



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:13 PM UTC

PDB ID : 1YMC / pdb_00001ymc
Title : THREE-DIMENSIONAL STRUCTURE OF CYANOMET-SULFMYOGLOBIN C
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Deposited on : 1993-09-27
Resolution : 2.00 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

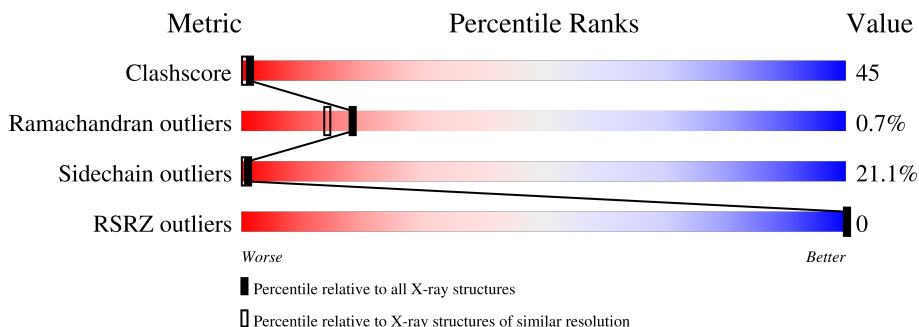
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	153	10% 44% 37% 8%

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
2	SO4	A	155	-	-	X	-
4	CLN	A	154	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 1423 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 CYANOMET-SULFMYOGLOBIN.

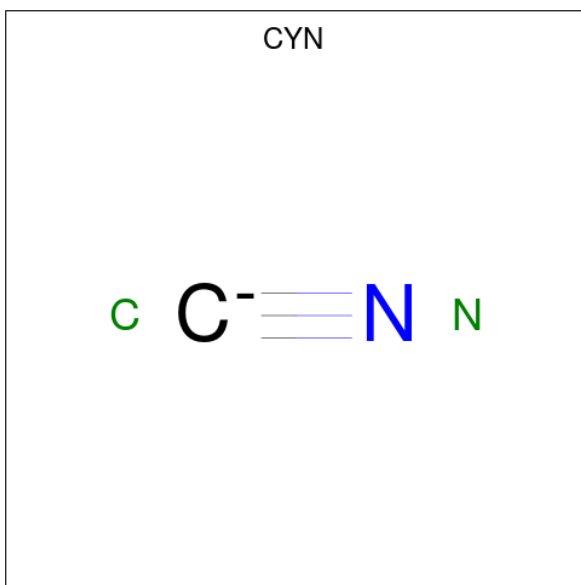
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	0	0
			1199	769	210	218	2			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



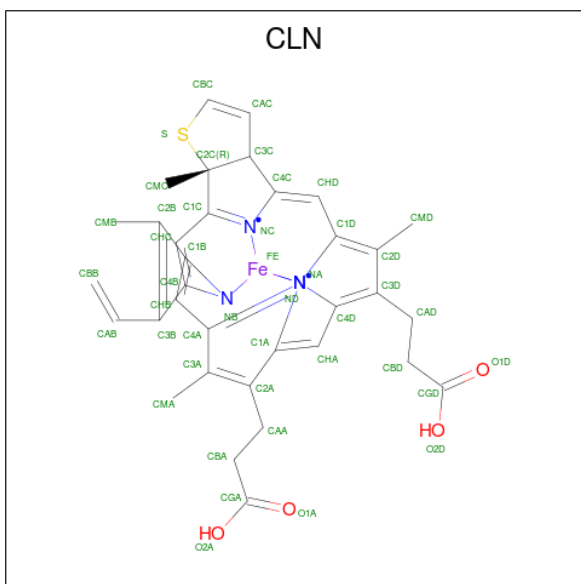
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CYANIDE ION (CCD ID: CYN) (formula: CN).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			2	1	1		

- Molecule 4 is SULFUR SUBSTITUTED PROTOPORPHYRIN IX (CCD ID: CLN) (formula: $C_{34}H_{32}FeN_4O_4S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	S	0	0
			44	34	1	4	4	1		

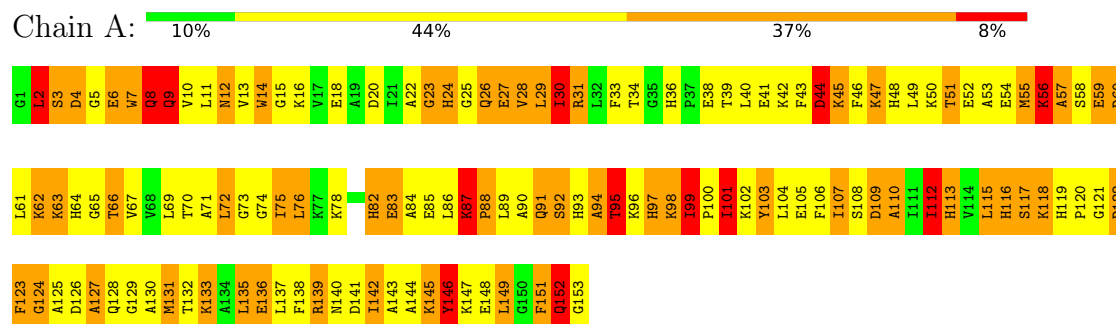
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	173	Total 173	O 173	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: CYANOMET-SULFMYOGLOBIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.50Å 28.91Å 35.66Å 90.00° 107.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.00 6.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.00) 61.4 (6.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.129 , (Not available) 0.129 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	9.8	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.06 , 49.6	EDS
L-test for twinning ¹	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.096 for -h-l,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1423	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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: CYN, SO4, CLN

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	2.34	49/1226 (4.0%)	3.40	204/1645 (12.4%)

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	ALA	C-O	12.40	1.38	1.24
1	A	133	LYS	C-O	8.76	1.34	1.24
1	A	91	GLN	N-CA	8.31	1.56	1.46
1	A	99	ILE	N-CA	7.96	1.52	1.46
1	A	121	GLY	C-O	7.81	1.34	1.23
1	A	65	GLY	C-N	-7.73	1.23	1.33
1	A	11	LEU	C-O	7.67	1.33	1.24
1	A	7	TRP	N-CA	7.29	1.55	1.46
1	A	132	THR	N-CA	7.25	1.55	1.46
1	A	23	GLY	N-CA	7.11	1.55	1.45
1	A	62	LYS	CA-CB	-7.09	1.42	1.53
1	A	31	ARG	CD-NE	-6.94	1.36	1.46
1	A	110	ALA	C-N	-6.83	1.25	1.33
1	A	103	TYR	N-CA	6.79	1.55	1.46
1	A	62	LYS	C-O	6.58	1.31	1.24
1	A	124	GLY	N-CA	-6.52	1.35	1.45
1	A	95	THR	C-N	-6.40	1.24	1.33
1	A	126	ASP	C-O	6.40	1.31	1.24
1	A	62	LYS	C-N	-6.33	1.25	1.34
1	A	20	ASP	CA-CB	-6.15	1.43	1.53
1	A	64	HIS	N-CA	6.14	1.54	1.46
1	A	123	PHE	N-CA	6.13	1.54	1.46
1	A	69	LEU	C-O	6.06	1.31	1.24
1	A	119	HIS	N-CA	6.03	1.53	1.46
1	A	103	TYR	CA-CB	-5.93	1.43	1.53
1	A	51	THR	CB-OG1	5.92	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	THR	CA-C	-5.90	1.45	1.52
1	A	30	ILE	CA-CB	5.85	1.60	1.54
1	A	113	HIS	N-CA	5.80	1.53	1.46
1	A	76	LEU	CB-CG	-5.70	1.42	1.53
1	A	93	HIS	ND1-CE1	-5.60	1.26	1.32
1	A	64	HIS	CG-ND1	-5.58	1.32	1.38
1	A	97	HIS	ND1-CE1	-5.56	1.26	1.32
1	A	110	ALA	N-CA	-5.56	1.39	1.46
1	A	89	LEU	N-CA	5.47	1.53	1.46
1	A	60	ASP	N-CA	5.42	1.53	1.46
1	A	91	GLN	CD-NE2	5.39	1.44	1.33
1	A	36	HIS	CA-C	-5.35	1.46	1.52
1	A	125	ALA	C-O	-5.32	1.18	1.24
1	A	54	GLU	C-O	-5.31	1.17	1.24
1	A	15	GLY	N-CA	-5.23	1.38	1.45
1	A	95	THR	CB-OG1	5.18	1.52	1.43
1	A	31	ARG	C-O	-5.17	1.17	1.24
1	A	43	PHE	C-O	-5.17	1.17	1.24
1	A	10	VAL	N-CA	5.15	1.52	1.46
1	A	138	PHE	N-CA	-5.13	1.40	1.46
1	A	22	ALA	N-CA	5.12	1.52	1.46
1	A	88	PRO	N-CA	-5.11	1.40	1.47
1	A	82	HIS	CA-CB	5.05	1.60	1.53

All (204) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	ASP	CA-CB-CG	26.82	139.42	112.60
1	A	62	LYS	CA-CB-CG	19.45	153.00	114.10
1	A	139	ARG	CD-NE-CZ	16.41	147.38	124.40
1	A	126	ASP	CA-CB-CG	15.28	127.88	112.60
1	A	148	GLU	CA-C-O	-13.20	106.96	120.82
1	A	148	GLU	O-C-N	12.92	135.38	122.07
1	A	7	TRP	CA-C-O	12.19	133.34	120.42
1	A	34	THR	CA-C-N	11.79	135.20	120.34
1	A	34	THR	C-N-CA	11.79	135.20	120.34
1	A	113	HIS	CA-C-O	11.65	133.02	120.55
1	A	31	ARG	CD-NE-CZ	11.43	140.41	124.40
1	A	152	GLN	CB-CG-CD	10.71	130.81	112.60
1	A	8	GLN	CA-CB-CG	10.47	135.04	114.10
1	A	151	PHE	CA-CB-CG	10.45	124.25	113.80
1	A	64	HIS	CA-CB-CG	10.40	124.20	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ARG	NH1-CZ-NH2	-10.26	105.96	119.30
1	A	109	ASP	CA-C-N	10.19	133.93	120.28
1	A	109	ASP	C-N-CA	10.19	133.93	120.28
1	A	65	GLY	CA-C-N	10.16	133.90	120.28
1	A	65	GLY	C-N-CA	10.16	133.90	120.28
1	A	101	ILE	CA-C-O	-10.11	109.62	120.64
1	A	123	PHE	CA-CB-CG	9.74	123.54	113.80
1	A	103	TYR	CA-CB-CG	9.57	131.13	113.90
1	A	33	PHE	CA-C-O	-9.53	110.45	120.55
1	A	9	GLN	O-C-N	-9.52	110.56	122.27
1	A	66	THR	CA-CB-CG2	9.46	126.59	110.50
1	A	85	GLU	CG-CD-OE1	9.28	139.74	118.40
1	A	67	VAL	CB-CA-C	9.11	124.79	112.22
1	A	73	GLY	CA-C-N	9.06	130.03	119.98
1	A	73	GLY	C-N-CA	9.06	130.03	119.98
1	A	5	GLY	N-CA-C	-8.89	102.19	112.50
1	A	38	GLU	O-C-N	8.88	133.19	122.27
1	A	20	ASP	CA-CB-CG	8.81	121.42	112.60
1	A	87	LYS	CA-C-N	8.64	128.64	119.05
1	A	87	LYS	C-N-CA	8.64	128.64	119.05
1	A	76	LEU	CA-C-O	-8.49	110.21	119.97
1	A	144	ALA	CA-C-O	-8.47	111.45	120.42
1	A	44	ASP	N-CA-C	-8.40	103.03	113.28
1	A	75	ILE	CA-C-O	8.33	130.00	121.17
1	A	31	ARG	CG-CD-NE	8.22	130.09	112.00
1	A	41	GLU	CB-CG-CD	8.21	126.56	112.60
1	A	70	THR	N-CA-C	-8.14	102.35	111.14
1	A	33	PHE	O-C-N	8.09	130.70	122.12
1	A	123	PHE	CB-CA-C	8.09	123.62	111.17
1	A	148	GLU	N-CA-CB	7.88	121.43	110.01
1	A	26	GLN	OE1-CD-NE2	7.87	130.47	122.60
1	A	30	ILE	O-C-N	7.83	129.78	121.94
1	A	85	GLU	CA-C-O	7.78	128.94	119.38
1	A	133	LYS	CA-C-O	7.62	128.73	120.20
1	A	4	ASP	N-CA-CB	7.57	122.01	110.28
1	A	139	ARG	NE-CZ-NH2	7.57	126.01	119.20
1	A	140	ASN	OD1-CG-ND2	7.56	130.16	122.60
1	A	147	LYS	CA-C-O	-7.46	112.64	120.55
1	A	135	LEU	N-CA-C	-7.40	102.90	112.23
1	A	27	GLU	CA-C-O	-7.39	113.08	120.70
1	A	55	MET	CG-SD-CE	7.39	117.17	100.90
1	A	127	ALA	N-CA-CB	7.22	120.48	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	HIS	N-CA-CB	7.16	121.06	110.33
1	A	98	LYS	CA-C-O	7.09	129.77	121.54
1	A	28	VAL	CA-C-O	7.08	128.63	121.27
1	A	70	THR	N-CA-CB	7.03	120.26	110.07
1	A	74	GLY	CA-C-N	-7.02	111.72	120.56
1	A	74	GLY	C-N-CA	-7.02	111.72	120.56
1	A	56	LYS	CA-C-O	-7.01	111.91	119.97
1	A	98	LYS	CG-CD-CE	6.95	127.28	111.30
1	A	113	HIS	N-CA-CB	-6.94	99.86	110.13
1	A	2	LEU	CA-CB-CG	6.94	140.59	116.30
1	A	54	GLU	N-CA-CB	6.88	120.81	110.22
1	A	113	HIS	CB-CA-C	6.87	122.33	110.79
1	A	151	PHE	CA-C-N	6.87	134.66	121.54
1	A	151	PHE	C-N-CA	6.87	134.66	121.54
1	A	62	LYS	CB-CA-C	6.86	122.52	110.85
1	A	67	VAL	N-CA-CB	-6.86	100.30	110.58
1	A	85	GLU	CG-CD-OE2	-6.81	102.73	118.40
1	A	116	HIS	CA-C-O	6.79	127.69	120.70
1	A	62	LYS	CA-C-O	-6.77	113.24	120.42
1	A	83	GLU	CA-C-N	6.76	129.83	120.63
1	A	83	GLU	C-N-CA	6.76	129.83	120.63
1	A	8	GLN	N-CA-C	-6.71	103.96	111.28
1	A	122	ASP	CA-C-N	-6.64	113.39	122.95
1	A	122	ASP	C-N-CA	-6.64	113.39	122.95
1	A	91	GLN	CB-CG-CD	6.62	123.85	112.60
1	A	38	GLU	CA-C-O	-6.55	112.43	119.97
1	A	139	ARG	NE-CZ-NH1	6.53	128.03	121.50
1	A	26	GLN	CG-CD-NE2	-6.51	106.63	116.40
1	A	103	TYR	N-CA-C	-6.50	104.27	111.82
1	A	144	ALA	CB-CA-C	6.50	121.91	110.85
1	A	8	GLN	CA-C-O	-6.49	113.67	120.55
1	A	85	GLU	O-C-N	-6.34	113.93	122.43
1	A	105	GLU	CB-CG-CD	6.33	123.36	112.60
1	A	102	LYS	CA-CB-CG	6.28	126.65	114.10
1	A	106	PHE	CA-CB-CG	6.27	120.07	113.80
1	A	135	LEU	CB-CA-C	6.25	123.14	110.38
1	A	26	GLN	CA-C-O	6.22	127.36	120.82
1	A	142	ILE	CB-CG1-CD1	6.21	126.84	113.80
1	A	27	GLU	CG-CD-OE2	6.20	132.66	118.40
1	A	58	SER	O-C-N	6.18	130.56	122.89
1	A	39	THR	CA-CB-OG1	-6.18	100.33	109.60
1	A	147	LYS	CB-CG-CD	6.17	125.50	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	GLN	CB-CA-C	6.15	122.47	110.67
1	A	133	LYS	N-CA-C	6.14	119.61	111.75
1	A	76	LEU	O-C-N	6.11	129.79	122.27
1	A	99	ILE	CA-C-O	-6.11	115.54	119.15
1	A	56	LYS	N-CA-CB	6.10	119.74	110.28
1	A	133	LYS	CA-CB-CG	-6.08	101.94	114.10
1	A	78	LYS	CA-C-N	-6.06	113.91	122.34
1	A	78	LYS	C-N-CA	-6.06	113.91	122.34
1	A	127	ALA	CA-C-N	6.04	128.65	120.38
1	A	127	ALA	C-N-CA	6.04	128.65	120.38
1	A	12	ASN	N-CA-C	-6.03	104.62	111.14
1	A	152	GLN	OE1-CD-NE2	-6.03	116.57	122.60
1	A	131	MET	N-CA-C	-6.02	104.29	111.69
1	A	93	HIS	CA-CB-CG	-6.00	107.81	113.80
1	A	82	HIS	ND1-CE1-NE2	5.99	114.39	108.40
1	A	56	LYS	O-C-N	5.98	129.62	122.27
1	A	139	ARG	CB-CG-CD	5.96	125.02	111.30
1	A	97	HIS	N-CA-CB	5.96	120.11	110.40
1	A	63	LYS	CA-C-O	-5.94	113.39	120.10
1	A	122	ASP	N-CA-CB	5.90	120.93	111.20
1	A	64	HIS	CA-C-O	-5.90	112.70	119.60
1	A	137	LEU	O-C-N	5.89	128.92	122.20
1	A	67	VAL	CA-C-O	5.88	127.08	120.85
1	A	72	LEU	N-CA-CB	-5.86	101.58	110.07
1	A	90	ALA	CA-C-O	5.82	127.12	120.90
1	A	123	PHE	CA-C-N	5.81	132.80	121.41
1	A	123	PHE	C-N-CA	5.81	132.80	121.41
1	A	38	GLU	N-CA-CB	5.79	119.26	110.28
1	A	132	THR	CA-CB-OG1	-5.78	100.93	109.60
1	A	24	HIS	N-CA-CB	5.78	119.23	110.28
1	A	12	ASN	CA-CB-CG	5.77	118.37	112.60
1	A	63	LYS	CA-CB-CG	5.76	125.63	114.10
1	A	147	LYS	O-C-N	5.75	128.22	122.12
1	A	4	ASP	CA-C-O	-5.75	113.36	119.97
1	A	58	SER	CB-CA-C	-5.72	102.77	109.80
1	A	142	ILE	CA-C-O	-5.71	114.79	120.85
1	A	88	PRO	O-C-N	5.69	129.05	122.23
1	A	14	TRP	N-CA-C	-5.67	105.09	112.23
1	A	82	HIS	CE1-NE2-CD2	-5.66	103.34	109.00
1	A	76	LEU	CA-CB-CG	5.66	136.10	116.30
1	A	84	ALA	N-CA-CB	-5.64	101.80	109.98
1	A	131	MET	CB-CA-C	5.64	121.02	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	ASN	N-CA-CB	-5.63	101.56	110.28
1	A	24	HIS	CA-CB-CG	-5.59	108.21	113.80
1	A	133	LYS	O-C-N	-5.58	115.84	122.20
1	A	146	TYR	CA-C-N	5.57	127.75	120.28
1	A	146	TYR	C-N-CA	5.57	127.75	120.28
1	A	91	GLN	CA-CB-CG	5.57	125.24	114.10
1	A	109	ASP	O-C-N	5.56	128.49	122.15
1	A	28	VAL	CA-C-N	5.54	127.97	120.44
1	A	28	VAL	C-N-CA	5.54	127.97	120.44
1	A	29	LEU	CA-C-O	-5.53	115.00	120.70
1	A	62	LYS	CA-C-N	5.50	128.19	120.28
1	A	62	LYS	C-N-CA	5.50	128.19	120.28
1	A	113	HIS	O-C-N	-5.50	115.52	122.17
1	A	57	ALA	CB-CA-C	5.49	120.18	110.85
1	A	36	HIS	CA-C-O	5.47	126.49	121.34
1	A	109	ASP	N-CA-C	-5.46	105.41	111.36
1	A	118	LYS	CG-CD-CE	5.46	123.86	111.30
1	A	112	ILE	CA-CB-CG2	5.46	119.78	110.50
1	A	39	THR	CA-CB-CG2	5.45	119.77	110.50
1	A	116	HIS	CA-CB-CG	-5.44	108.36	113.80
1	A	52	GLU	CB-CG-CD	5.42	121.81	112.60
1	A	103	TYR	CB-CA-C	5.38	121.00	110.67
1	A	152	GLN	CG-CD-NE2	5.38	124.47	116.40
1	A	93	HIS	ND1-CE1-NE2	5.37	113.77	108.40
1	A	69	LEU	O-C-N	-5.35	115.96	122.22
1	A	44	ASP	CA-C-N	-5.34	113.73	122.54
1	A	44	ASP	C-N-CA	-5.34	113.73	122.54
1	A	12	ASN	OD1-CG-ND2	-5.33	117.27	122.60
1	A	100	PRO	CA-C-O	5.33	127.74	121.56
1	A	71	ALA	N-CA-CB	5.33	117.95	110.12
1	A	6	GLU	CA-CB-CG	5.32	124.75	114.10
1	A	126	ASP	CA-C-O	-5.32	115.22	120.70
1	A	99	ILE	N-CA-CB	-5.30	104.41	111.08
1	A	44	ASP	CB-CA-C	5.28	119.85	109.72
1	A	149	LEU	CA-C-O	5.27	127.35	118.91
1	A	144	ALA	N-CA-C	-5.27	105.61	111.36
1	A	53	ALA	N-CA-C	-5.26	105.22	111.69
1	A	92	SER	CA-CB-OG	-5.26	100.59	111.10
1	A	143	ALA	O-C-N	5.26	128.37	122.22
1	A	64	HIS	N-CA-C	-5.23	106.05	112.90
1	A	3	SER	CA-C-N	5.22	128.25	120.31
1	A	3	SER	C-N-CA	5.22	128.25	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	LYS	CB-CA-C	-5.21	102.15	110.79
1	A	132	THR	OG1-CB-CG2	5.20	119.70	109.30
1	A	64	HIS	CB-CG-CD2	-5.19	124.46	131.20
1	A	116	HIS	N-CA-CB	5.18	117.58	110.07
1	A	11	LEU	N-CA-CB	-5.16	101.83	110.39
1	A	64	HIS	CB-CG-ND1	5.14	130.42	122.70
1	A	135	LEU	CA-CB-CG	5.14	134.29	116.30
1	A	136	GLU	CA-C-N	5.13	127.87	120.38
1	A	136	GLU	C-N-CA	5.13	127.87	120.38
1	A	12	ASN	CB-CA-C	5.11	118.97	110.90
1	A	54	GLU	N-CA-C	-5.11	105.84	111.71
1	A	113	HIS	N-CA-C	-5.10	105.18	111.40
1	A	146	TYR	N-CA-C	-5.07	105.83	111.36
1	A	94	ALA	CA-C-O	-5.07	114.43	120.56
1	A	85	GLU	CB-CG-CD	5.05	121.19	112.60
1	A	99	ILE	CB-CA-C	5.05	116.11	110.71
1	A	124	GLY	N-CA-C	5.04	125.13	113.18
1	A	86	LEU	CA-C-O	-5.01	114.67	120.24
1	A	117	SER	CA-C-N	-5.01	112.70	120.31
1	A	117	SER	C-N-CA	-5.01	112.70	120.31
1	A	143	ALA	N-CA-C	-5.00	105.96	111.71

There are no chirality outliers.

There are no planarity outliers.

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	1199	0	1212	111	5
2	A	5	0	0	2	0
3	A	2	0	0	0	0
4	A	44	0	29	5	0
5	A	173	0	0	52	5
All	All	1423	0	1241	112	8

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 45.

All (112) 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:24:HIS:HA	1:A:118:LYS:HZ1	1.24	1.00
1:A:62:LYS:HB3	5:A:276:HOH:O	1.66	0.95
1:A:152:GLN:HG2	5:A:228:HOH:O	1.79	0.83
1:A:104:LEU:HD23	4:A:154:CLN:CMC	2.10	0.81
1:A:115:LEU:HD13	5:A:321:HOH:O	1.79	0.81
1:A:87:LYS:HA	5:A:273:HOH:O	1.82	0.80
1:A:4:ASP:O	1:A:8:GLN:HB2	1.82	0.80
1:A:131:MET:HB3	5:A:274:HOH:O	1.81	0.79
1:A:51:THR:O	1:A:55:MET:HG3	1.82	0.79
1:A:104:LEU:HD23	4:A:154:CLN:HMC1	1.66	0.78
1:A:24:HIS:HA	1:A:118:LYS:NZ	2.00	0.77
1:A:9:GLN:HG2	5:A:182:HOH:O	1.83	0.77
1:A:94:ALA:O	1:A:98:LYS:HD3	1.86	0.76
1:A:30:ILE:CG1	1:A:55:MET:HE3	2.17	0.75
1:A:122:ASP:HB2	5:A:249:HOH:O	1.86	0.74
1:A:124:GLY:HA3	5:A:252:HOH:O	1.88	0.73
1:A:60:ASP:HB2	2:A:155:SO4:O4	1.90	0.72
1:A:27:GLU:OE2	1:A:118:LYS:HD2	1.90	0.71
1:A:6:GLU:HA	5:A:245:HOH:O	1.92	0.69
1:A:110:ALA:HA	5:A:189:HOH:O	1.93	0.68
1:A:27:GLU:CD	1:A:118:LYS:HD2	2.20	0.67
1:A:146:TYR:HA	5:A:271:HOH:O	1.95	0.66
1:A:123:PHE:HA	5:A:299:HOH:O	1.95	0.65
1:A:145:LYS:HD2	5:A:222:HOH:O	1.97	0.65
1:A:112:ILE:HD13	5:A:327:HOH:O	1.97	0.64
1:A:45:LYS:HD2	5:A:202:HOH:O	1.98	0.64
1:A:130:ALA:HB2	5:A:245:HOH:O	1.98	0.63
1:A:59:GLU:HA	5:A:276:HOH:O	1.97	0.63
1:A:30:ILE:HG12	1:A:55:MET:HE3	1.82	0.61
1:A:24:HIS:O	1:A:28:VAL:HG23	2.01	0.60
1:A:48:HIS:HD2	5:A:310:HOH:O	1.84	0.60
1:A:44:ASP:HA	1:A:47:LYS:HD2	1.82	0.59
1:A:104:LEU:HD23	4:A:154:CLN:HMC2	1.84	0.59
1:A:40:LEU:HD11	1:A:46:PHE:O	2.03	0.59
1:A:151:PHE:C	1:A:152:GLN:HG3	2.27	0.59
1:A:112:ILE:HD11	1:A:135:LEU:HD12	1.85	0.58
1:A:30:ILE:CD1	1:A:56:LYS:HG3	2.33	0.58
1:A:95:THR:O	1:A:98:LYS:HE2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:GLN:HA	5:A:274:HOH:O	2.04	0.57
1:A:87:LYS:N	1:A:88:PRO:HD2	2.20	0.57
1:A:24:HIS:CD2	1:A:118:LYS:NZ	2.73	0.56
1:A:127:ALA:HB3	5:A:188:HOH:O	2.04	0.56
1:A:91:GLN:HB3	5:A:305:HOH:O	2.05	0.56
1:A:99:ILE:HB	5:A:248:HOH:O	2.05	0.56
1:A:127:ALA:N	5:A:188:HOH:O	2.39	0.55
1:A:113:HIS:HB3	5:A:189:HOH:O	2.06	0.55
1:A:82:HIS:HE1	1:A:141:ASP:OD2	1.90	0.54
1:A:59:GLU:CA	5:A:276:HOH:O	2.55	0.54
1:A:108:SER:O	1:A:112:ILE:HD12	2.07	0.54
1:A:49:LEU:HD21	5:A:254:HOH:O	2.09	0.53
1:A:59:GLU:C	5:A:276:HOH:O	2.52	0.53
1:A:112:ILE:CD1	1:A:135:LEU:HD12	2.38	0.53
1:A:30:ILE:HG13	1:A:55:MET:HE3	1.91	0.52
1:A:101:ILE:O	1:A:104:LEU:HB2	2.10	0.52
1:A:124:GLY:C	5:A:188:HOH:O	2.52	0.52
1:A:87:LYS:HD3	5:A:305:HOH:O	2.08	0.52
1:A:29:LEU:HB3	1:A:61:LEU:HD11	1.91	0.52
1:A:47:LYS:HD3	5:A:231:HOH:O	2.10	0.51
1:A:83:GLU:HG3	5:A:172:HOH:O	2.09	0.51
1:A:75:ILE:HG23	1:A:82:HIS:CB	2.41	0.51
1:A:110:ALA:HB2	5:A:313:HOH:O	2.11	0.50
1:A:13:VAL:HG21	1:A:127:ALA:HB1	1.92	0.50
1:A:97:HIS:HB2	5:A:248:HOH:O	2.10	0.50
1:A:25:GLY:O	1:A:29:LEU:HB2	2.12	0.49
1:A:57:ALA:HB2	5:A:277:HOH:O	2.11	0.49
1:A:2:LEU:HD11	1:A:133:LYS:HB3	1.93	0.49
1:A:63:LYS:HG2	5:A:261:HOH:O	2.11	0.49
1:A:62:LYS:HE2	5:A:307:HOH:O	2.12	0.49
1:A:26:GLN:HG2	1:A:30:ILE:HD12	1.96	0.48
1:A:30:ILE:HD11	1:A:56:LYS:HG3	1.93	0.48
1:A:117:SER:HB2	5:A:234:HOH:O	2.13	0.48
1:A:83:GLU:H	1:A:83:GLU:CD	2.20	0.48
1:A:60:ASP:N	2:A:155:SO4:O4	2.47	0.48
1:A:24:HIS:CA	1:A:118:LYS:HZ1	2.11	0.48
1:A:88:PRO:HG3	5:A:318:HOH:O	2.12	0.48
1:A:42:LYS:HG3	1:A:99:ILE:HD11	1.95	0.48
1:A:14:TRP:O	1:A:18:GLU:HG3	2.14	0.48
1:A:30:ILE:HD13	1:A:56:LYS:HG3	1.95	0.47
1:A:44:ASP:HA	1:A:47:LYS:CD	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:LYS:HD3	5:A:165:HOH:O	2.15	0.47
1:A:116:HIS:NE2	1:A:128:GLN:NE2	2.63	0.46
1:A:141:ASP:O	1:A:145:LYS:HE2	2.15	0.46
1:A:42:LYS:HG3	1:A:99:ILE:CD1	2.46	0.46
1:A:149:LEU:HD12	5:A:271:HOH:O	2.15	0.46
1:A:24:HIS:CD2	1:A:118:LYS:HZ1	2.34	0.46
1:A:60:ASP:HB3	5:A:283:HOH:O	2.16	0.46
1:A:99:ILE:HD12	1:A:103:TYR:HD2	1.81	0.46
1:A:24:HIS:CG	1:A:118:LYS:HZ1	2.35	0.45
1:A:145:LYS:HB3	5:A:281:HOH:O	2.17	0.44
1:A:23:GLY:HA2	5:A:307:HOH:O	2.17	0.44
1:A:109:ASP:HB3	5:A:298:HOH:O	2.18	0.44
1:A:87:LYS:HG2	5:A:273:HOH:O	2.17	0.44
1:A:31:ARG:CG	5:A:189:HOH:O	2.65	0.43
1:A:107:ILE:O	1:A:110:ALA:HB3	2.18	0.43
1:A:127:ALA:HB2	5:A:182:HOH:O	2.18	0.43
1:A:98:LYS:HD2	1:A:151:PHE:HE1	1.84	0.43
1:A:30:ILE:HA	1:A:55:MET:HE3	2.00	0.43
1:A:82:HIS:CE1	1:A:141:ASP:OD2	2.71	0.43
1:A:99:ILE:CD1	4:A:154:CLN:HAC	2.49	0.43
1:A:87:LYS:HD3	1:A:91:GLN:OE1	2.19	0.42
1:A:92:SER:O	1:A:96:LYS:HB3	2.19	0.42
1:A:98:LYS:HA	1:A:151:PHE:CZ	2.54	0.42
1:A:2:LEU:CD1	1:A:133:LYS:HB3	2.49	0.42
4:A:154:CLN:HAA1	5:A:170:HOH:O	2.19	0.42
1:A:12:ASN:ND2	5:A:324:HOH:O	2.52	0.42
1:A:4:ASP:HA	1:A:7:TRP:HB2	2.02	0.41
1:A:61:LEU:O	1:A:61:LEU:HD12	2.21	0.41
1:A:141:ASP:O	1:A:145:LYS:CE	2.68	0.41
1:A:12:ASN:HA	5:A:241:HOH:O	2.21	0.40
1:A:14:TRP:C	1:A:16:LYS:N	2.78	0.40
1:A:97:HIS:CD2	5:A:223:HOH:O	2.74	0.40
1:A:152:GLN:N	5:A:312:HOH:O	2.53	0.40

All (8) 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:129:GLY:CA	5:A:318:HOH:O[1_545]	1.42	0.78
5:A:165:HOH:O	5:A:289:HOH:O[1_565]	1.54	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLN:NE2	1:A:153:GLY:C[2_555]	2.00	0.20
1:A:91:GLN:NE2	1:A:153:GLY:O[2_555]	2.05	0.15
1:A:129:GLY:N	5:A:318:HOH:O[1_545]	2.09	0.11
5:A:192:HOH:O	5:A:272:HOH:O[1_546]	2.12	0.08
5:A:255:HOH:O	5:A:326:HOH:O[2_555]	2.14	0.06
1:A:136:GLU:OE1	1:A:153:GLY:OXT[2_545]	2.19	0.01

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	151/153 (99%)	142 (94%)	8 (5%)	1 (1%)	18	14

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	GLN

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	123/123 (100%)	97 (79%)	26 (21%)	1	0

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	3	SER
1	A	8	GLN
1	A	9	GLN
1	A	30	ILE
1	A	44	ASP
1	A	45	LYS
1	A	47	LYS
1	A	50	LYS
1	A	56	LYS
1	A	59	GLU
1	A	66	THR
1	A	72	LEU
1	A	76	LEU
1	A	87	LYS
1	A	95	THR
1	A	99	ILE
1	A	101	ILE
1	A	107	ILE
1	A	112	ILE
1	A	115	LEU
1	A	120	PRO
1	A	139	ARG
1	A	142	ILE
1	A	145	LYS
1	A	146	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	48	HIS
1	A	81	HIS
1	A	119	HIS
1	A	128	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
4	CLN	A	154	1,3	48,52,52	3.31	14 (29%)	58,87,87	1.88	14 (24%)
3	CYN	A	156	4	1,1,1	0.29	0	-		
2	SO4	A	155	-	4,4,4	0.97	0	6,6,6	1.87	1 (16%)

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
4	CLN	A	154	1,3	1/1/8/15	6/12/83/83	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	154	CLN	CBC-S	11.30	1.89	1.74
4	A	154	CLN	CBC-CAC	10.61	1.45	1.31
4	A	154	CLN	C1C-NC	8.41	1.40	1.35
4	A	154	CLN	C3C-CAC	-8.35	1.34	1.52
4	A	154	CLN	FE-NC	5.07	2.10	1.94
4	A	154	CLN	CMB-C2B	4.33	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	154	CLN	FE-NA	4.05	2.07	1.94
4	A	154	CLN	CAB-C3B	3.56	1.56	1.47
4	A	154	CLN	C1A-C2A	2.57	1.49	1.45
4	A	154	CLN	C4A-C3A	2.51	1.49	1.44
4	A	154	CLN	CBA-CAA	2.41	1.60	1.51
4	A	154	CLN	CHD-C4C	2.40	1.43	1.37
4	A	154	CLN	CBB-CAB	2.17	1.40	1.30
4	A	154	CLN	FE-NB	2.04	2.01	1.95

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	154	CLN	C4C-NC-C1C	5.63	108.94	106.48
4	A	154	CLN	O1A-CGA-CBA	-4.59	108.55	123.09
4	A	154	CLN	CAD-CBD-CGD	4.52	125.64	113.67
4	A	154	CLN	C4B-CHC-C1C	4.11	132.63	125.99
2	A	155	SO4	O3-S-O2	3.62	128.46	109.56
4	A	154	CLN	CBB-CAB-C3B	-3.46	110.24	127.53
4	A	154	CLN	O2A-CGA-O1A	2.78	130.49	123.33
4	A	154	CLN	CMA-C3A-C2A	2.77	133.64	126.15
4	A	154	CLN	CMA-C3A-C4A	-2.70	120.82	125.03
4	A	154	CLN	CMC-C2C-C1C	2.68	114.61	109.75
4	A	154	CLN	C3C-C2C-C1C	-2.64	97.43	100.83
4	A	154	CLN	C2C-C1C-CHC	2.42	127.10	123.35
4	A	154	CLN	CHB-C4A-NA	2.34	126.94	124.42
4	A	154	CLN	CAA-C2A-C1A	-2.22	120.84	124.70
4	A	154	CLN	O2A-CGA-CBA	2.20	120.94	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	154	CLN	C3C

All (6) torsion outliers are listed below:

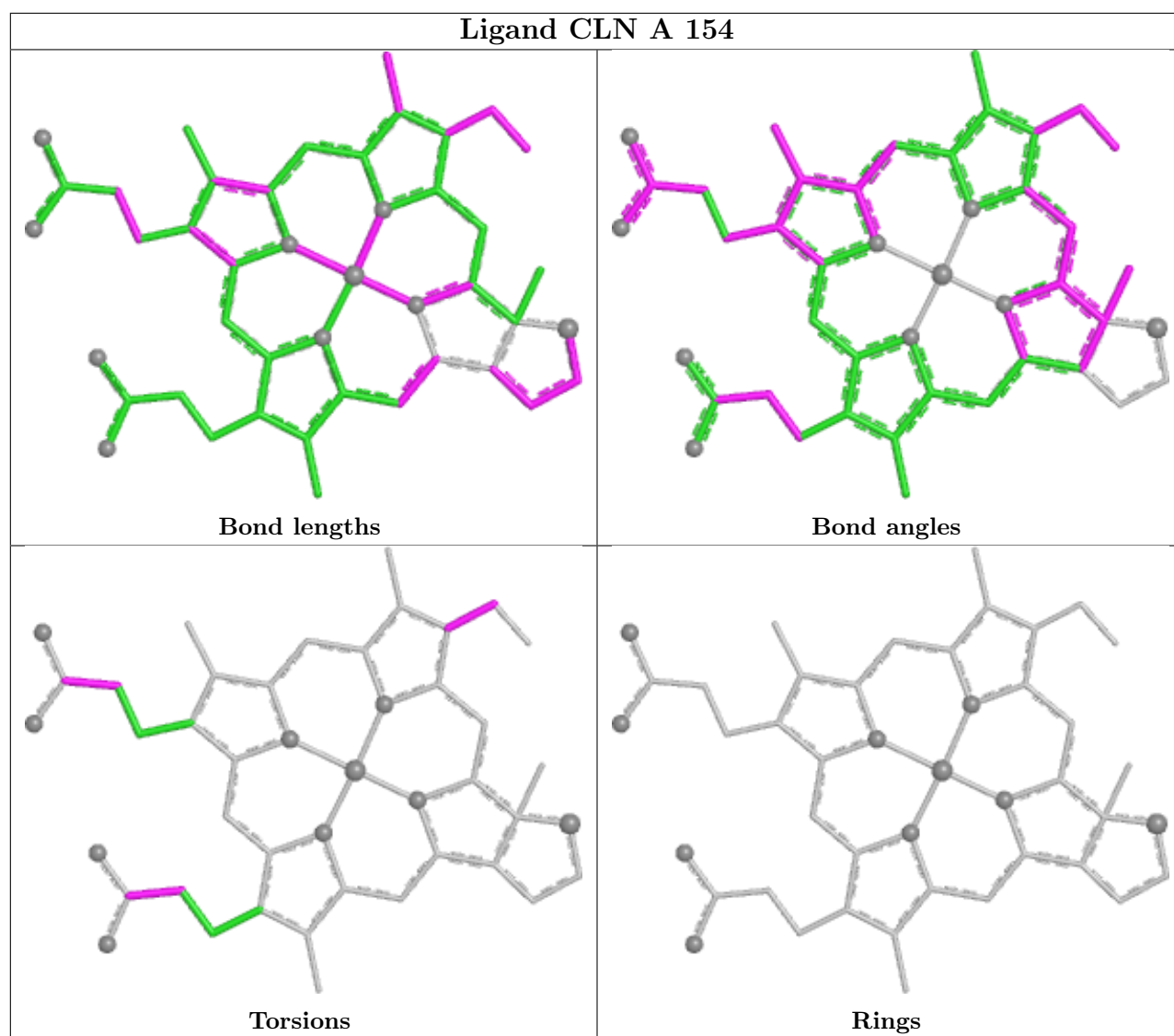
Mol	Chain	Res	Type	Atoms
4	A	154	CLN	C2B-C3B-CAB-CBB
4	A	154	CLN	C4B-C3B-CAB-CBB
4	A	154	CLN	CAA-CBA-CGA-O2A
4	A	154	CLN	CAD-CBD-CGD-O2D
4	A	154	CLN	CAA-CBA-CGA-O1A
4	A	154	CLN	CAD-CBD-CGD-O1D

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	154	CLN	5	0
2	A	155	SO4	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	153/153 (100%)	-1.14	0 100 100	3, 12, 24, 31	0

There are no RSRZ outliers to report.

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](#)

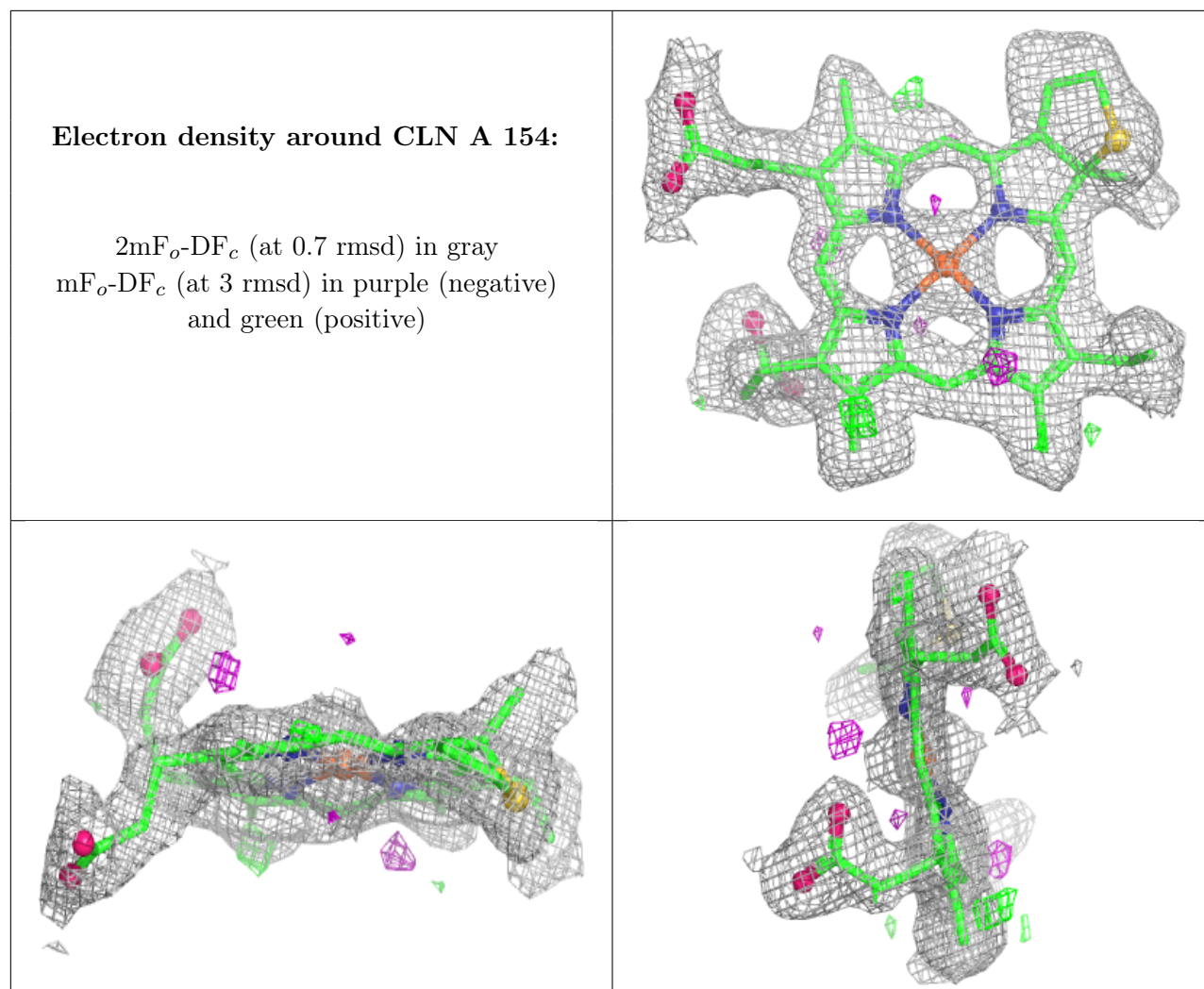
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
3	CYN	A	156	2/2	0.90	0.08	14,14,14,15	0
2	SO4	A	155	5/5	0.91	0.14	53,53,54,54	0
4	CLN	A	154	44/44	0.97	0.05	13,18,20,22	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.