B	612	ARG

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

5.3.2 Protein sidechains ⓘ

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%)	590 (96%)	22 (4%)	31	23
1	B	612/636 (96%)	577 (94%)	35 (6%)	18	11
1	C	613/636 (96%)	579 (94%)	34 (6%)	19	11
1	D	613/636 (96%)	584 (95%)	29 (5%)	23	15
All	All	2450/2544 (96%)	2330 (95%)	120 (5%)	22	14

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	37	ARG
1	A	41	GLU
1	A	73	LYS
1	A	191	THR
1	A	195	ILE
1	A	205	ILE
1	A	252	ASN
1	A	341	ILE
1	A	348	LYS
1	A	375	LEU
1	A	432	PRO
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	612	ARG
1	A	617	LEU

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Mol	Chain	Res	Type
1	A	707	THR
1	A	713	GLN
1	A	716	GLU
1	A	732	LEU
1	A	750	LYS
1	B	191	THR
1	B	195	ILE
1	B	198	LEU
1	B	205	ILE
1	B	213	LYS
1	B	252	ASN
1	B	283	GLU
1	B	321	GLU
1	B	344	GLU
1	B	369	ARG
1	B	370	VAL
1	B	375	LEU
1	B	398	PRO
1	B	432	PRO
1	B	440	TYR
1	B	459	ASN
1	B	521	ARG
1	B	552	LEU
1	B	562	LEU
1	B	565	GLU
1	B	566	LEU
1	B	571	LEU
1	B	583	LYS
1	B	595	ASP
1	B	610	GLU
1	B	612	ARG
1	B	616	LEU
1	B	621	LYS
1	B	633	LEU
1	B	639	GLU
1	B	703	LYS
1	B	708	ILE
1	B	713	GLN
1	B	732	LEU
1	B	751	ILE
1	C	32	GLU
1	C	159	ILE

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Mol	Chain	Res	Type
1	C	191	THR
1	C	198	LEU
1	C	205	ILE
1	C	213	LYS
1	C	252	ASN
1	C	375	LEU
1	C	377	ARG
1	C	398	PRO
1	C	432	PRO
1	C	440	TYR
1	C	459	ASN
1	C	478	LYS
1	C	488	ARG
1	C	521	ARG
1	C	531	LEU
1	C	571	LEU
1	C	583	LYS
1	C	584	LYS
1	C	606	LEU
1	C	610	GLU
1	C	612	ARG
1	C	616	LEU
1	C	617	LEU
1	C	621	LYS
1	C	633	LEU
1	C	636	ARG
1	C	648	LEU
1	C	660	LEU
1	C	709	LYS
1	C	713	GLN
1	C	732	LEU
1	C	733	LEU
1	D	48	GLN
1	D	73	LYS
1	D	191	THR
1	D	198	LEU
1	D	205	ILE
1	D	252	ASN
1	D	340	LEU
1	D	344	GLU
1	D	369	ARG
1	D	375	LEU

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Mol	Chain	Res	Type
1	D	432	PRO
1	D	440	TYR
1	D	459	ASN
1	D	490	GLU
1	D	546[A]	GLN
1	D	546[B]	GLN
1	D	554	LEU
1	D	574	THR
1	D	582	LEU
1	D	584	LYS
1	D	593	ILE
1	D	598	VAL
1	D	612	ARG
1	D	616	LEU
1	D	633	LEU
1	D	648	LEU
1	D	716	GLU
1	D	732	LEU
1	D	747	LYS

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

Mol	Chain	Res	Type
1	A	36	HIS
1	A	139	GLN
1	A	252	ASN
1	A	419	GLN
1	A	459	ASN
1	A	713	GLN
1	B	252	ASN
1	B	419	GLN
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	507	HIS
1	C	556	GLN
1	C	572	ASN
1	C	629	HIS

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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	A	801	3,1	46,52,52	2.06	17 (36%)	62,89,89	2.69	21 (33%)
2	HDD	D	801	3,1	46,52,52	2.17	16 (34%)	62,89,89	2.22	17 (27%)
2	HDD	B	801	3,1	46,52,52	2.33	17 (36%)	62,89,89	2.82	24 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HDD	C	801	1	46,52,52	2.04	15 (32%)	62,89,89	2.52	22 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HDD	A	801	3,1	-	2/9/89/89	0/1/9/9
2	HDD	D	801	3,1	-	4/9/89/89	0/1/9/9
2	HDD	B	801	3,1	-	2/9/89/89	0/1/9/9
2	HDD	C	801	1	-	2/9/89/89	0/1/9/9

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HDD	CHC-C4B	6.42	1.51	1.38
2	A	801	HDD	O1D-CGD	5.68	1.44	1.35
2	C	801	HDD	CHB-C4A	5.08	1.50	1.39
2	C	801	HDD	CHC-C4B	4.77	1.47	1.38
2	B	801	HDD	O1D-C3D	4.60	1.54	1.46
2	D	801	HDD	CHD-C4C	4.54	1.49	1.39
2	A	801	HDD	CHB-C1B	4.46	1.47	1.38
2	D	801	HDD	CHB-C1B	4.45	1.47	1.38
2	C	801	HDD	CHB-C1B	4.38	1.47	1.38
2	D	801	HDD	C3B-C2B	4.19	1.45	1.37
2	D	801	HDD	CHC-C4B	4.18	1.46	1.38
2	B	801	HDD	CHB-C4A	4.07	1.48	1.39
2	B	801	HDD	C1B-NB	-3.88	1.32	1.39
2	D	801	HDD	CHC-C1C	3.87	1.48	1.39
2	D	801	HDD	O1D-CGD	3.87	1.41	1.35
2	B	801	HDD	O1D-CGD	3.86	1.41	1.35
2	A	801	HDD	CHC-C4B	3.80	1.45	1.38
2	B	801	HDD	C3B-C2B	3.75	1.44	1.37
2	D	801	HDD	CHA-C1A	3.73	1.47	1.39
2	A	801	HDD	CHD-C4C	3.65	1.47	1.39
2	D	801	HDD	C4B-NB	-3.51	1.33	1.39
2	B	801	HDD	C2A-C3A	3.49	1.48	1.38
2	A	801	HDD	C3B-C2B	3.46	1.44	1.37
2	B	801	HDD	CHD-C4C	3.38	1.47	1.39
2	B	801	HDD	C4B-NB	-3.36	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HDD	CHC-C1C	3.35	1.46	1.39
2	A	801	HDD	CHC-C1C	3.34	1.46	1.39
2	A	801	HDD	CHA-C1A	3.32	1.46	1.39
2	D	801	HDD	CHB-C4A	3.31	1.46	1.39
2	C	801	HDD	CHC-C1C	3.29	1.46	1.39
2	C	801	HDD	O1D-CGD	3.08	1.40	1.35
2	B	801	HDD	C4A-NA	-3.05	1.33	1.39
2	D	801	HDD	OND-C2D	3.01	1.48	1.42
2	D	801	HDD	C2A-C3A	2.97	1.46	1.38
2	B	801	HDD	CHB-C1B	2.92	1.44	1.38
2	C	801	HDD	CHA-C1A	2.81	1.45	1.39
2	B	801	HDD	C4A-C3A	2.80	1.49	1.43
2	C	801	HDD	C4C-NC	-2.76	1.34	1.39
2	A	801	HDD	C4C-NC	-2.70	1.34	1.39
2	A	801	HDD	OND-C2D	2.70	1.47	1.42
2	C	801	HDD	C4B-NB	-2.68	1.34	1.39
2	B	801	HDD	CHA-C1A	2.68	1.45	1.39
2	D	801	HDD	C1A-NA	-2.61	1.34	1.39
2	D	801	HDD	C1B-NB	-2.57	1.34	1.39
2	C	801	HDD	C3B-C2B	2.55	1.42	1.37
2	A	801	HDD	CHB-C4A	2.55	1.45	1.39
2	C	801	HDD	C1A-C2A	2.52	1.49	1.44
2	C	801	HDD	C2A-C3A	2.50	1.45	1.38
2	A	801	HDD	C4B-NB	-2.50	1.34	1.39
2	B	801	HDD	C1C-NC	-2.48	1.35	1.39
2	D	801	HDD	C1C-NC	-2.41	1.35	1.39
2	C	801	HDD	C3C-C2C	2.38	1.49	1.41
2	A	801	HDD	C4A-C3A	2.36	1.48	1.43
2	B	801	HDD	C4C-NC	-2.34	1.35	1.39
2	A	801	HDD	C1B-NB	-2.34	1.35	1.39
2	C	801	HDD	CHD-C4C	2.28	1.44	1.39
2	C	801	HDD	CMC-C2C	2.23	1.55	1.50
2	D	801	HDD	C4C-NC	-2.19	1.35	1.39
2	C	801	HDD	C1A-NA	-2.17	1.35	1.39
2	A	801	HDD	C1A-NA	-2.13	1.35	1.39
2	A	801	HDD	O2A-CGA	-2.13	1.23	1.30
2	D	801	HDD	C3B-C4B	2.12	1.49	1.46
2	A	801	HDD	C2A-C3A	2.12	1.44	1.38
2	A	801	HDD	CMC-C2C	2.10	1.55	1.50
2	B	801	HDD	C3D-C2D	-2.02	1.50	1.55

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HDD	O1D-CGD-O2D	9.19	128.55	120.81
2	A	801	HDD	O1D-CGD-O2D	8.48	127.95	120.81
2	A	801	HDD	C3B-C2B-C1B	-7.95	99.52	107.05
2	D	801	HDD	C3B-C2B-C1B	-7.89	99.58	107.05
2	C	801	HDD	C3C-C2C-C1C	-7.81	97.97	107.17
2	B	801	HDD	C3B-C2B-C1B	-7.76	99.71	107.05
2	C	801	HDD	C3B-C2B-C1B	-7.70	99.76	107.05
2	B	801	HDD	O1D-CGD-CBD	-6.92	103.86	110.17
2	A	801	HDD	O1D-CGD-CBD	-6.52	104.23	110.17
2	B	801	HDD	C3C-C2C-C1C	-5.72	100.43	107.17
2	B	801	HDD	C3D-O1D-CGD	5.63	116.39	111.14
2	A	801	HDD	OND-C2D-CMD	-5.59	98.63	109.45
2	A	801	HDD	C3D-O1D-CGD	5.50	116.27	111.14
2	A	801	HDD	CMC-C2C-C1C	5.45	133.72	125.42
2	A	801	HDD	C3C-C2C-C1C	-5.38	100.82	107.17
2	C	801	HDD	O1D-CGD-O2D	5.25	125.23	120.81
2	D	801	HDD	C3C-C2C-C1C	-5.09	101.17	107.17
2	D	801	HDD	O1D-CGD-O2D	4.54	124.64	120.81
2	D	801	HDD	CMC-C2C-C1C	4.46	132.21	125.42
2	B	801	HDD	C2D-C1D-CHD	-4.45	117.36	124.27
2	D	801	HDD	C2B-C1B-NB	4.37	117.72	109.64
2	C	801	HDD	OND-C2D-CMD	-4.36	101.02	109.45
2	B	801	HDD	CAA-CBA-CGA	-4.28	102.33	113.67
2	C	801	HDD	C2C-C1C-NC	4.27	116.99	110.14
2	D	801	HDD	CAA-CBA-CGA	-4.20	102.53	113.67
2	C	801	HDD	CHB-C1B-NB	-4.16	119.92	124.45
2	B	801	HDD	OND-C2D-CMD	-4.16	101.41	109.45
2	C	801	HDD	CAA-CBA-CGA	-4.02	103.00	113.67
2	D	801	HDD	C2D-C1D-CHD	-3.96	118.12	124.27
2	A	801	HDD	C2B-C1B-NB	3.87	116.79	109.64
2	A	801	HDD	C2D-C1D-CHD	-3.81	118.34	124.27
2	C	801	HDD	CMB-C2B-C1B	3.81	131.44	124.73
2	C	801	HDD	CBD-CAD-C3D	3.79	109.38	103.98
2	B	801	HDD	C2C-C1C-NC	3.74	116.13	110.14
2	B	801	HDD	C2B-C1B-NB	3.72	116.53	109.64
2	A	801	HDD	CAA-CBA-CGA	-3.65	103.99	113.67
2	B	801	HDD	CBD-CAD-C3D	3.55	109.04	103.98
2	C	801	HDD	CMC-C2C-C1C	3.52	130.77	125.42
2	B	801	HDD	CHB-C1B-NB	-3.50	120.64	124.45
2	B	801	HDD	C2A-C1A-NA	3.46	113.99	110.15
2	B	801	HDD	CAD-CBD-CGD	3.43	109.57	104.48
2	D	801	HDD	C4A-C3A-C2A	-3.40	102.92	106.82
2	D	801	HDD	OND-C2D-CMD	-3.35	102.98	109.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HDD	C2A-C1A-NA	3.34	113.86	110.15
2	C	801	HDD	C2D-C1D-CHD	-3.28	119.17	124.27
2	B	801	HDD	CMB-C2B-C1B	3.24	130.44	124.73
2	C	801	HDD	C3D-O1D-CGD	3.15	114.08	111.14
2	C	801	HDD	C2B-C1B-NB	3.12	115.41	109.64
2	B	801	HDD	C4A-C3A-C2A	-3.08	103.29	106.82
2	A	801	HDD	CBD-CAD-C3D	3.03	108.30	103.98
2	C	801	HDD	CMD-C2D-C3D	3.03	123.07	115.11
2	B	801	HDD	CAA-C2A-C1A	3.03	130.85	124.94
2	C	801	HDD	CBC-CAC-C3C	-2.67	114.16	127.53
2	D	801	HDD	CHB-C1B-NB	-2.66	121.56	124.45
2	C	801	HDD	CBB-CAB-C3B	-2.65	114.29	127.53
2	C	801	HDD	CMA-C3A-C2A	2.63	131.19	125.62
2	B	801	HDD	C3D-C4D-CHA	-2.58	116.64	124.14
2	A	801	HDD	C2C-C1C-NC	2.56	114.25	110.14
2	C	801	HDD	CHB-C4A-C3A	-2.54	120.05	127.43
2	D	801	HDD	C2A-C1A-NA	2.50	112.93	110.15
2	B	801	HDD	C1A-C2A-C3A	-2.50	103.00	106.87
2	D	801	HDD	C2C-C1C-NC	2.49	114.13	110.14
2	B	801	HDD	CHC-C1C-C2C	-2.46	120.30	127.43
2	C	801	HDD	C4A-C3A-C2A	-2.44	104.02	106.82
2	C	801	HDD	C3D-C4D-CHA	-2.37	117.27	124.14
2	C	801	HDD	CHC-C1C-C2C	-2.34	120.62	127.43
2	D	801	HDD	CBD-CAD-C3D	2.33	107.30	103.98
2	D	801	HDD	CHB-C1B-C2B	-2.30	120.70	125.49
2	A	801	HDD	CHB-C1B-C2B	-2.29	120.72	125.49
2	A	801	HDD	CBC-CAC-C3C	-2.28	116.16	127.53
2	D	801	HDD	CAA-C2A-C1A	2.27	129.37	124.94
2	C	801	HDD	C2A-C1A-NA	2.25	112.65	110.15
2	B	801	HDD	C3A-C4A-NA	2.22	113.69	110.14
2	A	801	HDD	C1A-C2A-C3A	-2.18	103.50	106.87
2	D	801	HDD	C3D-C4D-CHA	-2.17	117.85	124.14
2	A	801	HDD	C3D-C4D-CHA	-2.16	117.86	124.14
2	A	801	HDD	CMD-C2D-C3D	2.13	120.72	115.11
2	A	801	HDD	CHD-C1D-ND	2.13	127.22	124.28
2	A	801	HDD	O1D-C3D-CAD	-2.11	99.15	103.06
2	B	801	HDD	CHB-C4A-C3A	-2.07	121.40	127.43
2	D	801	HDD	CHB-C4A-C3A	-2.07	121.42	127.43
2	A	801	HDD	CMB-C2B-C1B	2.03	128.31	124.73
2	B	801	HDD	CBA-CAA-C2A	-2.03	106.93	112.53
2	B	801	HDD	CHA-C4D-ND	2.01	127.05	124.28

There are no chirality outliers.

All (10) torsion outliers are listed below:

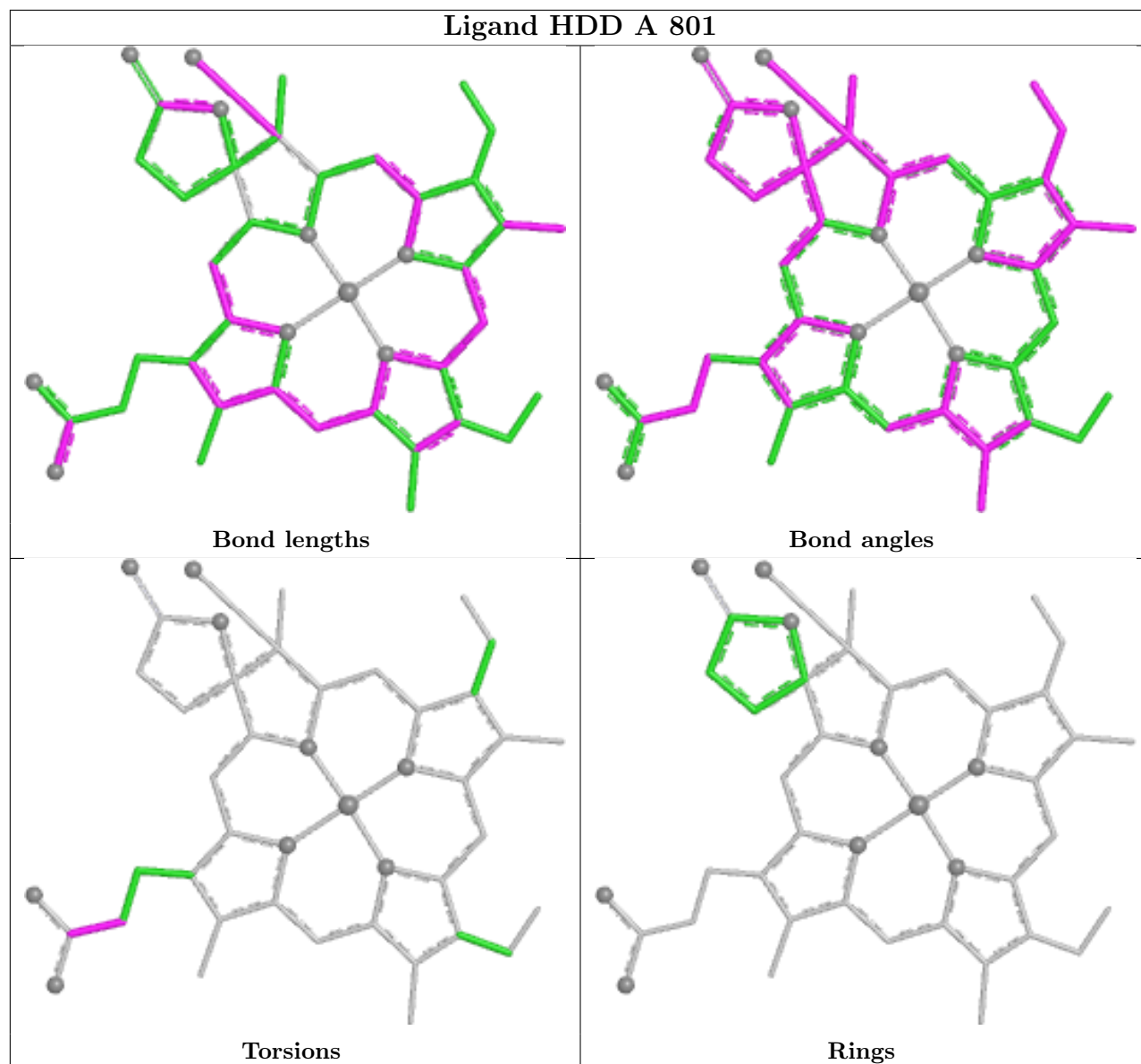
Mol	Chain	Res	Type	Atoms
2	B	801	HDD	CAA-CBA-CGA-O1A
2	A	801	HDD	CAA-CBA-CGA-O1A
2	D	801	HDD	CAA-CBA-CGA-O2A
2	B	801	HDD	CAA-CBA-CGA-O2A
2	A	801	HDD	CAA-CBA-CGA-O2A
2	D	801	HDD	C2C-C3C-CAC-CBC
2	D	801	HDD	CAA-CBA-CGA-O1A
2	C	801	HDD	CAA-CBA-CGA-O1A
2	C	801	HDD	CAA-CBA-CGA-O2A
2	D	801	HDD	C4C-C3C-CAC-CBC

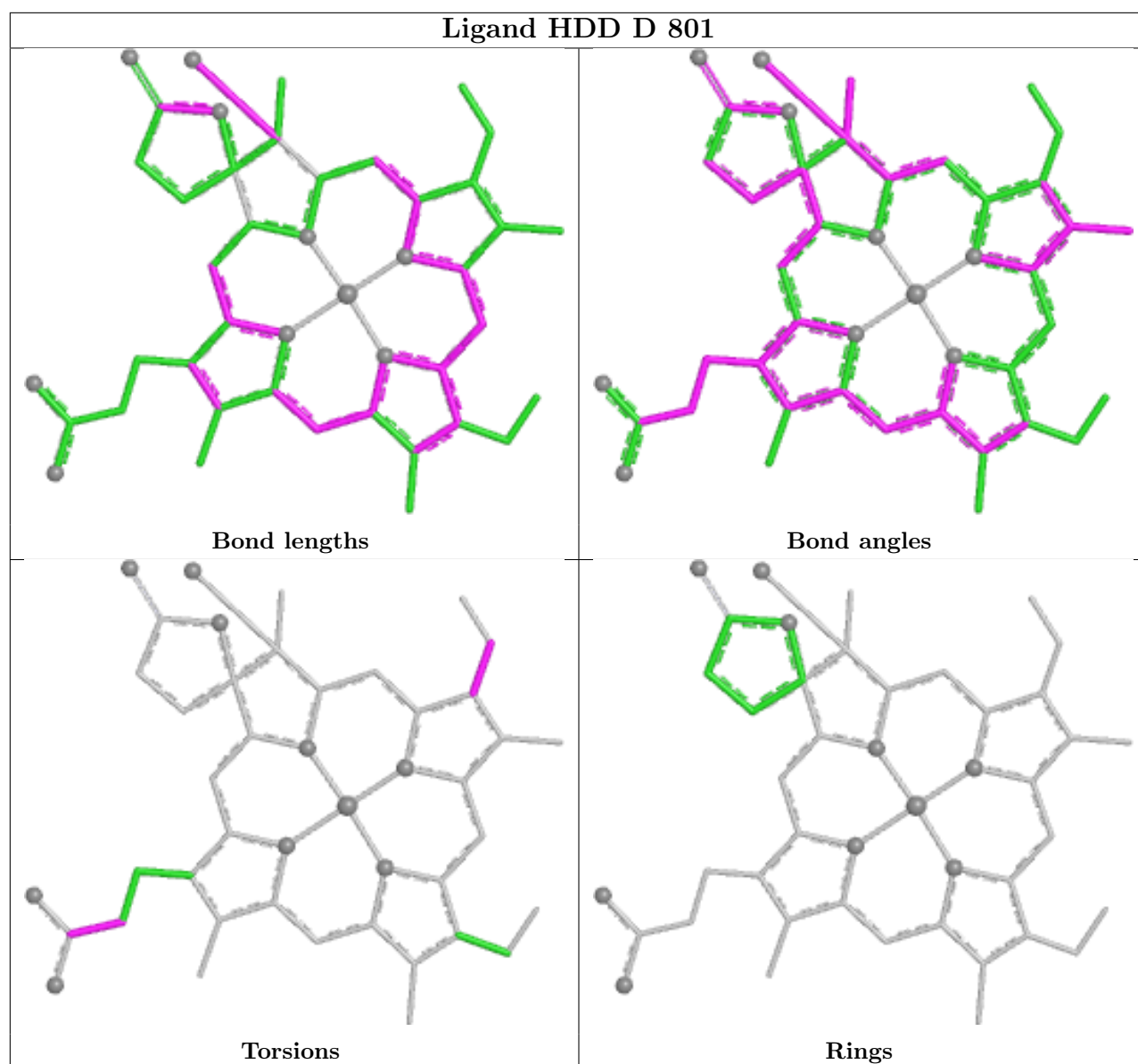
There are no ring outliers.

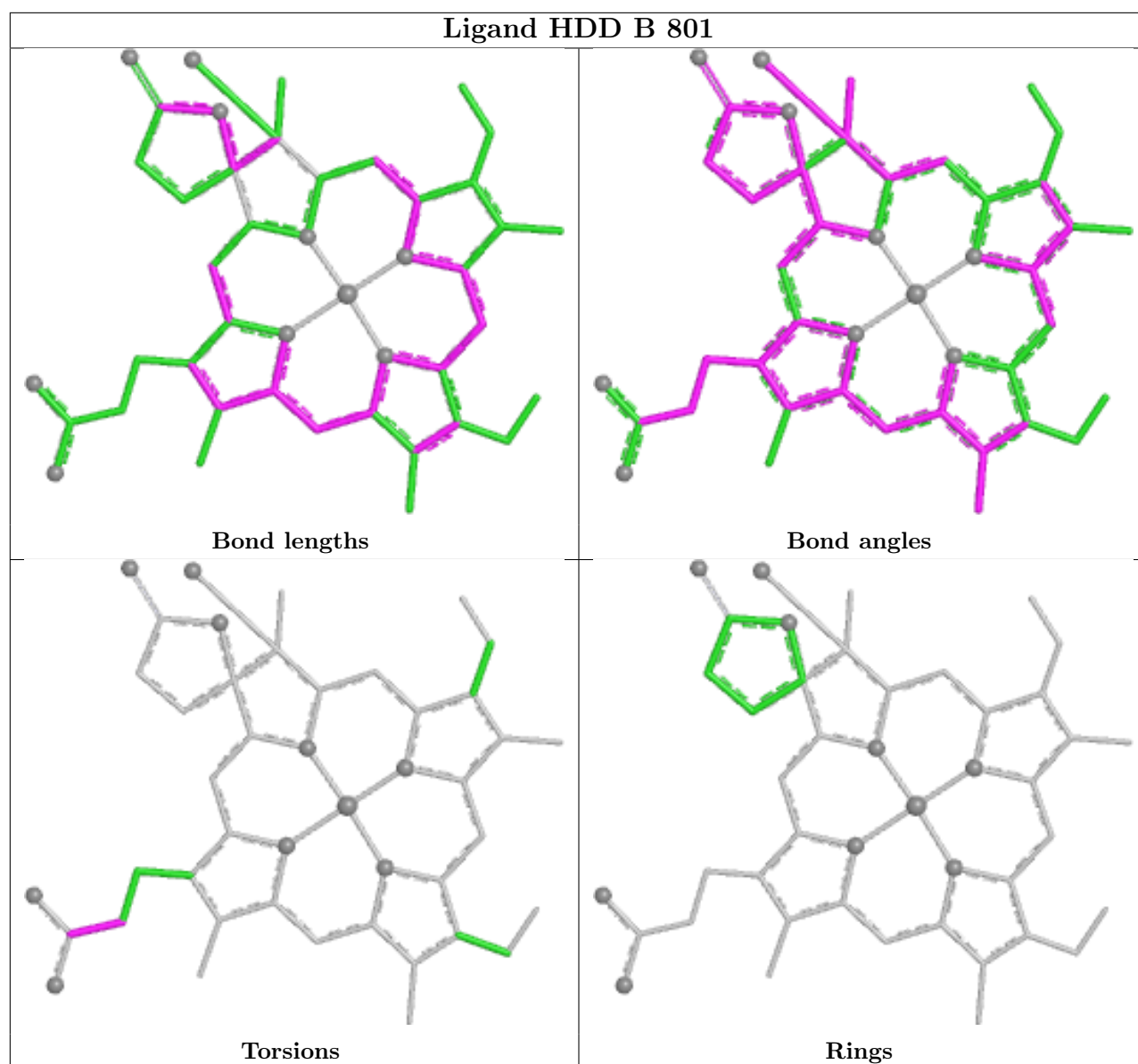
4 monomers are involved in 11 short contacts:

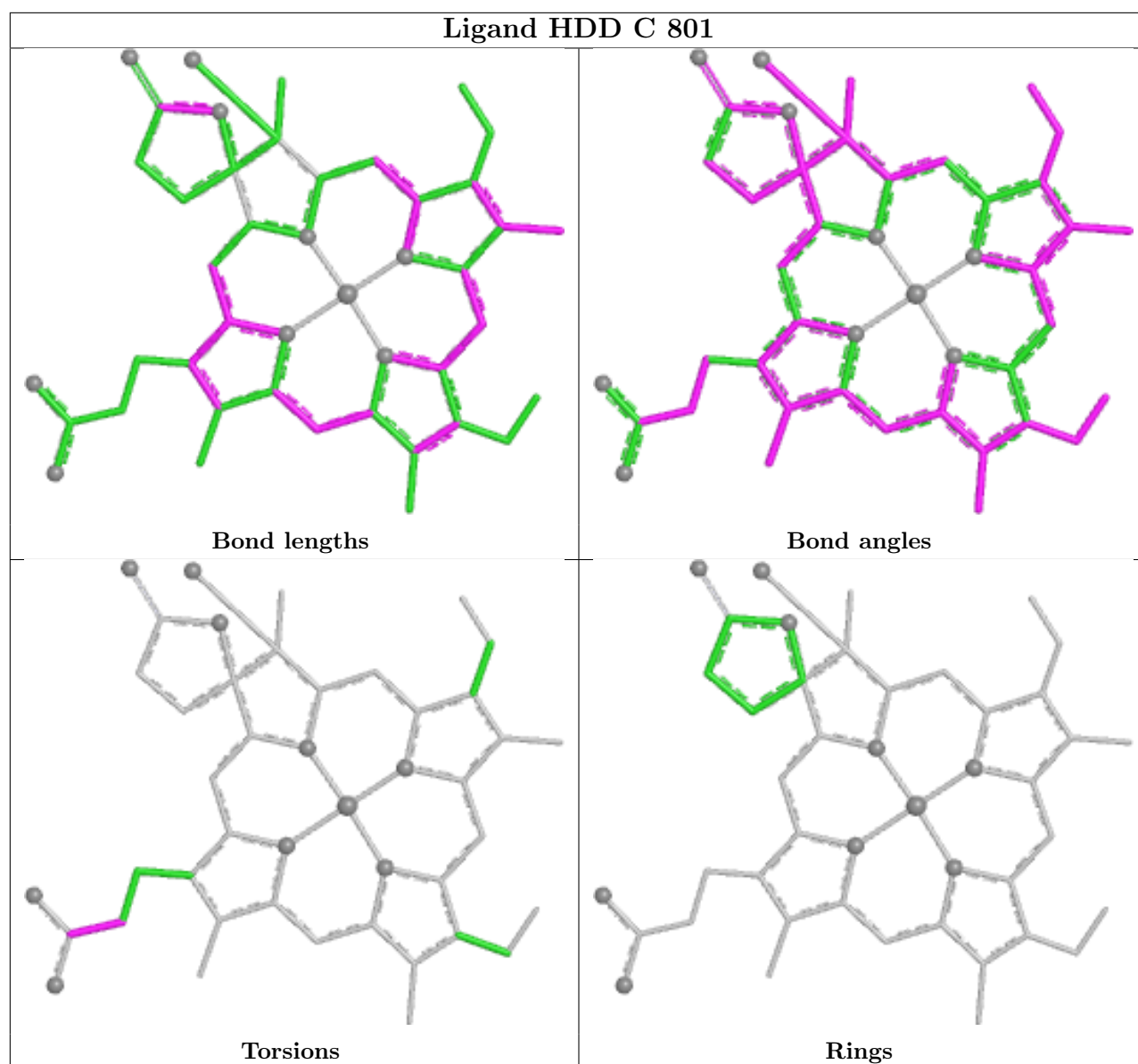
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	HDD	2	0
2	D	801	HDD	2	0
2	B	801	HDD	4	0
2	C	801	HDD	3	0

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 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	726/753 (96%)	-0.61	4 (0%) 85 87	5, 12, 26, 51	2 (0%)
1	B	726/753 (96%)	-0.48	4 (0%) 85 87	5, 13, 35, 56	2 (0%)
1	C	726/753 (96%)	-0.49	4 (0%) 85 87	6, 13, 33, 52	3 (0%)
1	D	726/753 (96%)	-0.56	3 (0%) 88 90	5, 12, 29, 54	3 (0%)
All	All	2904/3012 (96%)	-0.53	15 (0%) 87 89	5, 12, 32, 56	10 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	725	ASP	3.3
1	D	28	SER	3.3
1	B	726	GLY	3.2
1	C	751	ILE	3.0
1	A	751	ILE	2.6
1	D	749	ASP	2.5
1	A	726	GLY	2.4
1	B	749	ASP	2.4
1	A	749	ASP	2.3
1	D	751	ILE	2.3
1	B	725	ASP	2.2
1	C	706	ALA	2.1
1	C	725	ASP	2.1
1	B	583	LYS	2.0
1	C	726	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

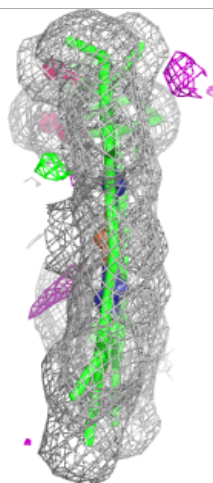
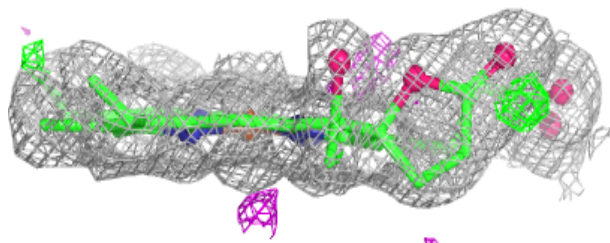
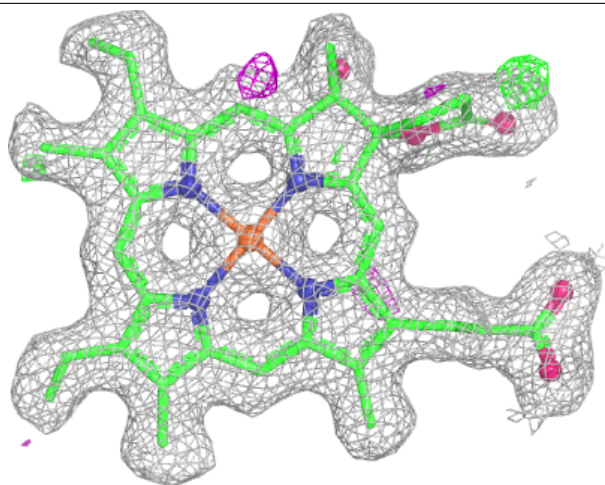
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.98	0.06	5,8,11,12	0
2	HDD	B	801	44/44	0.98	0.05	6,9,11,12	0
2	HDD	C	801	44/44	0.98	0.05	7,8,13,17	0
2	HDD	D	801	44/44	0.98	0.05	6,7,12,14	0

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

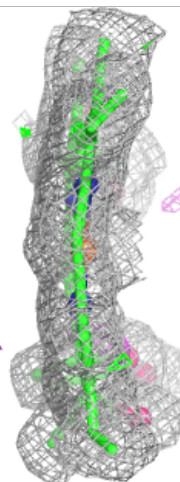
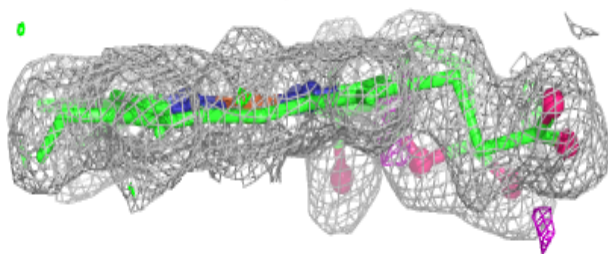
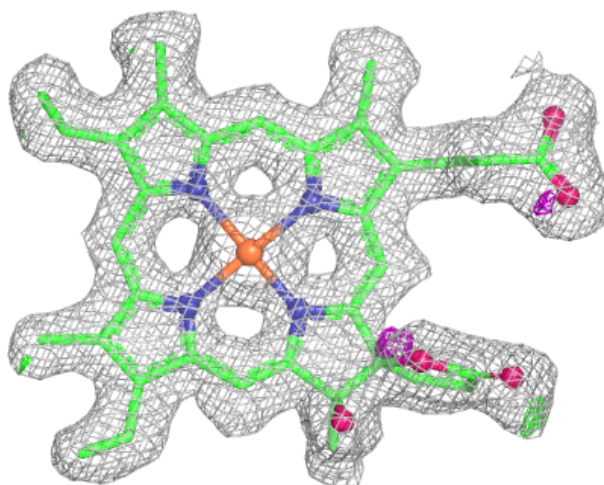
Electron density around HDD A 801:

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



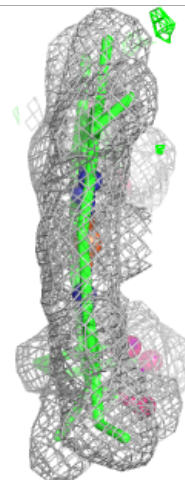
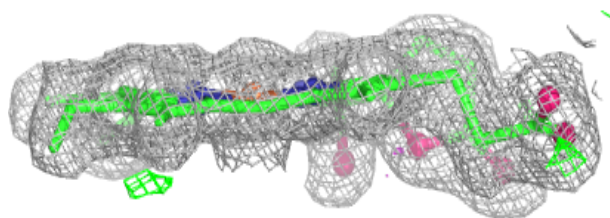
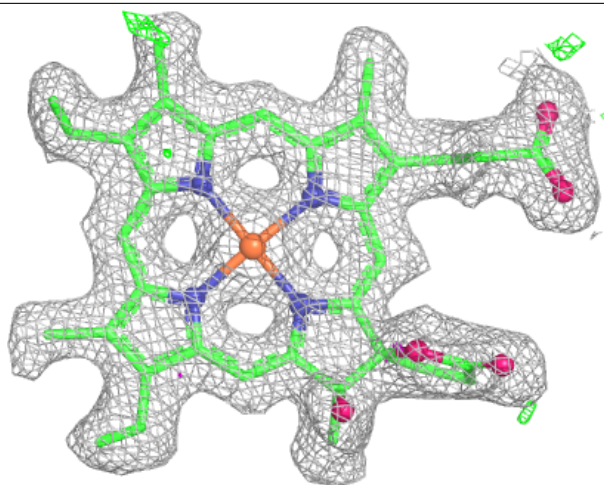
Electron density around HDD B 801:

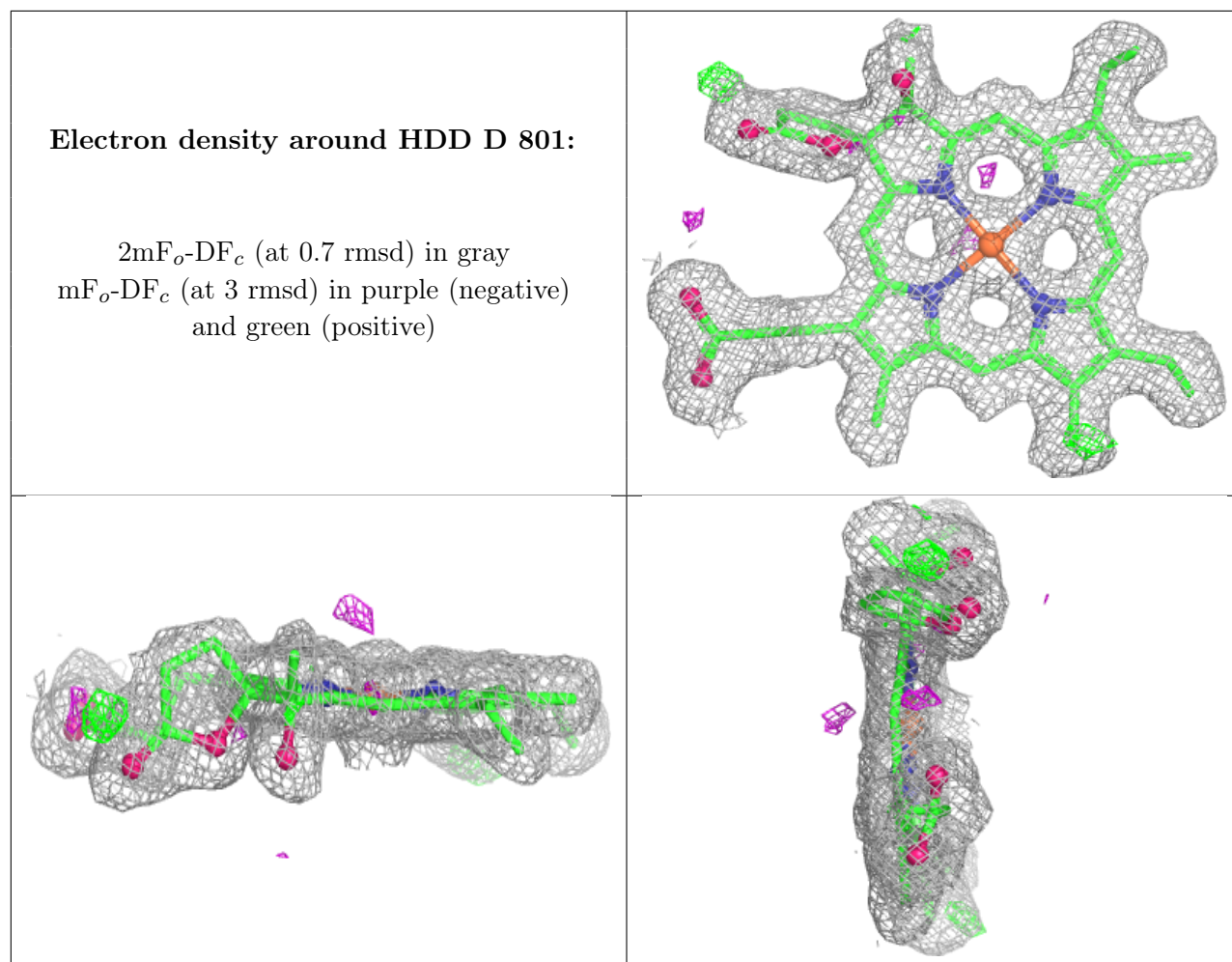
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HDD C 801:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.