



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 05:31 AM UTC

PDB ID : 1NOL / pdb_00001nol
Title : OXYGENATED HEMOCYANIN (SUBUNIT TYPE II)
Authors : Hazes, B.; Hol, W.G.J.
Deposited on : 1995-10-17
Resolution : 2.40 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
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

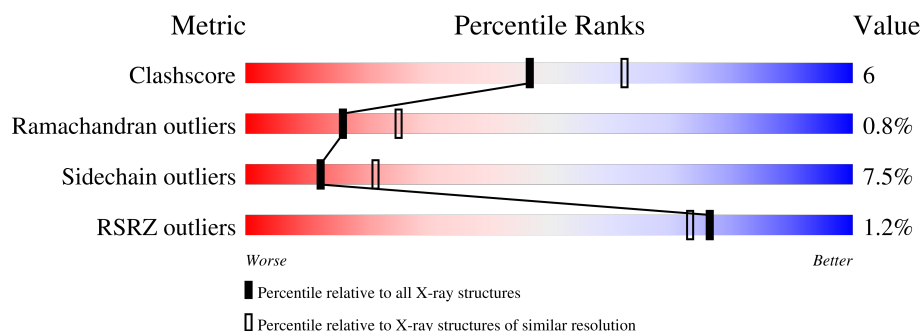
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	628	64% 26% 6% ..

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5154 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 HEMOCYANIN (SUBUNIT TYPE II).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	607	Total	C	N	O	S	0	0	0
			4933	3145	862	904	22			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	ILE	VAL	conflict	UNP P04253

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cu	0	0
			2	2		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

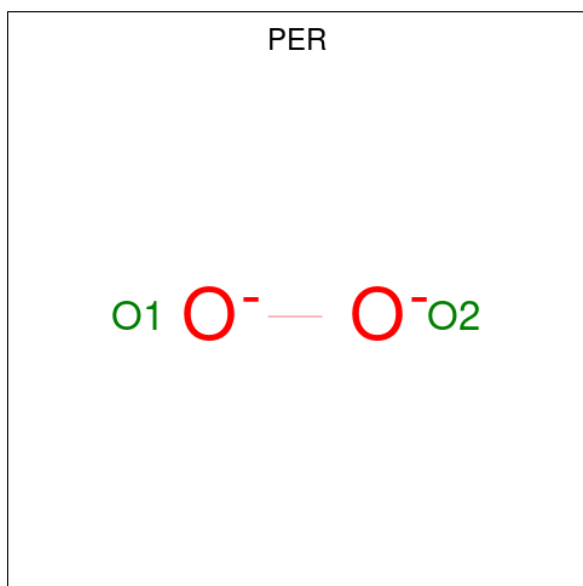
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	N	O	0	0
			4	1	3		

- Molecule 5 is PEROXIDE ION (CCD ID: PER) (formula: O₂).



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

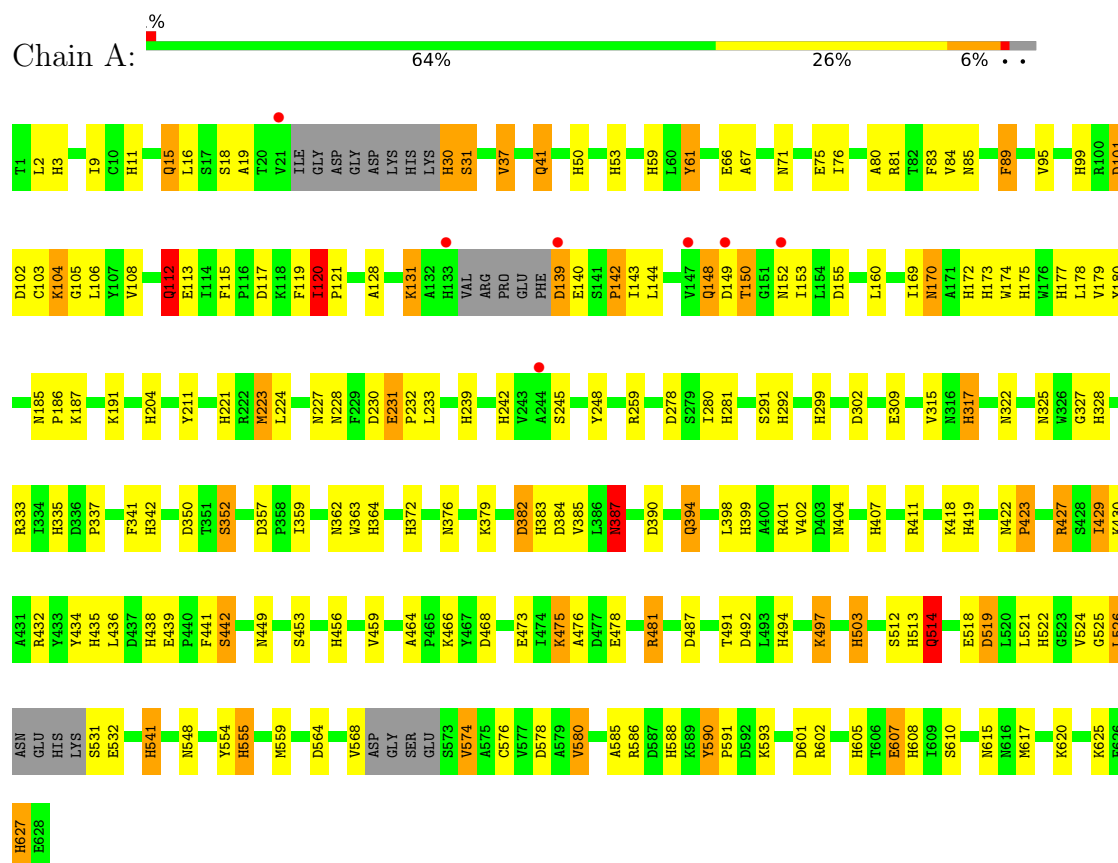
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	212	Total 212	O 212	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: HEMOCYANIN (SUBUNIT TYPE II)



4 Data and refinement statistics

Property	Value	Source
Space group	R 3 2	Depositor
Cell constants a, b, c, α , β , γ	117.00Å 117.00Å 117.00Å 60.02° 60.02° 60.02°	Depositor
Resolution (Å)	8.00 – 2.40 8.00 – 2.41	Depositor EDS
% Data completeness (in resolution range)	83.4 (8.00-2.40) 80.9 (8.00-2.41)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR 2.1	Depositor
R, R_{free}	0.181 , (Not available) 0.168 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 75.6	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5154	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CA, CU, PER, NO3

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	1.26	50/5077 (1.0%)	1.88	147/6880 (2.1%)

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	A	0	2

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	173	HIS	CD2-NE2	-7.12	1.30	1.37
1	A	292	HIS	CD2-NE2	-7.09	1.30	1.37
1	A	514	GLN	CA-CB	7.03	1.63	1.52
1	A	53	HIS	CD2-NE2	-6.85	1.30	1.37
1	A	281	HIS	CD2-NE2	-6.72	1.30	1.37
1	A	53	HIS	CG-ND1	-6.63	1.30	1.38
1	A	50	HIS	CD2-NE2	-6.58	1.30	1.37
1	A	555	HIS	CD2-NE2	-6.55	1.30	1.37
1	A	419	HIS	CD2-NE2	-6.48	1.30	1.37
1	A	3	HIS	CD2-NE2	-6.47	1.30	1.37
1	A	503	HIS	CD2-NE2	-6.43	1.30	1.37
1	A	204	HIS	CG-ND1	-6.42	1.31	1.38
1	A	399	HIS	CD2-NE2	-6.37	1.30	1.37
1	A	173	HIS	CG-ND1	-6.26	1.31	1.38
1	A	99	HIS	CD2-NE2	-6.24	1.30	1.37
1	A	59	HIS	CD2-NE2	-6.20	1.31	1.37
1	A	177	HIS	CD2-NE2	-6.20	1.31	1.37
1	A	522	HIS	CD2-NE2	-6.19	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	30	HIS	CD2-NE2	-6.01	1.31	1.37
1	A	221	HIS	CD2-NE2	-6.00	1.31	1.37
1	A	239	HIS	CD2-NE2	-5.98	1.31	1.37
1	A	335	HIS	CD2-NE2	-5.98	1.31	1.37
1	A	438	HIS	CD2-NE2	-5.93	1.31	1.37
1	A	435	HIS	CD2-NE2	-5.93	1.31	1.37
1	A	456	HIS	CD2-NE2	-5.80	1.31	1.37
1	A	372	HIS	CD2-NE2	-5.79	1.31	1.37
1	A	281	HIS	CG-ND1	-5.77	1.31	1.38
1	A	242	HIS	CD2-NE2	-5.74	1.31	1.37
1	A	588	HIS	CD2-NE2	-5.72	1.31	1.37
1	A	608	HIS	CD2-NE2	-5.71	1.31	1.37
1	A	328	HIS	CD2-NE2	-5.67	1.31	1.37
1	A	383	HIS	CD2-NE2	-5.63	1.31	1.37
1	A	317	HIS	CG-CD2	5.48	1.41	1.35
1	A	608	HIS	CG-ND1	-5.47	1.32	1.38
1	A	407	HIS	CD2-NE2	-5.40	1.31	1.37
1	A	494	HIS	CD2-NE2	-5.38	1.31	1.37
1	A	328	HIS	CG-ND1	-5.37	1.32	1.38
1	A	541	HIS	CD2-NE2	-5.35	1.31	1.37
1	A	99	HIS	CG-ND1	-5.32	1.32	1.38
1	A	459	VAL	CA-CB	5.32	1.60	1.54
1	A	204	HIS	CD2-NE2	-5.31	1.32	1.37
1	A	555	HIS	CG-ND1	-5.31	1.32	1.38
1	A	175	HIS	CD2-NE2	-5.30	1.32	1.37
1	A	605	HIS	CD2-NE2	-5.28	1.32	1.37
1	A	342	HIS	CD2-NE2	-5.28	1.32	1.37
1	A	172	HIS	CD2-NE2	-5.22	1.32	1.37
1	A	113	GLU	CA-CB	-5.16	1.45	1.53
1	A	11	HIS	CD2-NE2	-5.07	1.32	1.37
1	A	513	HIS	CG-CD2	5.02	1.41	1.35
1	A	494	HIS	CG-ND1	-5.00	1.32	1.38

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ASP	CA-CB-CG	12.04	124.64	112.60
1	A	387	ASN	OD1-CG-ND2	-11.10	111.50	122.60
1	A	422	ASN	CA-CB-CG	-9.20	103.40	112.60
1	A	376	ASN	OD1-CG-ND2	-8.89	113.71	122.60
1	A	117	ASP	CA-CB-CG	8.44	121.04	112.60
1	A	580	VAL	CB-CA-C	-8.37	101.08	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	419	HIS	CB-CG-CD2	-8.27	120.45	131.20
1	A	309	GLU	CA-C-O	-8.21	112.19	120.82
1	A	578	ASP	CA-CB-CG	8.03	120.63	112.60
1	A	387	ASN	CA-CB-CG	8.02	120.62	112.60
1	A	102	ASP	CA-CB-CG	7.76	120.36	112.60
1	A	514	GLN	OE1-CD-NE2	-7.63	114.97	122.60
1	A	387	ASN	CB-CG-ND2	7.60	127.80	116.40
1	A	85	ASN	OD1-CG-ND2	-7.52	115.08	122.60
1	A	281	HIS	CA-CB-CG	-7.48	106.32	113.80
1	A	3	HIS	CA-CB-CG	-7.29	106.51	113.80
1	A	31	SER	N-CA-C	-7.25	95.36	110.80
1	A	11	HIS	CB-CG-CD2	-7.22	121.81	131.20
1	A	399	HIS	CB-CG-CD2	-7.16	121.89	131.20
1	A	325	ASN	OD1-CG-ND2	-7.16	115.44	122.60
1	A	449	ASN	OD1-CG-ND2	-7.16	115.44	122.60
1	A	67	ALA	N-CA-C	-7.14	97.61	108.96
1	A	350	ASP	CA-CB-CG	7.09	119.69	112.60
1	A	435	HIS	CB-CG-CD2	-7.07	122.01	131.20
1	A	384	ASP	CA-CB-CG	7.03	119.63	112.60
1	A	468	ASP	CA-CB-CG	7.02	119.62	112.60
1	A	41	GLN	N-CA-C	6.84	117.99	109.57
1	A	180	TYR	CA-C-N	6.82	126.79	119.76
1	A	180	TYR	C-N-CA	6.82	126.79	119.76
1	A	291	SER	N-CA-C	6.76	119.67	110.55
1	A	441	PHE	CA-CB-CG	6.68	120.48	113.80
1	A	382	ASP	CA-CB-CG	6.65	119.25	112.60
1	A	50	HIS	CB-CG-CD2	-6.55	122.68	131.20
1	A	439	GLU	CA-C-N	6.50	126.53	119.90
1	A	439	GLU	C-N-CA	6.50	126.53	119.90
1	A	503	HIS	CB-CG-CD2	-6.46	122.81	131.20
1	A	605	HIS	CB-CG-CD2	-6.43	122.84	131.20
1	A	476	ALA	N-CA-C	6.39	118.78	111.11
1	A	402	VAL	N-CA-C	-6.37	98.94	108.12
1	A	627	HIS	CB-CG-ND1	6.33	132.20	122.70
1	A	11	HIS	CB-CG-ND1	6.33	132.20	122.70
1	A	481	ARG	NE-CZ-NH2	-6.30	113.53	119.20
1	A	627	HIS	CB-CG-CD2	-6.25	123.07	131.20
1	A	521	LEU	N-CA-C	-6.25	104.55	111.36
1	A	30	HIS	CB-CG-CD2	-6.21	123.13	131.20
1	A	615	ASN	OD1-CG-ND2	-6.20	116.40	122.60
1	A	601	ASP	CA-CB-CG	6.14	118.74	112.60
1	A	120	ILE	CA-C-N	6.13	126.08	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	ILE	C-N-CA	6.13	126.08	119.76
1	A	541	HIS	CB-CG-CD2	-6.09	123.28	131.20
1	A	394	GLN	CG-CD-NE2	-6.09	107.27	116.40
1	A	15	GLN	CA-C-O	6.07	128.88	121.84
1	A	50	HIS	CA-C-N	6.06	125.27	118.97
1	A	50	HIS	C-N-CA	6.06	125.27	118.97
1	A	148	GLN	N-CA-C	6.05	123.69	110.80
1	A	383	HIS	CB-CG-CD2	-5.97	123.44	131.20
1	A	555	HIS	CB-CG-CD2	-5.96	123.45	131.20
1	A	512	SER	CA-CB-OG	5.94	122.97	111.10
1	A	174	TRP	CG-CD2-CE3	5.93	139.83	133.90
1	A	442	SER	CA-CB-OG	5.91	122.91	111.10
1	A	115	PHE	CA-C-N	5.88	126.29	119.47
1	A	115	PHE	C-N-CA	5.88	126.29	119.47
1	A	580	VAL	N-CA-CB	5.85	117.78	110.47
1	A	83	PHE	CA-CB-CG	5.84	119.64	113.80
1	A	131	LYS	N-CA-C	-5.84	105.41	112.54
1	A	335	HIS	CB-CG-CD2	-5.82	123.64	131.20
1	A	108	VAL	CA-C-N	5.80	126.36	120.38
1	A	108	VAL	C-N-CA	5.80	126.36	120.38
1	A	105	GLY	N-CA-C	-5.79	107.39	114.92
1	A	112	GLN	OE1-CD-NE2	-5.74	116.86	122.60
1	A	37	VAL	N-CA-CB	-5.74	102.79	112.44
1	A	399	HIS	CB-CG-ND1	5.70	131.25	122.70
1	A	120	ILE	N-CA-CB	-5.68	103.25	111.21
1	A	590	TYR	CA-C-N	5.68	126.94	119.84
1	A	590	TYR	C-N-CA	5.68	126.94	119.84
1	A	564	ASP	N-CA-C	-5.67	105.86	112.89
1	A	120	ILE	CA-CB-CG1	-5.62	100.85	110.40
1	A	588	HIS	CB-CG-CD2	-5.59	123.93	131.20
1	A	503	HIS	CB-CG-ND1	5.57	131.06	122.70
1	A	149	ASP	CA-C-N	5.57	132.17	121.54
1	A	149	ASP	C-N-CA	5.57	132.17	121.54
1	A	112	GLN	CG-CD-NE2	5.56	124.73	116.40
1	A	411	ARG	N-CA-C	-5.51	100.34	108.99
1	A	191	LYS	N-CA-C	5.50	122.51	110.80
1	A	280	ILE	O-C-N	-5.49	116.51	121.89
1	A	564	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	341	PHE	CA-CB-CG	-5.47	108.33	113.80
1	A	497	LYS	CA-CB-CG	-5.46	103.18	114.10
1	A	177	HIS	CB-CG-CD2	-5.44	124.13	131.20
1	A	407	HIS	CB-CG-CD2	-5.44	124.13	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	435	HIS	CB-CG-ND1	5.43	130.85	122.70
1	A	172	HIS	CB-CG-CD2	-5.43	124.14	131.20
1	A	3	HIS	CB-CG-CD2	-5.42	124.16	131.20
1	A	89	PHE	CA-C-O	-5.42	115.13	120.82
1	A	607	GLU	CB-CG-CD	5.40	121.78	112.60
1	A	322	ASN	CA-CB-CG	5.40	118.00	112.60
1	A	299	HIS	CB-CG-CD2	-5.40	124.18	131.20
1	A	221	HIS	CB-CG-CD2	-5.40	124.19	131.20
1	A	142	PRO	N-CA-C	5.38	119.03	110.21
1	A	487	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	364	HIS	CB-CG-CD2	-5.37	124.22	131.20
1	A	379	LYS	CA-C-O	-5.37	114.76	120.23
1	A	228	ASN	OD1-CG-ND2	-5.36	117.24	122.60
1	A	419	HIS	CB-CG-ND1	5.36	130.73	122.70
1	A	514	GLN	CA-CB-CG	5.36	124.81	114.10
1	A	302	ASP	O-C-N	-5.35	116.05	122.15
1	A	155	ASP	CA-C-N	5.34	124.98	119.05
1	A	155	ASP	C-N-CA	5.34	124.98	119.05
1	A	429	ILE	N-CA-C	-5.34	98.78	107.28
1	A	478	GLU	CA-CB-CG	5.34	124.79	114.10
1	A	357	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	242	HIS	CB-CG-CD2	-5.32	124.29	131.20
1	A	61	TYR	CA-CB-CG	5.32	123.47	113.90
1	A	248	TYR	N-CA-C	-5.31	101.28	109.52
1	A	325	ASN	CA-CB-CG	5.29	117.89	112.60
1	A	224	LEU	CA-C-N	5.27	125.19	119.76
1	A	224	LEU	C-N-CA	5.27	125.19	119.76
1	A	481	ARG	CG-CD-NE	-5.25	100.44	112.00
1	A	50	HIS	CB-CG-ND1	5.24	130.56	122.70
1	A	394	GLN	OE1-CD-NE2	5.24	127.83	122.60
1	A	464	ALA	CA-C-N	5.23	125.17	119.78
1	A	464	ALA	C-N-CA	5.23	125.17	119.78
1	A	227	ASN	OD1-CG-ND2	-5.23	117.37	122.60
1	A	179	VAL	CB-CA-C	-5.22	103.64	112.16
1	A	602	ARG	CA-C-N	5.22	125.51	119.93
1	A	602	ARG	C-N-CA	5.22	125.51	119.93
1	A	317	HIS	CB-CG-CD2	-5.21	124.43	131.20
1	A	131	LYS	CA-CB-CG	-5.21	103.68	114.10
1	A	390	ASP	CA-CB-CG	5.19	117.79	112.60
1	A	152	ASN	N-CA-C	-5.16	101.71	109.15
1	A	456	HIS	CB-CG-CD2	-5.16	124.49	131.20
1	A	150	THR	CA-CB-CG2	5.16	119.27	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	LEU	N-CA-C	-5.13	100.80	109.07
1	A	16	LEU	N-CA-C	-5.13	105.77	112.23
1	A	66	GLU	O-C-N	-5.10	115.81	122.59
1	A	230	ASP	CB-CA-C	-5.08	99.96	109.72
1	A	71	ASN	OD1-CG-ND2	-5.08	117.52	122.60
1	A	170	ASN	CA-CB-CG	-5.06	107.54	112.60
1	A	155	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	357	ASP	O-C-N	-5.06	117.01	121.31
1	A	75	GLU	CA-CB-CG	-5.05	104.01	114.10
1	A	120	ILE	CA-CB-CG2	5.05	119.08	110.50
1	A	519	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	174	TRP	CE2-CD2-CG	-5.03	101.16	107.20
1	A	372	HIS	CB-CG-CD2	-5.03	124.67	131.20
1	A	59	HIS	CB-CG-CD2	-5.02	124.67	131.20
1	A	554	TYR	O-C-N	-5.01	116.72	123.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	434	TYR	Sidechain
1	A	525	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	4933	0	4680	55	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	4	0	0	1	0
5	A	2	0	0	0	0
6	A	212	0	0	7	0
All	All	5154	0	4680	55	0

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 6.

All (55) 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:223:MET:HB3	6:A:808:HOH:O	1.80	0.82
1:A:112:GLN:HE21	1:A:112:GLN:H	1.35	0.75
1:A:559:MET:HG3	1:A:617:MET:HG2	1.70	0.73
1:A:211:TYR:HE2	1:A:223:MET:HG3	1.53	0.72
1:A:144:LEU:HD21	1:A:432:ARG:HH21	1.55	0.70
1:A:359:ILE:HA	1:A:362:ASN:HD22	1.58	0.69
1:A:559:MET:HE3	1:A:617:MET:HE2	1.78	0.66
1:A:442:SER:HB3	1:A:503:HIS:HD2	1.63	0.63
1:A:95:VAL:HG23	1:A:178:LEU:HD22	1.81	0.62
1:A:9:ILE:HD12	1:A:106:LEU:HD13	1.83	0.61
1:A:259:ARG:HG3	6:A:809:HOH:O	2.03	0.57
1:A:481:ARG:HD2	6:A:690:HOH:O	2.04	0.57
1:A:144:LEU:HD21	1:A:432:ARG:NH2	2.22	0.55
1:A:259:ARG:HE	1:A:337:PRO:HG3	1.73	0.54
1:A:128:ALA:HB1	1:A:429:ILE:HG21	1.89	0.54
1:A:574:VAL:HA	6:A:807:HOH:O	2.08	0.54
1:A:233:LEU:HD23	1:A:359:ILE:HG12	1.90	0.53
1:A:359:ILE:HD12	1:A:362:ASN:HD22	1.74	0.52
1:A:80:ALA:O	1:A:84:VAL:HG22	2.10	0.51
1:A:576:CYS:HB2	1:A:586:ARG:HB2	1.93	0.50
1:A:524:VAL:O	1:A:526:LEU:HG	2.12	0.50
1:A:103:CYS:HA	1:A:106:LEU:HD12	1.95	0.48
1:A:404:ASN:ND2	1:A:620:LYS:HE2	2.29	0.48
1:A:112:GLN:H	1:A:112:GLN:NE2	2.08	0.47
1:A:387:ASN:ND2	6:A:786:HOH:O	2.47	0.47
1:A:514:GLN:HG3	6:A:720:HOH:O	2.13	0.47
1:A:475:LYS:HD2	1:A:607:GLU:HG2	1.97	0.47
1:A:327:GLY:HA3	1:A:363:TRP:CZ2	2.51	0.46
1:A:590:TYR:HA	1:A:591:PRO:HD3	1.67	0.46
1:A:315:VAL:HG13	6:A:784:HOH:O	2.14	0.46
1:A:170:ASN:HB3	1:A:352:SER:O	2.16	0.45
1:A:359:ILE:HD12	1:A:362:ASN:ND2	2.31	0.45
1:A:519:ASP:HA	1:A:524:VAL:HB	1.99	0.45
1:A:394:GLN:OE1	1:A:497:LYS:HE2	2.17	0.44
1:A:333:ARG:NH2	4:A:633:NO3:O3	2.51	0.44
1:A:120:ILE:HA	1:A:121:PRO:HD3	1.77	0.43
1:A:574:VAL:CG1	1:A:585:ALA:HB1	2.48	0.43
1:A:532:GLU:OE1	1:A:576:CYS:HA	2.18	0.43
1:A:101:ASP:O	1:A:104:LYS:HB2	2.19	0.43
1:A:15:GLN:NE2	1:A:418:LYS:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ALA:HB2	1:A:81:ARG:HH21	1.84	0.42
1:A:568:VAL:HG23	1:A:593:LYS:HG3	2.02	0.42
1:A:231:GLU:HG3	1:A:232:PRO:HD2	2.02	0.42
1:A:112:GLN:HA	1:A:119:PHE:CD1	2.54	0.42
1:A:81:ARG:HB3	1:A:89:PHE:CE1	2.55	0.41
1:A:76:ILE:HD12	1:A:76:ILE:HA	1.84	0.41
1:A:142:PRO:HG3	1:A:427:ARG:HE	1.85	0.41
1:A:359:ILE:HA	1:A:359:ILE:HD12	1.95	0.41
1:A:131:LYS:HE3	1:A:143:ILE:HG23	2.02	0.41
1:A:473:GLU:OE1	1:A:475:LYS:HE2	2.21	0.41
1:A:475:LYS:HA	1:A:475:LYS:HD3	1.88	0.41
1:A:548:ASN:O	1:A:625:LYS:HA	2.20	0.40
1:A:185:ASN:HA	1:A:186:PRO:HD3	1.83	0.40
1:A:466:LYS:HG3	1:A:555:HIS:CE1	2.56	0.40
1:A:436:LEU:O	1:A:541:HIS:HB2	2.22	0.40

There are no symmetry-related clashes.

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	597/628 (95%)	554 (93%)	38 (6%)	5 (1%)	16 25

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	140	GLU
1	A	245	SER
1	A	148	GLN
1	A	423	PRO

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	530/558 (95%)	490 (92%)	40 (8%)	12	21

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	18	SER
1	A	30	HIS
1	A	37	VAL
1	A	41	GLN
1	A	61	TYR
1	A	101	ASP
1	A	104	LYS
1	A	112	GLN
1	A	120	ILE
1	A	139	ASP
1	A	150	THR
1	A	153	ILE
1	A	160	LEU
1	A	169	ILE
1	A	187	LYS
1	A	223	MET
1	A	231	GLU
1	A	278	ASP
1	A	317	HIS
1	A	352	SER
1	A	382	ASP
1	A	385	VAL
1	A	387	ASN
1	A	401	ARG
1	A	423	PRO
1	A	427	ARG
1	A	430	LYS
1	A	453	SER
1	A	475	LYS

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Mol	Chain	Res	Type
1	A	491	THR
1	A	492	ASP
1	A	514	GLN
1	A	518	GLU
1	A	526	LEU
1	A	531	SER
1	A	574	VAL
1	A	580	VAL
1	A	610	SER
1	A	627	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	126	ASN
1	A	239	HIS
1	A	362	ASN
1	A	372	HIS
1	A	399	HIS
1	A	446	ASN
1	A	503	HIS
1	A	514	GLN
1	A	522	HIS

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 [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

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	NO3	A	633	-	1,3,3	0.36	0	0,3,3	-	-
5	PER	A	631	2	1,1,1	0.43	0	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	633	NO3	1	0

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	607/628 (96%)	-0.77	7 (1%) 76 73	4, 15, 31, 45	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	244	ALA	3.0
1	A	133	HIS	2.9
1	A	21	VAL	2.9
1	A	149	ASP	2.6
1	A	147	VAL	2.6
1	A	152	ASN	2.5
1	A	139	ASP	2.2

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
2	CU	A	630	1/1	0.99	0.07	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	A	632	1/1	0.99	0.01	21,21,21,21	0
4	NO3	A	633	4/4	0.99	0.04	15,16,16,16	0
5	PER	A	631	2/2	0.99	0.06	7,7,7,7	0
2	CU	A	629	1/1	1.00	0.05	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.