



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:44 PM UTC

PDB ID : 3P9R / pdb_00003p9r
Title : Structure of I274G variant of E. coli KatE
Authors : Loewen, P.C.; Jha, V.; Louis, S.; Chelikani, P.; Carpena, X.; Fita, I.
Deposited on : 2010-10-18
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

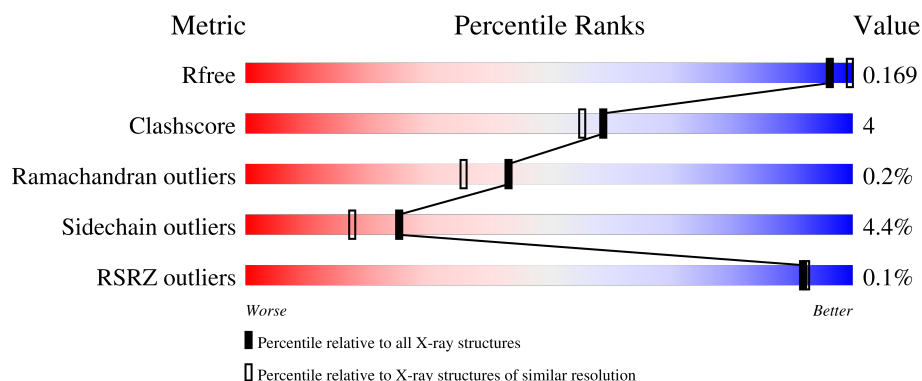
1 Overall quality at a glance

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	
1	B	753	
1	C	753	
1	D	753	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	OCS	D	669	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26363 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.

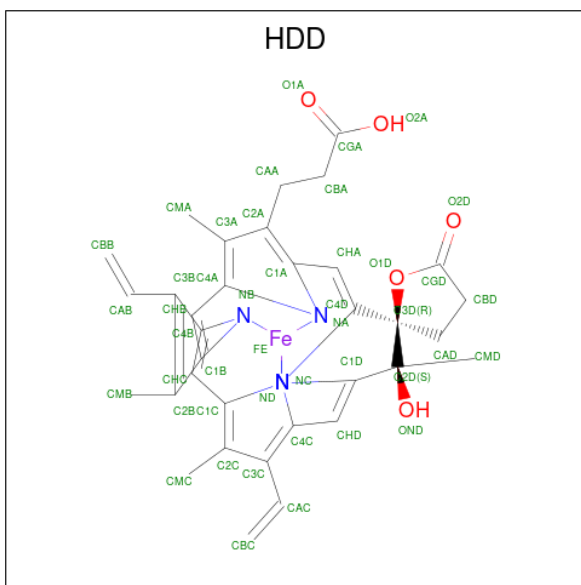
- Molecule 1 is a protein called Catalase HP11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	4	0
			5748	3645	1006	1085	12			
1	B	726	Total	C	N	O	S	0	4	0
			5750	3645	1007	1086	12			
1	C	726	Total	C	N	O	S	0	3	0
			5744	3642	1006	1084	12			
1	D	726	Total	C	N	O	S	0	3	0
			5749	3645	1007	1085	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	274	GLY	ILE	engineered mutation	UNP P21179
B	274	GLY	ILE	engineered mutation	UNP P21179
C	274	GLY	ILE	engineered mutation	UNP P21179
D	274	GLY	ILE	engineered mutation	UNP P21179

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



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

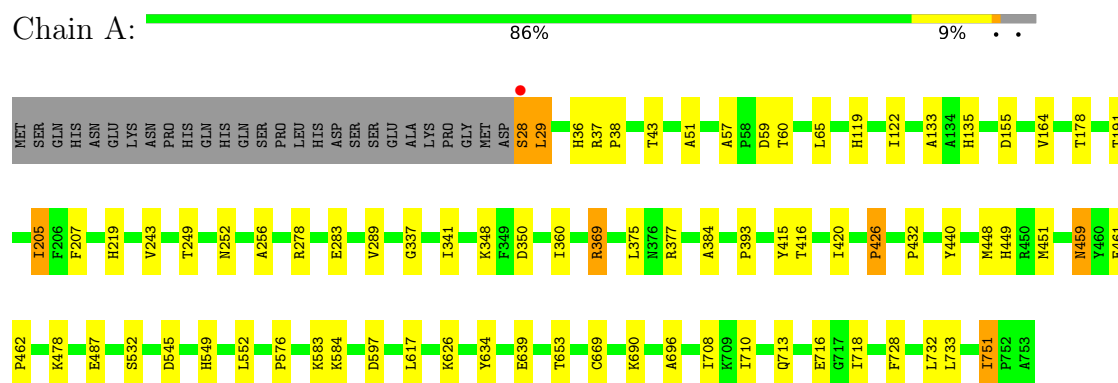
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	832	Total O 832 832	0	0
3	B	742	Total O 742 742	0	0
3	C	767	Total O 767 767	0	0
3	D	855	Total O 855 855	0	0

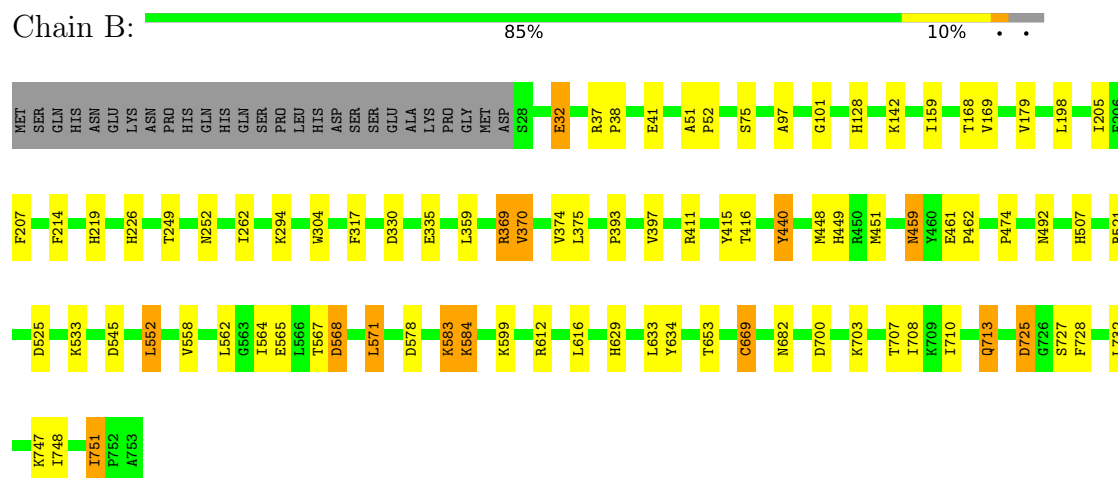
3 Residue-property plots [i](#)

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.

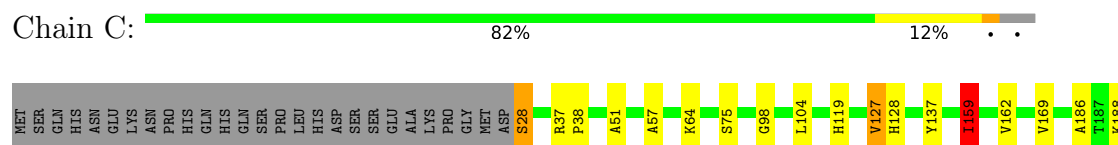
• Molecule 1: Catalase HP11

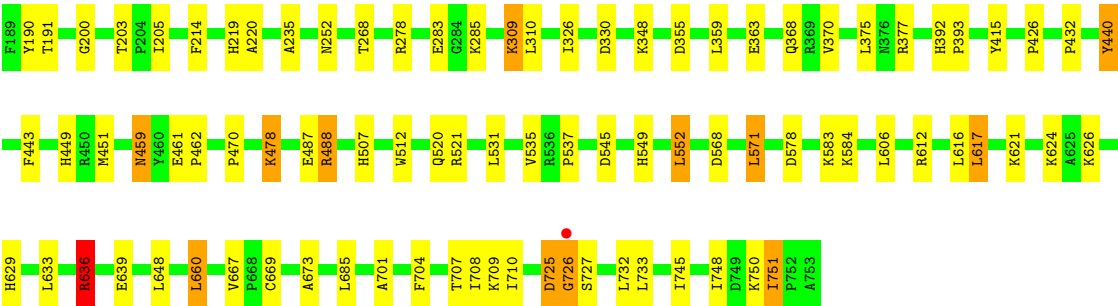


• Molecule 1: Catalase HP11

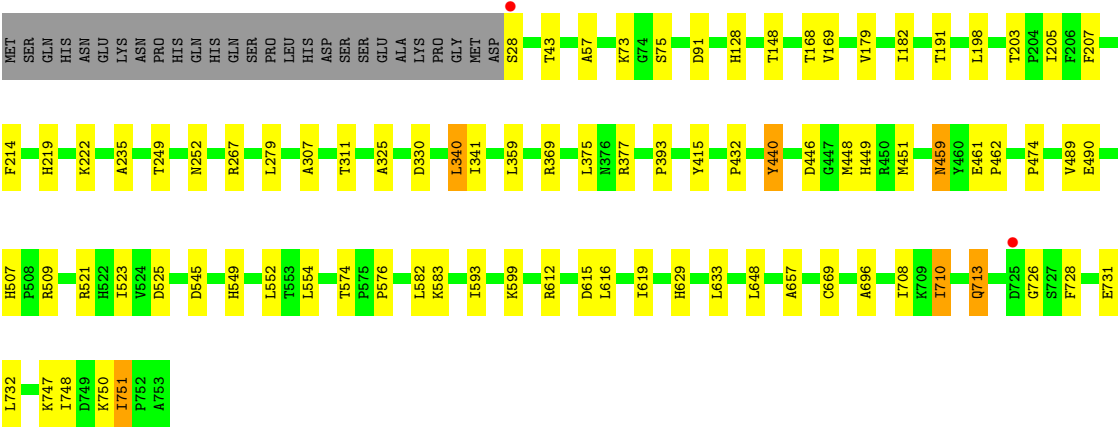
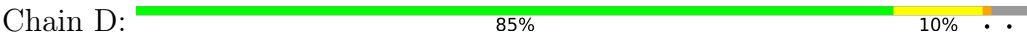


• Molecule 1: Catalase HP11





● Molecule 1: Catalase HP1I



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.41Å 133.18Å 122.74Å 90.00° 109.21° 90.00°	Depositor
Resolution (Å)	35.24 – 1.90 35.24 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (35.24-1.90) 99.4 (35.24-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 1.89Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.133 , 0.184 (Not available) , 0.169	Depositor DCC
R_{free} test set	11178 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	13.8	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.9	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	26363	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 3.54% 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 [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	1.35	14/5913 (0.2%)	1.14	10/8037 (0.1%)
1	B	1.33	6/5912 (0.1%)	1.14	9/8035 (0.1%)
1	C	1.32	13/5906 (0.2%)	1.16	15/8027 (0.2%)
1	D	1.36	14/5906 (0.2%)	1.14	7/8027 (0.1%)
All	All	1.34	47/23637 (0.2%)	1.14	41/32126 (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	1

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	745	ILE	CA-CB	11.52	1.59	1.54
1	C	214	PHE	C-O	-7.62	1.17	1.24
1	D	474	PRO	CA-C	7.39	1.55	1.51
1	C	200	GLY	N-CA	6.72	1.50	1.44
1	A	420	ILE	CA-CB	6.45	1.62	1.54
1	D	57	ALA	CA-CB	6.36	1.60	1.53
1	A	205	ILE	CA-CB	6.20	1.62	1.54
1	D	341	ILE	CA-C	6.11	1.57	1.52
1	D	307	ALA	CA-CB	6.09	1.62	1.53
1	D	214	PHE	C-O	-6.02	1.19	1.24
1	A	426	PRO	CA-C	6.01	1.60	1.52
1	A	377	ARG	CZ-NH2	6.01	1.41	1.33
1	B	262	ILE	CA-CB	5.98	1.61	1.54
1	C	57	ALA	CA-CB	5.90	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	179	VAL	CA-CB	5.84	1.62	1.54
1	A	243	VAL	CA-CB	-5.81	1.48	1.54
1	D	311	THR	CA-CB	5.78	1.62	1.53
1	B	226	HIS	C-O	5.77	1.30	1.24
1	C	186	ALA	CA-CB	5.71	1.62	1.53
1	D	710	ILE	CA-CB	5.67	1.61	1.54
1	C	725	ASP	CA-C	5.67	1.61	1.53
1	A	57	ALA	CA-CB	5.63	1.59	1.53
1	C	220	ALA	CA-C	5.62	1.60	1.52
1	C	370	VAL	CA-CB	5.61	1.62	1.54
1	A	337	GLY	C-O	5.52	1.30	1.23
1	B	397	VAL	N-CA	5.52	1.51	1.46
1	A	43	THR	CA-CB	5.52	1.61	1.54
1	B	168	THR	N-CA	5.46	1.51	1.46
1	D	43	THR	C-O	5.43	1.29	1.24
1	C	268	THR	CA-CB	5.42	1.60	1.53
1	A	178	THR	N-CA	5.36	1.52	1.46
1	D	222	LYS	C-O	5.31	1.30	1.23
1	A	256	ALA	CA-CB	5.30	1.61	1.53
1	D	489	VAL	CA-CB	5.29	1.60	1.54
1	B	179	VAL	CA-CB	5.29	1.60	1.54
1	C	235	ALA	CA-CB	5.22	1.59	1.52
1	A	122	ILE	CA-CB	5.21	1.59	1.55
1	B	474	PRO	CA-C	5.20	1.54	1.51
1	C	127	VAL	C-O	5.16	1.29	1.23
1	D	203	THR	CA-C	5.16	1.57	1.52
1	C	326	ILE	C-O	5.16	1.30	1.24
1	C	203	THR	CA-CB	5.14	1.60	1.54
1	D	235	ALA	CA-CB	5.11	1.59	1.52
1	A	289	VAL	C-O	5.06	1.29	1.24
1	A	384	ALA	CA-CB	5.04	1.61	1.53
1	A	60	THR	CA-CB	5.03	1.60	1.53
1	D	523	ILE	N-CA	5.03	1.52	1.46

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	98	GLY	N-CA-C	-6.93	104.09	112.48
1	B	370	VAL	N-CA-CB	-6.33	103.58	112.12
1	A	350	ASP	CB-CA-C	6.31	121.59	110.37
1	B	304	TRP	N-CA-C	6.27	117.78	111.07
1	B	521	ARG	NE-CZ-NH2	6.23	124.81	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	568	ASP	N-CA-C	6.05	118.37	111.11
1	C	159	ILE	CB-CG1-CD1	-6.04	101.12	113.80
1	C	355	ASP	CA-C-N	-6.00	114.71	120.83
1	C	355	ASP	C-N-CA	-6.00	114.71	120.83
1	D	446	ASP	CB-CA-C	-5.92	108.07	115.89
1	A	360	ILE	CA-C-N	-5.91	113.85	119.76
1	A	360	ILE	C-N-CA	-5.91	113.85	119.76
1	C	725	ASP	O-C-N	-5.74	116.52	122.84
1	A	155	ASP	CA-C-N	-5.74	114.20	119.82
1	A	155	ASP	C-N-CA	-5.74	114.20	119.82
1	B	317	PHE	N-CA-C	5.73	117.20	111.07
1	C	159	ILE	CA-CB-CG2	5.70	120.19	110.50
1	C	636	ARG	NE-CZ-NH2	-5.69	114.08	119.20
1	A	751	ILE	N-CA-CB	5.67	115.36	110.08
1	D	657	ALA	CA-C-N	5.61	125.92	119.92
1	D	657	ALA	C-N-CA	5.61	125.92	119.92
1	D	377	ARG	CG-CD-NE	-5.58	99.73	112.00
1	A	29	LEU	CB-CA-C	5.57	119.79	110.43
1	B	558	VAL	N-CA-C	-5.52	105.34	110.53
1	C	636	ARG	CG-CD-NE	-5.49	99.93	112.00
1	C	309	LYS	N-CA-C	-5.39	105.57	111.82
1	A	348	LYS	N-CA-C	5.31	119.63	113.20
1	B	41	GLU	CA-C-N	-5.29	114.47	119.76
1	B	41	GLU	C-N-CA	-5.29	114.47	119.76
1	C	363	GLU	N-CA-C	5.27	117.70	111.33
1	A	751	ILE	N-CA-C	5.26	114.10	108.95
1	C	348	LYS	CA-CB-CG	-5.18	103.75	114.10
1	C	57	ALA	CA-C-N	5.14	124.94	119.28
1	C	57	ALA	C-N-CA	5.14	124.94	119.28
1	B	374	VAL	N-CA-C	-5.10	100.78	108.12
1	A	733	LEU	N-CA-C	5.10	116.84	111.28
1	D	340	LEU	CA-C-N	-5.09	118.42	122.85
1	D	340	LEU	C-N-CA	-5.09	118.42	122.85
1	D	325	ALA	N-CA-C	-5.07	105.83	111.36
1	C	745	ILE	O-C-N	5.06	123.66	120.42
1	C	673	ALA	N-CA-C	-5.00	106.44	112.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	726	GLY	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	5748	0	5577	45	1
1	B	5750	0	5573	58	1
1	C	5744	0	5569	61	0
1	D	5749	0	5572	38	0
2	A	44	0	31	2	0
2	B	44	0	31	5	0
2	C	44	0	31	2	0
2	D	44	0	31	2	0
3	A	832	0	0	16	0
3	B	742	0	0	17	0
3	C	767	0	0	23	0
3	D	855	0	0	18	1
All	All	26363	0	22415	199	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 4.

All (199) 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:D:549:HIS:HE1	3:D:3214:HOH:O	1.04	1.26
1:C:449[B]:HIS:CD2	3:C:3402:HOH:O	1.70	1.24
1:B:416:THR:HG21	3:D:2464:HOH:O	1.39	1.18
1:A:549:HIS:HE1	3:A:3355:HOH:O	1.29	1.15
1:C:451:MET:SD	3:C:3402:HOH:O	2.08	1.10
1:B:451:MET:HE2	1:D:451:MET:HE2	1.14	1.08
1:C:392:HIS:CE1	1:C:415:TYR:HB2	1.88	1.08
1:C:392:HIS:CG	1:C:415:TYR:HB2	1.89	1.08
1:C:392:HIS:ND1	1:C:415:TYR:HB2	0.74	1.06
1:B:451:MET:SD	3:B:3409:HOH:O	2.19	1.00
1:C:751:ILE:HB	3:C:2367:HOH:O	1.63	0.98
1:B:369:ARG:HG2	3:B:1639:HOH:O	1.63	0.95
1:A:451:MET:HE2	1:C:451:MET:HE2	1.53	0.89
1:C:727:SER:HA	3:C:2714:HOH:O	1.72	0.88
1:B:545:ASP:OD1	3:B:3218:HOH:O	1.91	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:731:GLU:OE2	3:D:3028:HOH:O	1.95	0.85
3:A:2649:HOH:O	1:C:28:SER:HA	1.76	0.84
1:D:748:ILE:O	1:D:751:ILE:HG22	1.77	0.84
1:B:294:LYS:HB2	3:B:1097:HOH:O	1.78	0.84
1:C:549:HIS:HE1	3:C:2940:HOH:O	1.61	0.82
1:B:578:ASP:HB2	3:B:2590:HOH:O	1.81	0.81
1:C:545:ASP:OD1	3:C:3210:HOH:O	2.00	0.79
1:A:532[A]:SER:OG	3:A:3278:HOH:O	1.99	0.78
1:C:449[B]:HIS:HD2	3:C:3402:HOH:O	1.23	0.77
1:D:267:ARG:HG3	3:D:1920:HOH:O	1.85	0.77
1:D:549:HIS:CE1	3:D:3214:HOH:O	1.93	0.77
1:B:748:ILE:O	1:B:751:ILE:HG22	1.86	0.75
1:B:37:ARG:NH1	3:B:2886:HOH:O	2.21	0.74
1:B:37:ARG:NH2	3:B:3231:HOH:O	2.20	0.73
1:A:549:HIS:CE1	3:A:3355:HOH:O	2.16	0.72
2:A:760:HDD:HBB1	2:A:760:HDD:HMB3	1.70	0.72
1:B:583:LYS:H	1:B:583:LYS:NZ	1.90	0.70
1:A:710:ILE:CD1	1:A:718:ILE:HG13	2.22	0.70
1:A:639:GLU:HG3	3:A:2414:HOH:O	1.93	0.69
2:D:760:HDD:HBB1	2:D:760:HDD:HMB3	1.73	0.69
1:D:545:ASP:OD1	3:D:3214:HOH:O	2.10	0.69
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.74	0.68
1:D:629:HIS:HD2	3:D:1554:HOH:O	1.77	0.68
1:A:710:ILE:HD13	1:A:718:ILE:HG13	1.75	0.67
1:A:545:ASP:OD1	3:A:2770:HOH:O	2.11	0.67
1:D:726:GLY:O	3:D:2447:HOH:O	2.14	0.66
1:B:525:ASP:OD2	3:B:819:HOH:O	2.14	0.65
1:D:449[A]:HIS:HD2	3:D:3408:HOH:O	1.79	0.65
1:B:451:MET:CE	1:D:451:MET:HE2	2.09	0.65
1:D:451:MET:SD	3:D:3406:HOH:O	2.54	0.64
1:C:725:ASP:HB2	1:C:726:GLY:HA3	1.79	0.64
1:C:725:ASP:HB2	1:C:726:GLY:CA	2.28	0.64
1:B:629:HIS:HD2	3:B:1060:HOH:O	1.80	0.63
1:C:748:ILE:O	1:C:751:ILE:HG23	1.99	0.62
1:A:708:ILE:HD12	1:A:710:ILE:HD11	1.79	0.62
1:B:449[B]:HIS:HE1	3:D:1789:HOH:O	1.81	0.62
2:A:760:HDD:HBB1	2:A:760:HDD:CMB	2.29	0.61
2:D:760:HDD:HBB1	2:D:760:HDD:CMB	2.31	0.61
1:C:552:LEU:HD21	1:C:571:LEU:HD12	1.83	0.61
1:C:392:HIS:ND1	1:C:415:TYR:CG	2.65	0.60
1:A:416[B]:THR:HG22	3:A:901:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:704:PHE:O	1:C:707:THR:HG22	2.02	0.59
1:A:478:LYS:HG2	3:A:1955:HOH:O	2.01	0.59
1:A:29:LEU:HB2	3:C:2405:HOH:O	2.01	0.59
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.18	0.59
1:A:29:LEU:HD22	3:C:2405:HOH:O	2.03	0.58
1:A:36:HIS:CD2	1:A:36:HIS:H	2.21	0.58
1:B:533:LYS:HE2	3:B:3100:HOH:O	2.02	0.58
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.12	0.58
1:D:440:TYR:HD1	3:D:3139:HOH:O	1.86	0.57
1:C:392:HIS:ND1	1:C:415:TYR:CA	2.65	0.57
1:A:716:GLU:HG3	3:A:2227:HOH:O	2.03	0.57
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.87	0.57
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.85	0.57
1:C:629:HIS:HD2	3:C:1129:HOH:O	1.88	0.56
1:D:448:MET:O	1:D:449[A]:HIS:HB2	2.06	0.56
1:C:549:HIS:CE1	3:C:2940:HOH:O	2.43	0.56
2:C:760:HDD:CMB	2:C:760:HDD:HBB1	2.36	0.55
1:D:449[A]:HIS:HE1	3:D:1789:HOH:O	1.89	0.55
1:A:545:ASP:O	1:A:549:HIS:HD2	1.89	0.55
1:B:214:PHE:CD1	2:B:760:HDD:HAC	2.41	0.55
2:B:760:HDD:CMB	2:B:760:HDD:HBB1	2.36	0.55
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.90	0.54
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.91	0.54
1:B:583:LYS:O	1:B:584:LYS:HB3	2.07	0.54
1:B:583:LYS:H	1:B:583:LYS:HZ2	1.56	0.54
1:C:359:LEU:H	1:C:507:HIS:HD2	1.56	0.54
1:C:392:HIS:CG	1:C:415:TYR:CB	2.69	0.53
1:B:294:LYS:HE2	3:B:3346:HOH:O	2.08	0.53
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.39	0.53
1:D:599:LYS:HD3	3:D:2048:HOH:O	2.07	0.53
1:B:369:ARG:CG	3:B:1639:HOH:O	2.39	0.52
1:D:359:LEU:H	1:D:507:HIS:HD2	1.56	0.52
1:B:708:ILE:HG13	1:B:710:ILE:HG12	1.91	0.52
1:B:335:GLU:OE1	1:B:369:ARG:HD2	2.10	0.52
1:C:478:LYS:HB3	3:C:3101:HOH:O	2.09	0.52
1:D:713:GLN:O	1:D:713:GLN:HG2	2.10	0.52
1:B:583:LYS:H	1:B:583:LYS:HZ3	1.58	0.51
1:C:368:GLN:NE2	3:C:1787:HOH:O	2.23	0.51
1:B:440:TYR:CE1	1:D:73:LYS:HE3	2.46	0.51
1:A:426:PRO:HG3	1:C:119:HIS:HB2	1.92	0.51
1:A:597:ASP:OD1	3:A:2719:HOH:O	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:509:ARG:HD2	1:D:576:PRO:HD2	1.92	0.50
1:C:725:ASP:HB2	1:C:726:GLY:C	2.37	0.50
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.28	0.49
1:A:36:HIS:HE1	3:A:1872:HOH:O	1.94	0.49
1:B:411:ARG:HG2	2:B:760:HDD:C2C	2.42	0.49
1:B:533:LYS:CE	3:C:2623:HOH:O	2.60	0.49
1:C:636:ARG:HD3	3:C:2717:HOH:O	2.12	0.49
1:B:564:ILE:O	3:B:2603:HOH:O	2.20	0.49
1:A:28:SER:O	1:A:28:SER:OG	2.29	0.48
1:C:359:LEU:H	1:C:507:HIS:CD2	2.31	0.48
1:C:488:ARG:NH1	3:C:2379:HOH:O	2.18	0.48
1:B:492:ASN:CG	3:B:2605:HOH:O	2.56	0.48
1:D:461:GLU:HA	1:D:462:PRO:C	2.38	0.48
1:C:461:GLU:HA	1:C:462:PRO:C	2.37	0.48
1:C:583:LYS:O	1:C:584:LYS:HB3	2.13	0.48
1:B:533:LYS:HD2	3:C:2623:HOH:O	2.14	0.48
1:B:38:PRO:HG2	1:B:51:ALA:HB2	1.96	0.48
1:B:669:OCS:OD2	1:B:700:ASP:HB2	2.14	0.47
1:B:634:TYR:O	1:B:653:THR:HA	2.14	0.47
1:A:448:MET:O	1:A:449[B]:HIS:HB2	2.15	0.47
1:B:393:PRO:HD2	1:B:415:TYR:CG	2.50	0.47
1:D:521:ARG:HD2	1:D:525:ASP:OD1	2.15	0.47
1:A:583:LYS:O	1:A:584:LYS:HB3	2.14	0.47
1:C:278:ARG:HH12	1:C:487:GLU:CD	2.23	0.47
1:C:667:VAL:CG1	1:C:701:ALA:HB1	2.44	0.47
1:B:448:MET:O	1:B:449[B]:HIS:HB2	2.15	0.46
1:C:535:VAL:O	1:C:537:PRO:HD3	2.15	0.46
2:B:760:HDD:HBB1	2:B:760:HDD:HMB3	1.96	0.46
1:A:708:ILE:CD1	1:A:710:ILE:HD11	2.44	0.46
3:A:2649:HOH:O	1:C:28:SER:CA	2.51	0.46
1:A:710:ILE:HD11	1:A:718:ILE:HG13	1.97	0.46
1:D:583:LYS:HD3	3:D:3374:HOH:O	2.15	0.46
1:C:667:VAL:HG12	1:C:701:ALA:CB	2.46	0.45
1:B:128:HIS:CE1	1:B:169:VAL:HG22	2.51	0.45
1:D:615:ASP:O	1:D:619:ILE:HG13	2.17	0.45
1:B:294:LYS:NZ	3:B:2778:HOH:O	2.49	0.45
1:D:128:HIS:HA	1:D:168:THR:O	2.17	0.45
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.32	0.45
1:C:309:LYS:CE	3:C:1232:HOH:O	2.64	0.45
1:C:309:LYS:HE3	3:C:1232:HOH:O	2.16	0.45
1:C:748:ILE:O	1:C:751:ILE:CG2	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:VAL:HG21	1:D:182:ILE:HB	1.99	0.45
1:B:32:GLU:OE1	1:B:32:GLU:HA	2.16	0.44
1:A:393:PRO:HD2	1:A:415:TYR:CG	2.52	0.44
1:C:38:PRO:HG2	1:C:51:ALA:HB2	1.99	0.44
1:B:214:PHE:CD2	2:B:760:HDD:HMC2	2.52	0.44
1:C:617:LEU:HD12	3:C:2230:HOH:O	2.17	0.44
1:D:549:HIS:HD2	3:D:2205:HOH:O	2.00	0.44
1:A:369:ARG:HG2	3:A:2410:HOH:O	2.17	0.44
1:C:310:LEU:HD13	1:C:660:LEU:HB3	2.00	0.44
1:A:29:LEU:CB	3:C:2405:HOH:O	2.61	0.44
1:A:549:HIS:O	1:A:576:PRO:HD3	2.17	0.44
1:A:696:ALA:HB1	1:A:728:PHE:CZ	2.52	0.44
1:B:207:PHE:O	1:B:249:THR:HA	2.18	0.44
1:A:461:GLU:HA	1:A:462:PRO:C	2.42	0.43
1:B:52:PRO:HG3	3:D:1451:HOH:O	2.17	0.43
2:C:760:HDD:HBB1	2:C:760:HDD:HMB3	1.99	0.43
1:B:725:ASP:OD2	1:B:727:SER:HB3	2.18	0.43
1:D:207:PHE:O	1:D:249:THR:HA	2.17	0.43
1:B:552:LEU:HB2	3:B:3202:HOH:O	2.17	0.43
1:D:393:PRO:HD2	1:D:415:TYR:CG	2.53	0.43
1:A:634:TYR:O	1:A:653:THR:HA	2.18	0.43
1:A:133:ALA:HA	1:A:164:VAL:O	2.18	0.43
1:B:599:LYS:NZ	3:B:2386:HOH:O	2.51	0.43
1:D:708:ILE:HG13	1:D:710:ILE:HG12	2.00	0.43
1:A:690:LYS:HG3	3:A:3093:HOH:O	2.19	0.43
1:C:127:VAL:O	1:C:128:HIS:HB2	2.19	0.43
1:C:392:HIS:HB2	1:C:415:TYR:HB3	2.01	0.43
1:A:37:ARG:HA	1:A:38:PRO:HD3	1.95	0.42
1:A:65:LEU:HD21	1:A:135:HIS:CG	2.54	0.42
1:A:207:PHE:O	1:A:249:THR:HA	2.19	0.42
1:B:567:THR:O	1:B:571:LEU:HD22	2.19	0.42
1:B:359:LEU:H	1:B:507:HIS:HD2	1.66	0.42
1:C:443:PHE:CZ	1:C:470:PRO:HD2	2.55	0.42
3:A:1016:HOH:O	1:C:104:LEU:HB3	2.19	0.42
1:C:330:ASP:OD1	1:C:629:HIS:HE1	2.01	0.42
1:C:393:PRO:HD2	1:C:415:TYR:CG	2.55	0.42
1:D:696:ALA:HB1	1:D:728:PHE:CZ	2.55	0.42
1:D:148:THR:HB	1:D:279:LEU:HB3	2.02	0.41
1:C:128:HIS:CE1	1:C:169:VAL:HG22	2.55	0.41
1:D:521:ARG:HG2	3:D:2917:HOH:O	2.20	0.41
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ALA:O	1:B:101:GLY:HA3	2.20	0.41
1:C:621:LYS:HG2	3:C:3116:HOH:O	2.21	0.41
1:A:459:ASN:H	1:A:459:ASN:HD22	1.68	0.41
1:C:64:LYS:HE2	1:C:190:TYR:CZ	2.55	0.41
1:A:119:HIS:HB2	1:C:426:PRO:HG3	2.02	0.41
1:A:369:ARG:NH1	3:A:3347:HOH:O	2.49	0.41
1:B:459:ASN:HD22	1:B:459:ASN:H	1.68	0.41
1:C:512:TRP:CH2	1:C:520:GLN:HB3	2.55	0.41
1:A:393:PRO:HD2	1:A:415:TYR:CD2	2.55	0.41
1:B:461:GLU:HA	1:B:462:PRO:C	2.45	0.41
1:B:533:LYS:CD	3:C:2623:HOH:O	2.69	0.41
1:B:713:GLN:H	1:B:713:GLN:HG3	1.55	0.41
1:B:747:LYS:HB3	1:B:747:LYS:HE3	1.89	0.41
1:C:440:TYR:CD2	1:C:440:TYR:C	2.99	0.41
1:D:448:MET:O	1:D:449[A]:HIS:CB	2.68	0.41
1:A:459:ASN:HD22	1:A:459:ASN:C	2.28	0.40
1:C:28:SER:O	1:C:28:SER:OG	2.37	0.40
1:A:38:PRO:HG2	1:A:51:ALA:HB2	2.03	0.40
1:C:162:VAL:HA	1:C:188:LYS:O	2.21	0.40
1:B:461:GLU:OE1	1:D:91:ASP:OD1	2.40	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)
1:A:59:ASP:OD1	1:B:369:ARG:NH2[2_545]	2.07	0.13
3:D:2178:HOH:O	3:D:2976:HOH:O[1_655]	2.18	0.02

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	727/753 (96%)	706 (97%)	21 (3%)	0	100	100
1	B	727/753 (96%)	706 (97%)	18 (2%)	3 (0%)	30	22
1	C	726/753 (96%)	707 (97%)	18 (2%)	1 (0%)	48	40
1	D	726/753 (96%)	709 (98%)	16 (2%)	1 (0%)	48	40
All	All	2906/3012 (96%)	2828 (97%)	73 (2%)	5 (0%)	43	36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	725	ASP
1	B	75	SER
1	B	584	LYS
1	C	75	SER
1	D	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	613/634 (97%)	596 (97%)	17 (3%)	38	32
1	B	613/634 (97%)	588 (96%)	25 (4%)	27	19
1	C	612/634 (96%)	574 (94%)	38 (6%)	16	9
1	D	612/634 (96%)	586 (96%)	26 (4%)	26	19
All	All	2450/2536 (97%)	2344 (96%)	106 (4%)	25	18

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	191	THR
1	A	205	ILE
1	A	252	ASN
1	A	283	GLU
1	A	341	ILE

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Mol	Chain	Res	Type
1	A	369	ARG
1	A	375	LEU
1	A	432	PRO
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	617	LEU
1	A	626	LYS
1	A	713	GLN
1	A	732	LEU
1	A	751	ILE
1	B	32	GLU
1	B	142	LYS
1	B	159	ILE
1	B	198	LEU
1	B	205	ILE
1	B	252	ASN
1	B	369	ARG
1	B	370	VAL
1	B	375	LEU
1	B	440	TYR
1	B	459	ASN
1	B	552	LEU
1	B	562	LEU
1	B	565	GLU
1	B	568	ASP
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	B	728	PHE
1	B	732	LEU
1	B	751	ILE
1	C	28	SER
1	C	37	ARG
1	C	159	ILE
1	C	191	THR
1	C	205	ILE
1	C	252	ASN

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Mol	Chain	Res	Type
1	C	283	GLU
1	C	285	LYS
1	C	375	LEU
1	C	377	ARG
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	552	LEU
1	C	568	ASP
1	C	571	LEU
1	C	578	ASP
1	C	606	LEU
1	C	612	ARG
1	C	616	LEU
1	C	617	LEU
1	C	624	LYS
1	C	626	LYS
1	C	633	LEU
1	C	636	ARG
1	C	639	GLU
1	C	648	LEU
1	C	660	LEU
1	C	685	LEU
1	C	709	LYS
1	C	732	LEU
1	C	733	LEU
1	C	750	LYS
1	C	751	ILE
1	D	28	SER
1	D	191	THR
1	D	198	LEU
1	D	205	ILE
1	D	252	ASN
1	D	340	LEU
1	D	369	ARG
1	D	375	LEU
1	D	432	PRO
1	D	440	TYR

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Mol	Chain	Res	Type
1	D	459	ASN
1	D	490	GLU
1	D	552	LEU
1	D	554	LEU
1	D	574	THR
1	D	582	LEU
1	D	593	ILE
1	D	612	ARG
1	D	616	LEU
1	D	633	LEU
1	D	648	LEU
1	D	713	GLN
1	D	732	LEU
1	D	747	LYS
1	D	750	LYS
1	D	751	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	77	ASN
1	A	252	ASN
1	A	368	GLN
1	A	459	ASN
1	A	515	GLN
1	A	549	HIS
1	A	713	GLN
1	B	157	ASN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	C	252	ASN
1	C	459	ASN
1	C	486	GLN
1	C	507	HIS
1	C	556	GLN
1	C	572	ASN
1	C	629	HIS
1	C	682	ASN
1	D	48	GLN

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Mol	Chain	Res	Type
1	D	84	GLN
1	D	252	ASN
1	D	368	GLN
1	D	459	ASN
1	D	507	HIS
1	D	549	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 ⓘ

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	A	669	1	6,8,9	3.32	1 (16%)	7,11,13	2.40	3 (42%)
1	OCS	D	669	1	6,8,9	3.77	1 (16%)	7,11,13	3.90	7 (100%)
1	OCS	B	669	1	6,8,9	1.69	1 (16%)	7,11,13	2.88	3 (42%)
1	OCS	C	669	1	6,8,9	1.83	1 (16%)	7,11,13	2.26	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	A	669	1	-	4/4/7/9	-
1	OCS	D	669	1	-	4/4/7/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OCS	B	669	1	-	2/4/7/9	-
1	OCS	C	669	1	-	4/4/7/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	669	OCS	CB-CA	9.07	1.60	1.53
1	A	669	OCS	CB-CA	8.01	1.59	1.53
1	C	669	OCS	CB-CA	4.25	1.56	1.53
1	B	669	OCS	CB-CA	3.87	1.56	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	669	OCS	OD3-SG-CB	7.42	117.84	106.76
1	B	669	OCS	OD2-SG-CB	4.88	115.39	105.97
1	B	669	OCS	CA-CB-SG	4.70	120.58	113.61
1	C	669	OCS	OD2-SG-CB	3.99	113.68	105.97
1	D	669	OCS	OD1-SG-CB	3.65	112.20	106.76
1	A	669	OCS	OD1-SG-CB	3.39	111.82	106.76
1	A	669	OCS	OD2-SG-CB	3.30	112.34	105.97
1	C	669	OCS	CA-CB-SG	3.28	118.49	113.61
1	D	669	OCS	OD3-SG-OD1	-3.12	103.67	113.82
1	D	669	OCS	CA-CB-SG	2.92	117.95	113.61
1	D	669	OCS	OD2-SG-CB	2.83	111.44	105.97
1	A	669	OCS	CA-CB-SG	2.76	117.71	113.61
1	D	669	OCS	OD2-SG-OD3	-2.56	105.00	111.40
1	D	669	OCS	OD2-SG-OD1	-2.29	105.68	111.40
1	B	669	OCS	OD2-SG-OD3	-2.06	106.24	111.40

There are no chirality outliers.

All (14) 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-OD1
1	A	669	OCS	CA-CB-SG-OD2
1	A	669	OCS	CA-CB-SG-OD3
1	B	669	OCS	N-CA-CB-SG
1	C	669	OCS	N-CA-CB-SG
1	D	669	OCS	N-CA-CB-SG

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Mol	Chain	Res	Type	Atoms
1	D	669	OCS	CA-CB-SG-OD1
1	D	669	OCS	CA-CB-SG-OD2
1	C	669	OCS	CA-CB-SG-OD1
1	C	669	OCS	CA-CB-SG-OD3
1	D	669	OCS	CA-CB-SG-OD3
1	C	669	OCS	CA-CB-SG-OD2
1	B	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HDD	B	760	3,1	46,52,52	1.48	9 (19%)	62,89,89	2.62	14 (22%)
2	HDD	C	760	3,1	46,52,52	1.43	7 (15%)	62,89,89	2.57	13 (20%)
2	HDD	D	760	1	46,52,52	1.43	8 (17%)	62,89,89	2.37	13 (20%)
2	HDD	A	760	3,1	46,52,52	1.62	8 (17%)	62,89,89	2.58	13 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HDD	B	760	3,1	-	4/9/89/89	0/1/9/9
2	HDD	C	760	3,1	-	2/9/89/89	0/1/9/9
2	HDD	D	760	1	-	3/9/89/89	0/1/9/9
2	HDD	A	760	3,1	-	2/9/89/89	0/1/9/9

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	760	HDD	CMC-C2C	4.50	1.60	1.50
2	A	760	HDD	CMB-C2B	3.62	1.58	1.50
2	C	760	HDD	CMC-C2C	3.44	1.57	1.50
2	A	760	HDD	CAB-C3B	3.34	1.56	1.47
2	D	760	HDD	OND-C2D	3.32	1.49	1.42
2	D	760	HDD	CAB-C3B	3.25	1.56	1.47
2	D	760	HDD	CMD-C2D	3.10	1.57	1.53
2	B	760	HDD	CAB-C3B	3.06	1.55	1.47
2	C	760	HDD	CMB-C2B	3.04	1.57	1.50
2	A	760	HDD	O1D-C3D	-3.00	1.41	1.46
2	C	760	HDD	O1D-C3D	-2.83	1.42	1.46
2	C	760	HDD	CAB-C3B	2.77	1.54	1.47
2	A	760	HDD	OND-C2D	2.72	1.47	1.42
2	D	760	HDD	CMB-C2B	2.72	1.56	1.50
2	A	760	HDD	C1A-C2A	2.66	1.49	1.44
2	A	760	HDD	CMA-C3A	2.62	1.56	1.50
2	B	760	HDD	O1D-C3D	-2.55	1.42	1.46
2	B	760	HDD	CMC-C2C	2.50	1.55	1.50
2	B	760	HDD	CAA-C2A	2.49	1.57	1.51
2	D	760	HDD	CMC-C2C	2.42	1.55	1.50
2	B	760	HDD	O1D-CGD	2.38	1.39	1.35
2	A	760	HDD	C1A-NA	-2.36	1.35	1.39
2	C	760	HDD	CMA-C3A	2.36	1.55	1.50
2	D	760	HDD	CAC-C3C	2.32	1.53	1.47
2	B	760	HDD	CMA-C3A	2.32	1.55	1.50
2	C	760	HDD	C2A-C3A	-2.26	1.33	1.38
2	B	760	HDD	C4D-ND	2.24	1.41	1.37
2	D	760	HDD	CAA-C2A	2.15	1.56	1.51
2	B	760	HDD	O2D-CGD	2.09	1.28	1.22
2	D	760	HDD	C3C-C2C	-2.09	1.34	1.41
2	B	760	HDD	C4A-C3A	2.07	1.48	1.43
2	C	760	HDD	C1A-C2A	2.07	1.48	1.44

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	760	HDD	O1D-CGD-O2D	13.40	132.09	120.81
2	C	760	HDD	O1D-CGD-O2D	12.33	131.19	120.81
2	A	760	HDD	O1D-CGD-O2D	11.35	130.37	120.81
2	D	760	HDD	O1D-CGD-O2D	9.69	128.97	120.81
2	D	760	HDD	O1D-CGD-CBD	-8.34	102.57	110.17
2	A	760	HDD	C3D-O1D-CGD	8.16	118.75	111.14
2	A	760	HDD	O1D-CGD-CBD	-8.00	102.88	110.17
2	B	760	HDD	C3D-O1D-CGD	7.50	118.14	111.14
2	C	760	HDD	O1D-CGD-CBD	-7.37	103.45	110.17
2	B	760	HDD	O1D-CGD-CBD	-6.70	104.06	110.17
2	D	760	HDD	C3D-O1D-CGD	6.53	117.23	111.14
2	C	760	HDD	C3D-O1D-CGD	6.11	116.84	111.14
2	A	760	HDD	CMD-C2D-C1D	-5.69	103.05	112.68
2	C	760	HDD	OND-C2D-CMD	-5.62	98.59	109.45
2	D	760	HDD	OND-C2D-CMD	-5.22	99.36	109.45
2	B	760	HDD	C3C-C4C-NC	-4.95	105.63	109.80
2	A	760	HDD	C3C-C4C-NC	-4.56	105.96	109.80
2	D	760	HDD	CAA-CBA-CGA	-4.29	102.28	113.67
2	C	760	HDD	C3C-C4C-NC	-4.21	106.26	109.80
2	B	760	HDD	CAA-CBA-CGA	-4.02	103.00	113.67
2	B	760	HDD	OND-C2D-CMD	-3.77	102.17	109.45
2	D	760	HDD	C3C-C4C-NC	-3.71	106.67	109.80
2	C	760	HDD	C4C-C3C-C2C	3.56	111.73	107.30
2	A	760	HDD	CAA-CBA-CGA	-3.38	104.71	113.67
2	C	760	HDD	CHD-C4C-NC	3.28	129.80	123.86
2	A	760	HDD	CHA-C4D-ND	-3.08	120.04	124.28
2	C	760	HDD	C2A-C1A-NA	-2.98	106.84	110.15
2	A	760	HDD	C4C-C3C-C2C	2.96	110.99	107.30
2	C	760	HDD	CHC-C4B-NB	2.92	127.63	124.45
2	C	760	HDD	CBC-CAC-C3C	-2.83	113.39	127.53
2	B	760	HDD	CHD-C4C-NC	2.82	128.98	123.86
2	D	760	HDD	CHA-C1A-NA	2.78	128.90	123.86
2	C	760	HDD	CAA-CBA-CGA	-2.71	106.48	113.67
2	B	760	HDD	C4C-NC-C1C	2.65	110.15	105.82
2	D	760	HDD	O1A-CGA-CBA	-2.60	114.86	123.09
2	D	760	HDD	C4A-NA-C1A	2.58	110.02	105.82
2	B	760	HDD	CHC-C1C-NC	2.51	128.42	123.86
2	D	760	HDD	C2A-C1A-NA	-2.46	107.42	110.15
2	A	760	HDD	CHD-C4C-NC	2.30	128.04	123.86
2	B	760	HDD	CMD-C2D-C1D	2.30	116.57	112.68
2	A	760	HDD	C2A-C1A-NA	-2.29	107.61	110.15
2	A	760	HDD	CBC-CAC-C3C	-2.28	116.12	127.53
2	B	760	HDD	C4B-C3B-C2B	2.25	108.77	106.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	760	HDD	C4B-NB-C1B	2.25	109.48	105.82
2	B	760	HDD	CAD-CBD-CGD	2.22	107.77	104.48
2	C	760	HDD	CHB-C4A-NA	2.19	127.84	123.86
2	B	760	HDD	C2C-C1C-NC	-2.19	106.63	110.14
2	A	760	HDD	CMC-C2C-C1C	2.18	128.74	125.42
2	D	760	HDD	C4B-NB-C1B	2.15	109.33	105.82
2	D	760	HDD	CHC-C1C-NC	2.10	127.68	123.86
2	C	760	HDD	C4A-NA-C1A	2.08	109.20	105.82
2	D	760	HDD	C4C-NC-C1C	2.05	109.16	105.82
2	A	760	HDD	C1A-CHA-C4D	2.03	129.75	125.81

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	760	HDD	C4C-C3C-CAC-CBC
2	B	760	HDD	CAA-CBA-CGA-O1A
2	A	760	HDD	CAA-CBA-CGA-O1A
2	A	760	HDD	CAA-CBA-CGA-O2A
2	B	760	HDD	CAA-CBA-CGA-O2A
2	D	760	HDD	CAA-CBA-CGA-O2A
2	B	760	HDD	C2C-C3C-CAC-CBC
2	C	760	HDD	CAA-CBA-CGA-O2A
2	D	760	HDD	CAA-CBA-CGA-O1A
2	C	760	HDD	CAA-CBA-CGA-O1A
2	D	760	HDD	C2C-C3C-CAC-CBC

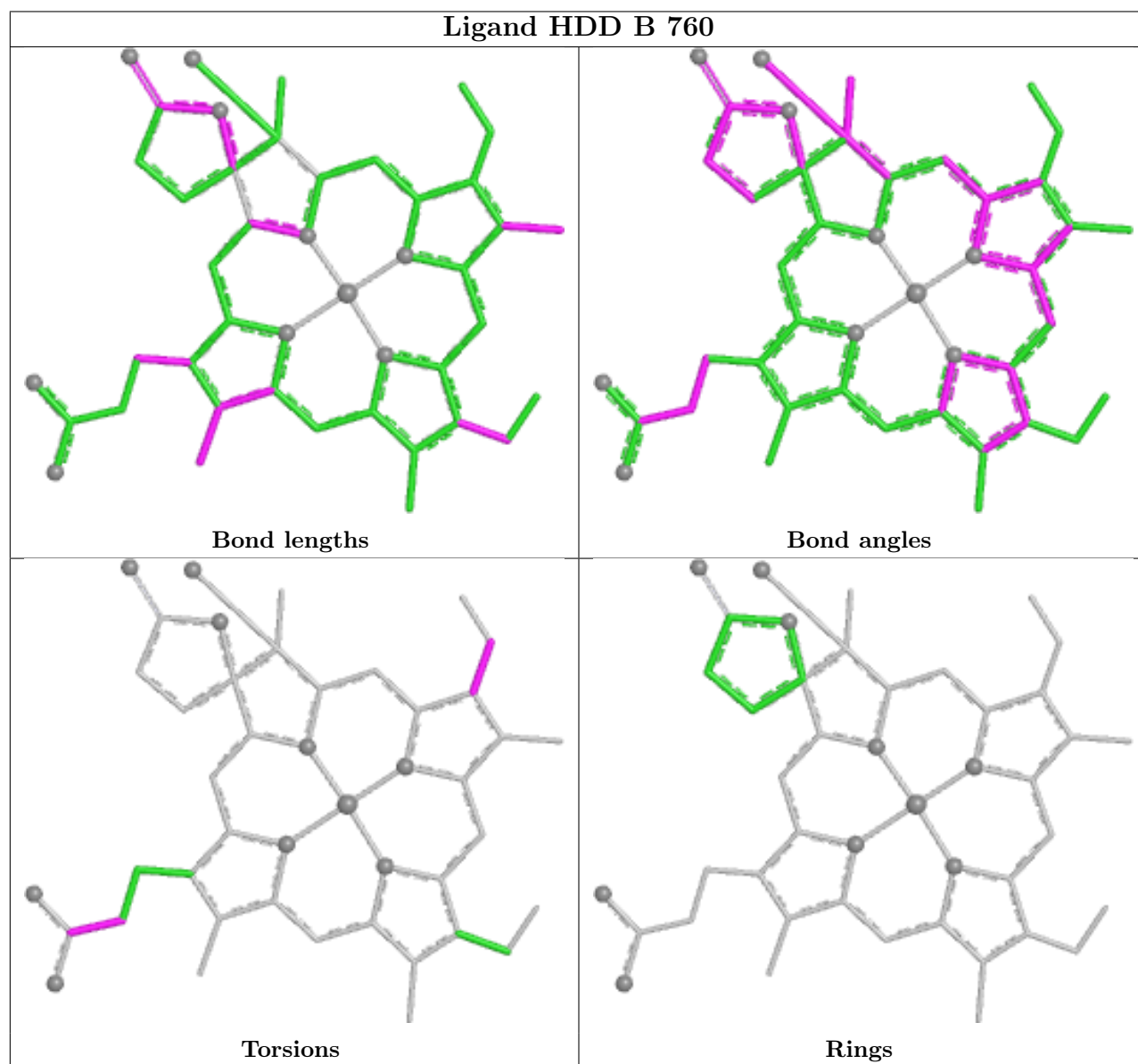
There are no ring outliers.

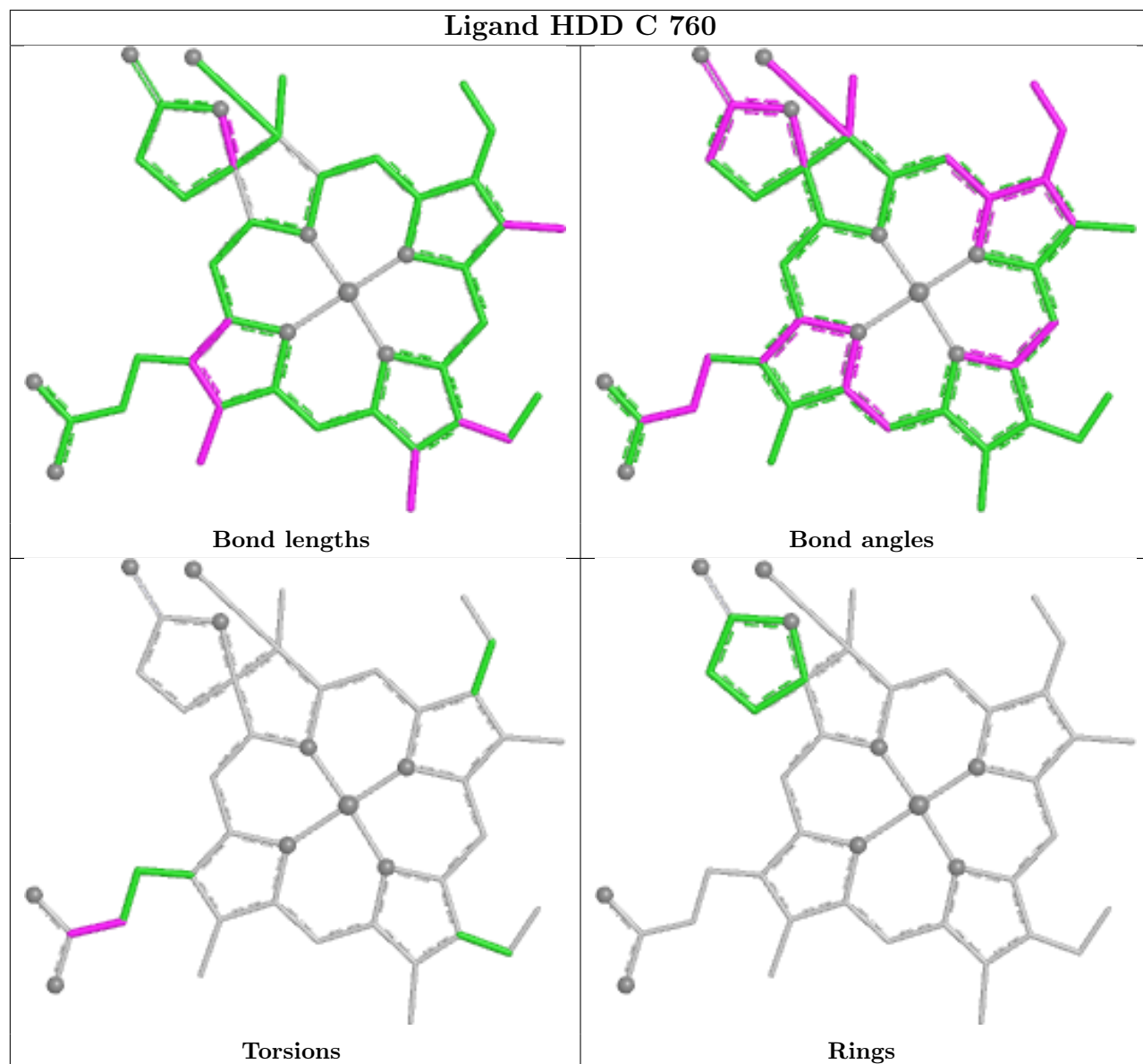
4 monomers are involved in 11 short contacts:

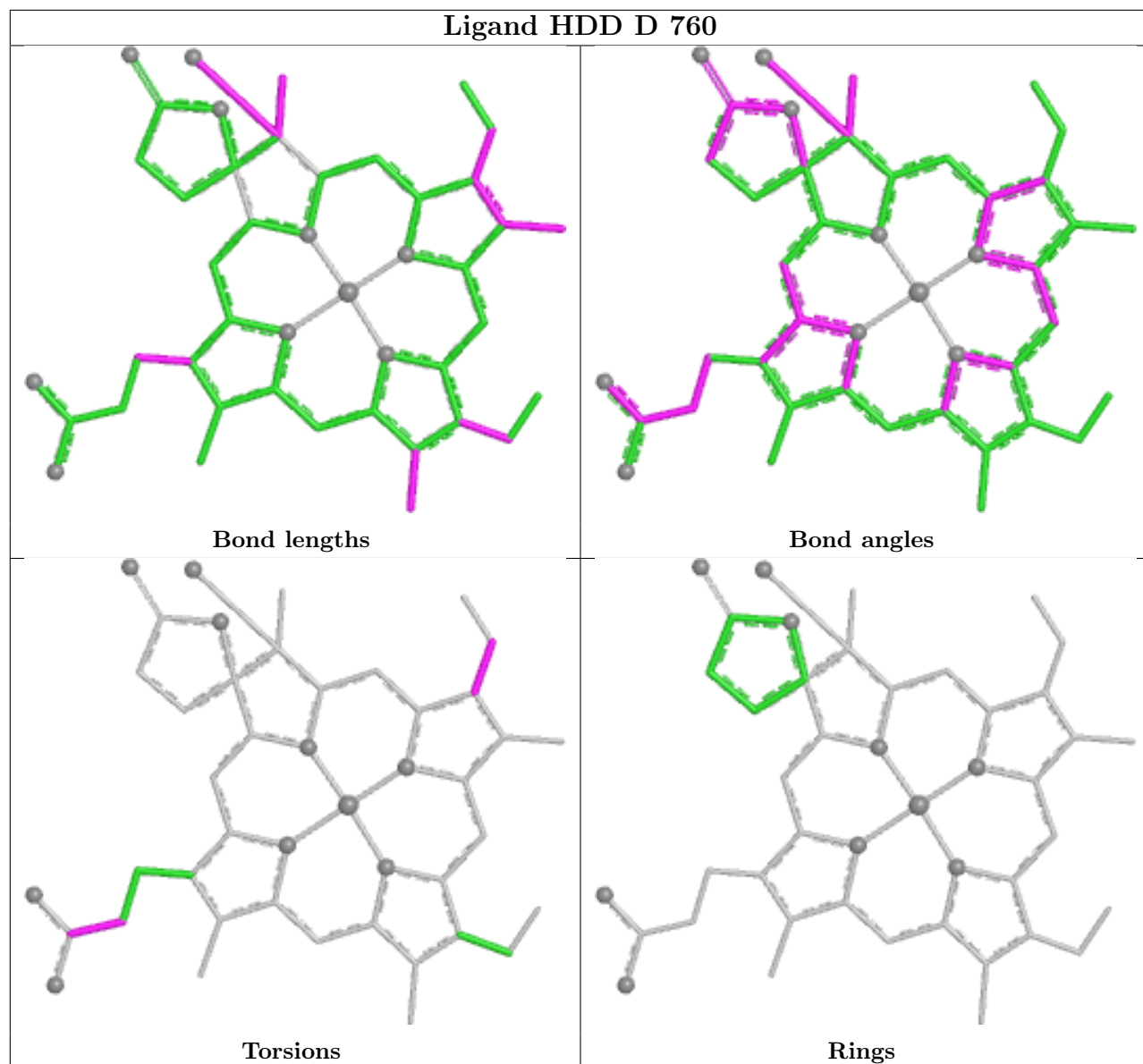
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	760	HDD	5	0
2	C	760	HDD	2	0
2	D	760	HDD	2	0
2	A	760	HDD	2	0

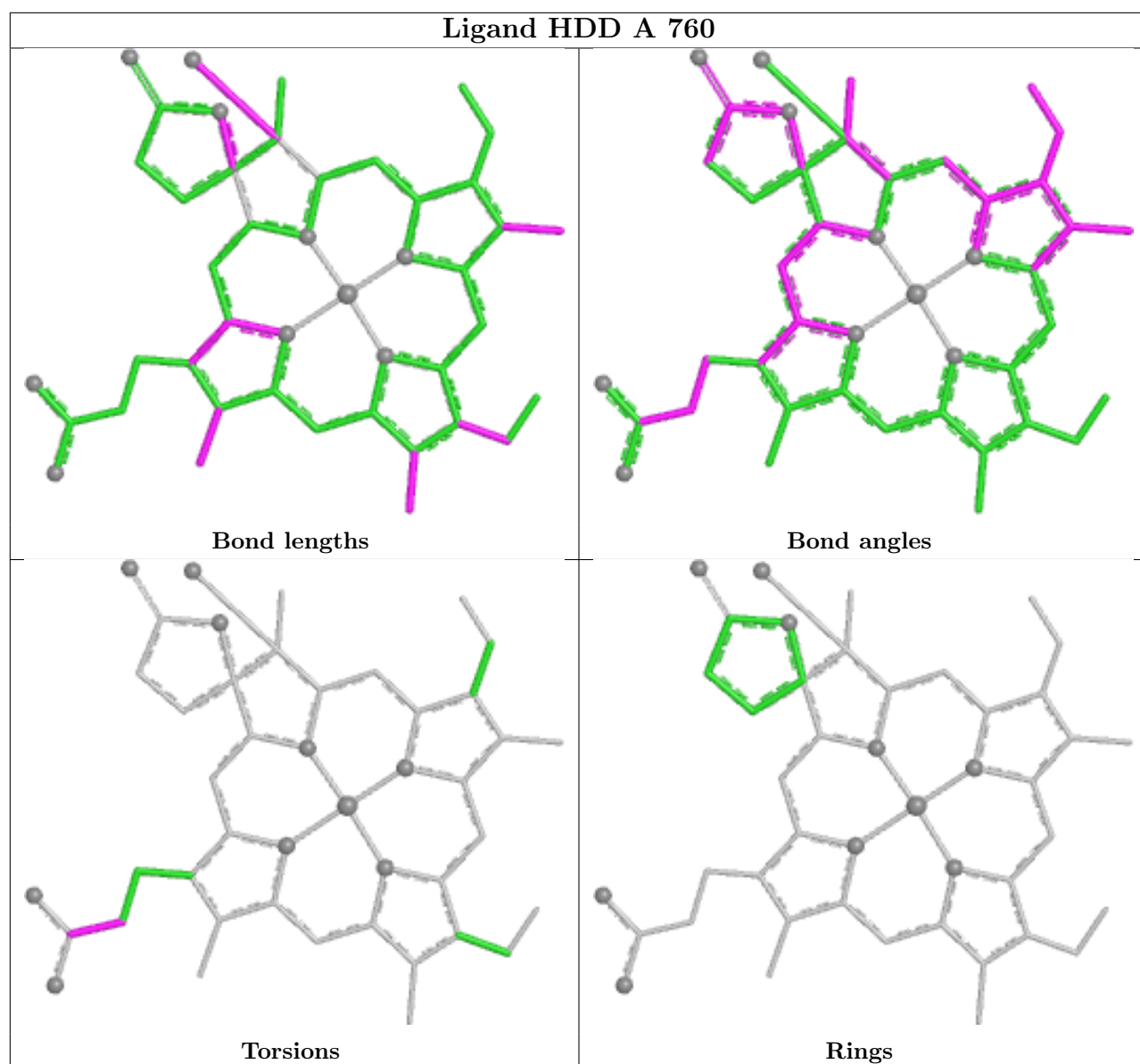
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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%)	-0.96	1 (0%) 92 92	5, 11, 27, 43	4 (0%)
1	B	725/753 (96%)	-0.86	0 100 100	4, 13, 33, 47	4 (0%)
1	C	725/753 (96%)	-0.88	1 (0%) 92 92	5, 12, 33, 47	3 (0%)
1	D	725/753 (96%)	-0.93	2 (0%) 90 91	4, 11, 29, 44	3 (0%)
All	All	2900/3012 (96%)	-0.91	4 (0%) 92 92	4, 12, 31, 47	14 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	SER	4.3
1	C	726	GLY	3.0
1	D	28	SER	2.2
1	D	725	ASP	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	D	669	9/10	0.88	0.11	23,27,43,45	0
1	OCS	B	669	9/10	0.89	0.10	30,33,49,49	0
1	OCS	C	669	9/10	0.90	0.09	30,33,48,48	0
1	OCS	A	669	9/10	0.92	0.08	20,24,39,42	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

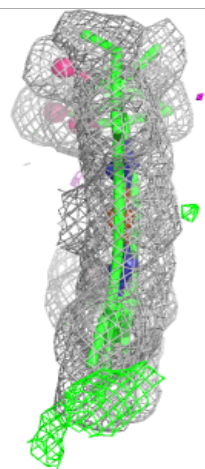
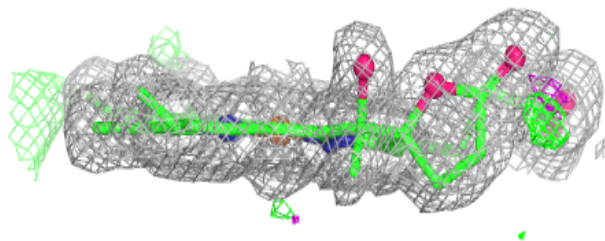
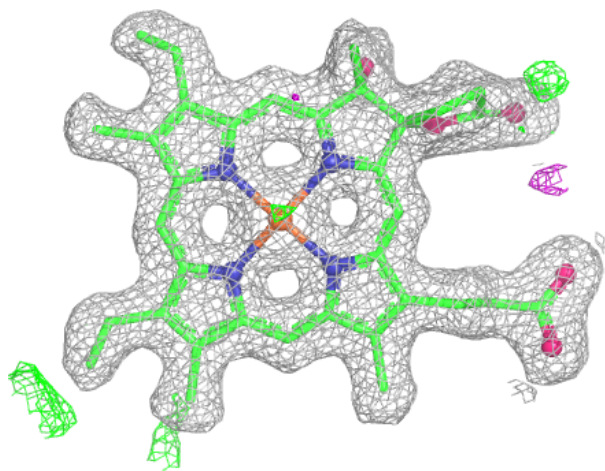
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	760	44/44	0.99	0.04	3,10,17,22	0
2	HDD	B	760	44/44	0.99	0.04	5,11,19,22	0
2	HDD	C	760	44/44	0.99	0.04	4,10,18,21	0
2	HDD	D	760	44/44	0.99	0.04	3,10,16,24	0

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

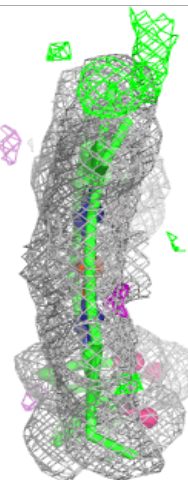
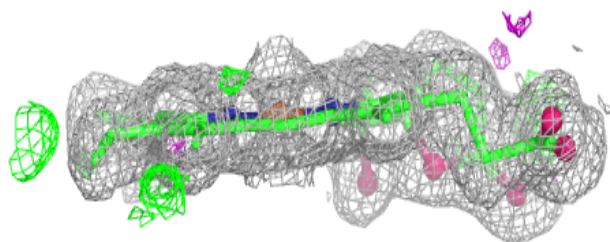
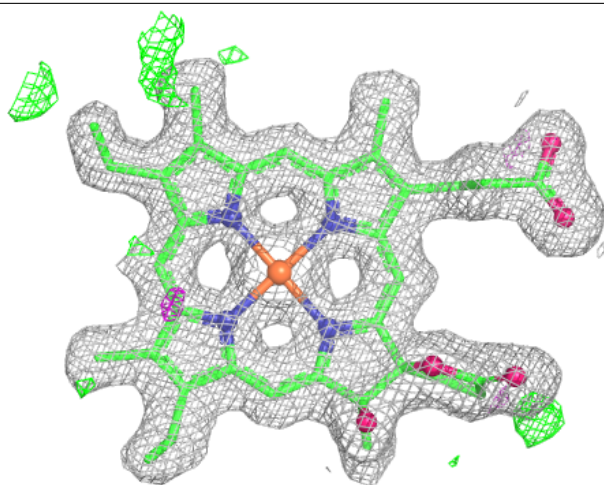
Electron density around HDD A 760:

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



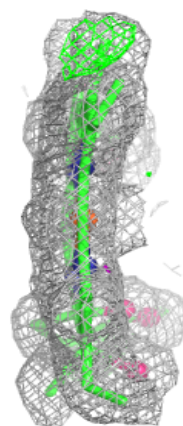
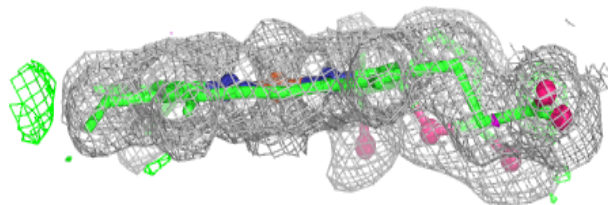
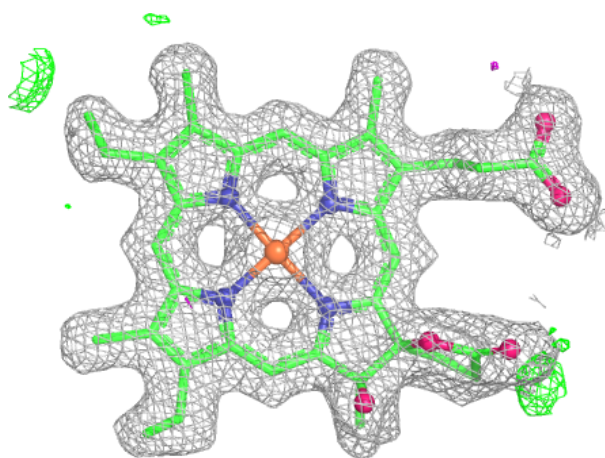
Electron density around HDD B 760:

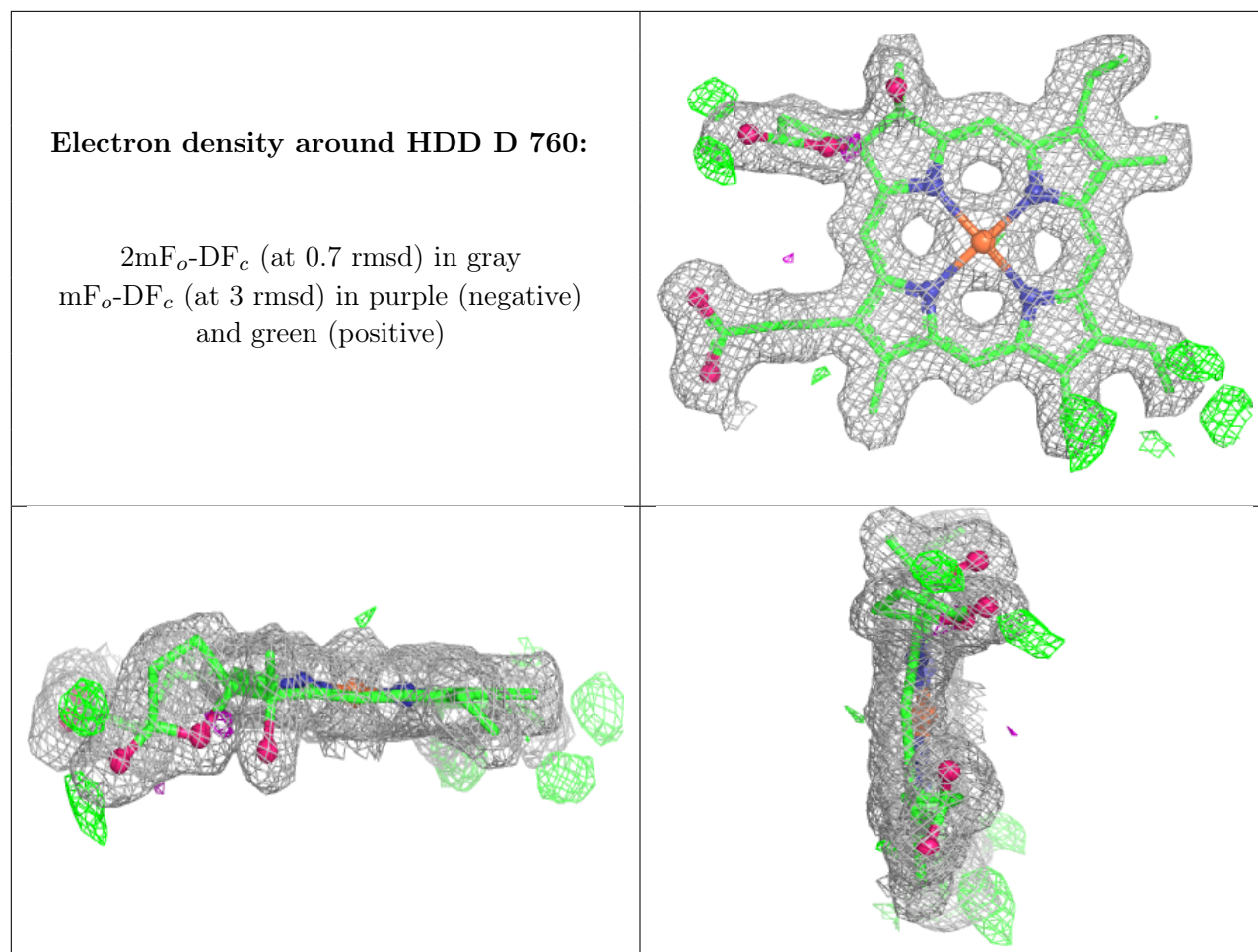
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HDD C 760:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.