



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:38 AM UTC

PDB ID : 1OXY / pdb_00001oxy
Title : CRYSTALLOGRAPHIC ANALYSIS OF OXYGENATED AND DEOXY-
GENATED STATES OF ARTHROPOD HEMOCYANIN SHOWS UNUSUAL
DIFFERENCES
Authors : Ton-that, H.; Magnus, K.
Deposited on : 1995-01-06
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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

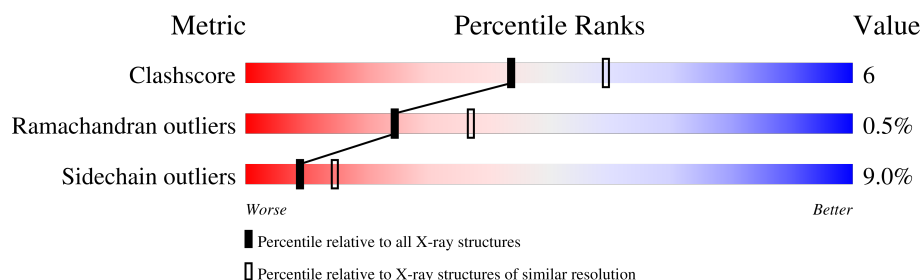
1 Overall quality at a glance

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)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	628	 60% 25% 5% • 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5006 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	573	Total	C	N	O	S	0	0	0
			4669	2986	812	849	22			

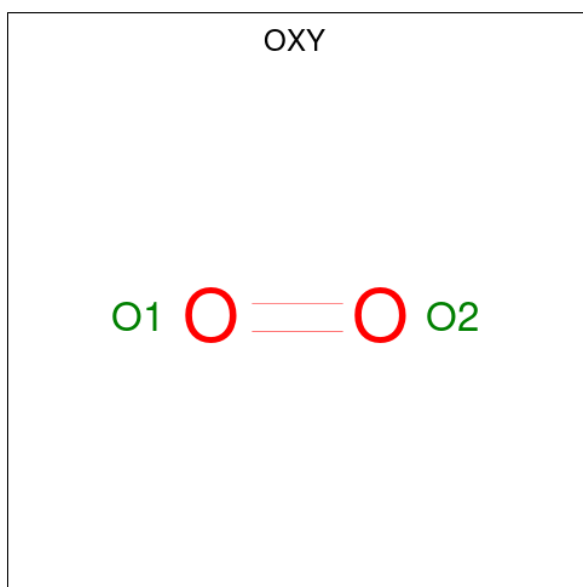
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	ILE	VAL	conflict	UNP P04253
A	408	THR	PHE	conflict	UNP P04253
A	409	PHE	THR	conflict	UNP P04253
A	432	LYS	ARG	conflict	UNP P04253
A	549	VAL	ILE	conflict	UNP P04253
A	550	ALA	LYS	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 OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



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

- Molecule 4 is water.

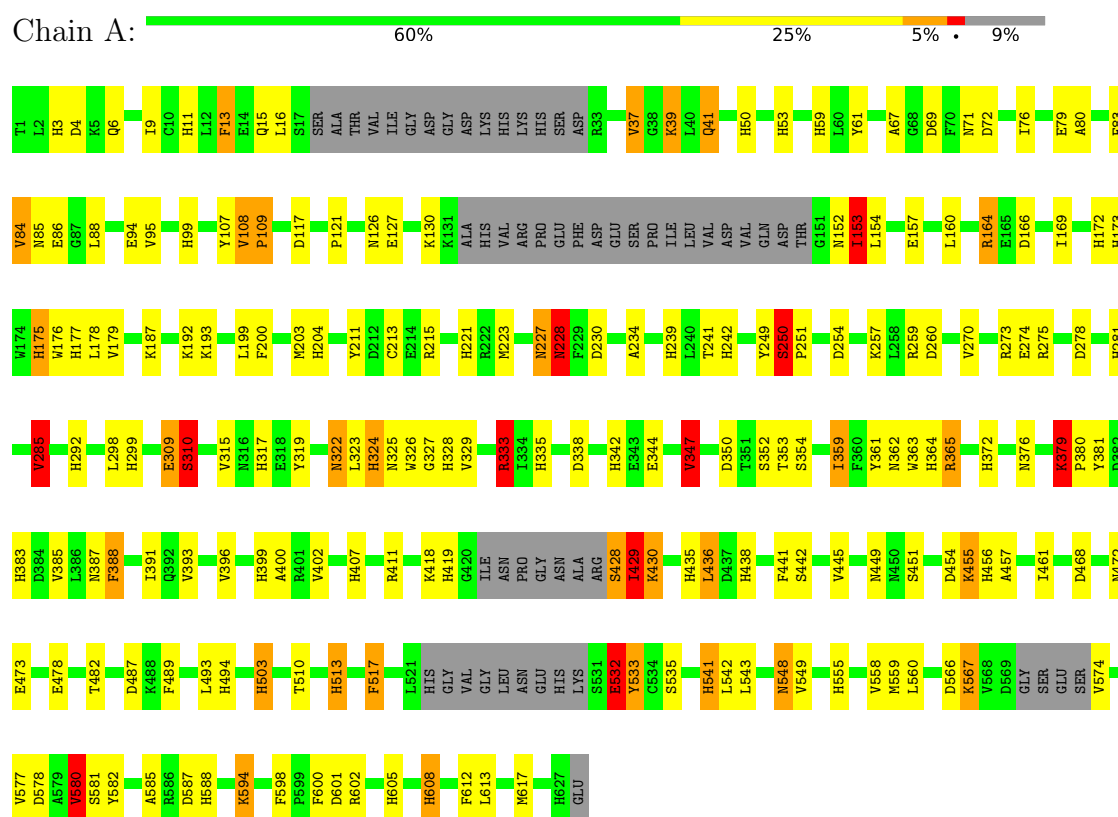
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	333	Total	O	0	0
			333	333		

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. 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. 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.

Note EDS was not executed.

• Molecule 1: HEMOCYANIN (SUBUNIT TYPE II)



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	117.24Å 117.24Å 285.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.171 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5006	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.07	47/4807 (1.0%)	1.76	116/6514 (1.8%)

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	1

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	407	HIS	CD2-NE2	-7.08	1.30	1.37
1	A	605	HIS	CD2-NE2	-6.93	1.30	1.37
1	A	503	HIS	CD2-NE2	-6.92	1.30	1.37
1	A	438	HIS	CD2-NE2	-6.85	1.30	1.37
1	A	50	HIS	CD2-NE2	-6.82	1.30	1.37
1	A	175	HIS	CD2-NE2	-6.66	1.30	1.37
1	A	435	HIS	CD2-NE2	-6.62	1.30	1.37
1	A	242	HIS	CD2-NE2	-6.60	1.30	1.37
1	A	173	HIS	CD2-NE2	-6.57	1.30	1.37
1	A	292	HIS	CD2-NE2	-6.57	1.30	1.37
1	A	456	HIS	CD2-NE2	-6.55	1.30	1.37
1	A	342	HIS	CD2-NE2	-6.48	1.30	1.37
1	A	239	HIS	CD2-NE2	-6.44	1.30	1.37
1	A	419	HIS	CD2-NE2	-6.39	1.30	1.37
1	A	399	HIS	CD2-NE2	-6.39	1.30	1.37
1	A	555	HIS	CD2-NE2	-6.34	1.30	1.37
1	A	11	HIS	CD2-NE2	-6.33	1.30	1.37
1	A	324	HIS	CD2-NE2	-6.32	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	HIS	CD2-NE2	-6.29	1.30	1.37
1	A	383	HIS	CD2-NE2	-6.26	1.30	1.37
1	A	608	HIS	CD2-NE2	-6.26	1.30	1.37
1	A	281	HIS	CD2-NE2	-6.25	1.30	1.37
1	A	588	HIS	CD2-NE2	-6.23	1.30	1.37
1	A	177	HIS	CD2-NE2	-6.23	1.31	1.37
1	A	53	HIS	CD2-NE2	-6.22	1.31	1.37
1	A	513	HIS	CD2-NE2	-6.21	1.31	1.37
1	A	541	HIS	CD2-NE2	-6.21	1.31	1.37
1	A	172	HIS	CD2-NE2	-6.20	1.31	1.37
1	A	364	HIS	CD2-NE2	-6.20	1.31	1.37
1	A	59	HIS	CD2-NE2	-6.18	1.31	1.37
1	A	99	HIS	CD2-NE2	-6.18	1.31	1.37
1	A	299	HIS	CD2-NE2	-6.10	1.31	1.37
1	A	335	HIS	CD2-NE2	-6.06	1.31	1.37
1	A	372	HIS	CD2-NE2	-6.02	1.31	1.37
1	A	3	HIS	CD2-NE2	-6.00	1.31	1.37
1	A	221	HIS	CD2-NE2	-5.83	1.31	1.37
1	A	328	HIS	CD2-NE2	-5.66	1.31	1.37
1	A	109	PRO	CA-CB	-5.52	1.49	1.54
1	A	494	HIS	CD2-NE2	-5.50	1.31	1.37
1	A	328	HIS	CG-ND1	-5.42	1.32	1.38
1	A	99	HIS	CG-ND1	-5.35	1.32	1.38
1	A	153	ILE	CA-CB	5.20	1.60	1.54
1	A	53	HIS	CG-ND1	-5.12	1.32	1.38
1	A	173	HIS	CG-ND1	-5.09	1.32	1.38
1	A	175	HIS	CG-ND1	-5.05	1.32	1.38
1	A	317	HIS	CD2-NE2	-5.03	1.32	1.37
1	A	204	HIS	CG-ND1	-5.01	1.32	1.38

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	532	GLU	N-CA-C	12.49	137.40	110.80
1	A	309	GLU	O-C-N	12.22	134.65	122.07
1	A	468	ASP	CA-CB-CG	9.67	122.27	112.60
1	A	533	TYR	N-CA-C	8.89	124.18	113.16
1	A	580	VAL	CB-CA-C	-8.73	100.70	111.88
1	A	292	HIS	N-CA-C	8.59	122.89	108.20
1	A	365	ARG	N-CA-C	-8.52	101.49	112.23
1	A	117	ASP	CA-CB-CG	8.45	121.05	112.60
1	A	153	ILE	N-CA-C	8.45	120.45	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	350	ASP	CA-CB-CG	8.17	120.77	112.60
1	A	254	ASP	CA-CB-CG	8.09	120.69	112.60
1	A	13	PHE	CA-CB-CG	7.71	121.51	113.80
1	A	399	HIS	CB-CG-CD2	-7.54	121.39	131.20
1	A	249	TYR	N-CA-C	-7.50	97.78	109.25
1	A	281	HIS	CA-CB-CG	-7.48	106.32	113.80
1	A	323	LEU	N-CA-C	7.48	119.12	110.97
1	A	130	LYS	CA-C-N	7.46	135.13	121.70
1	A	130	LYS	C-N-CA	7.46	135.13	121.70
1	A	130	LYS	N-CA-C	-7.45	102.70	112.24
1	A	594	LYS	CA-CB-CG	-7.21	99.69	114.10
1	A	578	ASP	CA-CB-CG	7.13	119.73	112.60
1	A	580	VAL	N-CA-C	7.11	117.82	110.36
1	A	228	ASN	OD1-CG-ND2	-7.10	115.50	122.60
1	A	72	ASP	CA-CB-CG	7.06	119.66	112.60
1	A	16	LEU	N-CA-C	-7.04	97.77	109.46
1	A	581	SER	N-CA-C	6.92	119.42	111.11
1	A	510	THR	N-CA-C	6.88	121.08	110.42
1	A	387	ASN	CA-CB-CG	6.82	119.42	112.60
1	A	613	LEU	N-CA-C	6.82	120.19	109.96
1	A	441	PHE	CA-CB-CG	6.80	120.60	113.80
1	A	309	GLU	CA-C-N	6.73	134.40	121.54
1	A	309	GLU	C-N-CA	6.73	134.40	121.54
1	A	347	VAL	N-CA-CB	-6.72	97.47	110.78
1	A	200	PHE	N-CA-C	-6.69	103.91	111.07
1	A	407	HIS	CB-CG-CD2	-6.66	122.54	131.20
1	A	487	ASP	CA-CB-CG	6.66	119.26	112.60
1	A	11	HIS	CB-CG-CD2	-6.60	122.62	131.20
1	A	567	LYS	N-CA-C	6.59	119.91	110.10
1	A	213	CYS	N-CA-C	-6.54	104.23	111.82
1	A	61	TYR	CA-CB-CG	6.49	125.58	113.90
1	A	260	ASP	CA-CB-CG	6.47	119.08	112.60
1	A	108	VAL	CA-C-N	6.46	124.31	119.66
1	A	108	VAL	C-N-CA	6.46	124.31	119.66
1	A	193	LYS	N-CA-C	-6.41	97.23	108.20
1	A	310	SER	CA-CB-OG	-6.40	98.31	111.10
1	A	164	ARG	N-CA-C	6.18	118.02	111.28
1	A	513	HIS	N-CA-C	6.13	119.52	108.48
1	A	566	ASP	CA-CB-CG	6.10	118.70	112.60
1	A	418	LYS	N-CA-C	6.03	120.25	113.01
1	A	179	VAL	N-CA-C	-6.02	104.44	111.00
1	A	175	HIS	CB-CG-CD2	-6.01	123.39	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	383	HIS	CB-CG-CD2	-5.99	123.41	131.20
1	A	285	VAL	N-CA-CB	-5.97	99.55	111.91
1	A	227	ASN	CA-CB-CG	5.97	118.57	112.60
1	A	342	HIS	CB-CG-CD2	-5.95	123.47	131.20
1	A	9	ILE	N-CA-C	-5.93	104.73	110.72
1	A	454	ASP	CA-CB-CG	5.91	118.51	112.60
1	A	457	ALA	N-CA-C	5.86	118.77	109.50
1	A	354	SER	N-CA-C	5.86	119.53	112.38
1	A	234	ALA	N-CA-C	-5.83	102.67	110.55
1	A	69	ASP	CA-CB-CG	5.83	118.43	112.60
1	A	322	ASN	CA-CB-CG	5.79	118.39	112.60
1	A	580	VAL	N-CA-CB	5.77	116.92	110.51
1	A	338	ASP	CA-CB-CG	5.77	118.37	112.60
1	A	601	ASP	CA-CB-CG	5.75	118.35	112.60
1	A	393	VAL	N-CA-C	-5.75	99.44	108.23
1	A	325	ASN	CA-CB-CG	5.72	118.32	112.60
1	A	478	GLU	CA-CB-CG	5.71	125.52	114.10
1	A	429	ILE	O-C-N	-5.67	115.49	122.57
1	A	438	HIS	CB-CG-CD2	-5.64	123.87	131.20
1	A	285	VAL	CB-CA-C	5.63	119.49	110.82
1	A	430	LYS	N-CA-C	5.62	119.14	110.42
1	A	399	HIS	CB-CG-ND1	5.60	131.10	122.70
1	A	548	ASN	CA-CB-CG	5.54	118.14	112.60
1	A	517	PHE	CA-CB-CG	5.52	119.32	113.80
1	A	364	HIS	CB-CG-CD2	-5.52	124.02	131.20
1	A	67	ALA	CA-C-N	5.47	126.15	120.03
1	A	67	ALA	C-N-CA	5.47	126.15	120.03
1	A	388	PHE	CA-C-N	5.46	124.81	118.85
1	A	388	PHE	C-N-CA	5.46	124.81	118.85
1	A	83	PHE	CA-CB-CG	5.46	119.26	113.80
1	A	71	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	A	39	LYS	N-CA-C	-5.45	106.31	113.12
1	A	177	HIS	CB-CG-CD2	-5.42	124.16	131.20
1	A	326	TRP	CG-CD2-CE3	5.41	139.31	133.90
1	A	335	HIS	CB-CG-CD2	-5.40	124.18	131.20
1	A	489	PHE	CA-CB-CG	5.38	119.18	113.80
1	A	376	ASN	OD1-CG-ND2	-5.37	117.23	122.60
1	A	228	ASN	CB-CG-ND2	5.37	124.45	116.40
1	A	250	SER	CA-C-N	5.33	125.31	120.03
1	A	250	SER	C-N-CA	5.33	125.31	120.03
1	A	494	HIS	CA-CB-CG	-5.31	108.49	113.80
1	A	587	ASP	CA-CB-CG	5.30	117.91	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	SER	N-CA-C	5.24	117.20	109.50
1	A	292	HIS	CA-CB-CG	5.24	119.03	113.80
1	A	472	ASN	CA-CB-CG	5.23	117.83	112.60
1	A	379	LYS	CA-C-N	5.19	125.10	119.76
1	A	379	LYS	C-N-CA	5.19	125.10	119.76
1	A	41	GLN	OE1-CD-NE2	-5.18	117.42	122.60
1	A	228	ASN	N-CA-C	-5.17	98.85	107.99
1	A	419	HIS	CB-CG-CD2	-5.16	124.49	131.20
1	A	179	VAL	CB-CA-C	-5.16	105.33	112.24
1	A	364	HIS	CA-CB-CG	-5.15	108.65	113.80
1	A	299	HIS	N-CA-C	5.15	119.66	113.17
1	A	535	SER	N-CA-C	5.14	119.54	113.16
1	A	59	HIS	CB-CG-CD2	-5.12	124.55	131.20
1	A	612	PHE	CA-CB-CG	5.09	118.89	113.80
1	A	326	TRP	CE2-CD2-CG	-5.09	101.09	107.20
1	A	600	PHE	N-CA-C	5.09	118.63	112.93
1	A	402	VAL	N-CA-C	-5.08	101.06	108.17
1	A	50	HIS	CB-CG-CD2	-5.07	124.61	131.20
1	A	333	ARG	CA-CB-CG	5.07	124.24	114.10
1	A	456	HIS	CB-CG-CD2	-5.07	124.61	131.20
1	A	372	HIS	CB-CG-CD2	-5.03	124.67	131.20
1	A	4	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	326	TRP	CB-CG-CD1	-5.01	119.38	126.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	388	PHE	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	4669	0	4417	55	0
2	A	2	0	0	0	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	333	0	0	4	0
All	All	5006	0	4417	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:94:GLU:HG3	1:A:108:VAL:HG21	1.67	0.75
1:A:347:VAL:HG22	1:A:353:THR:HB	1.68	0.74
1:A:223:MET:SD	1:A:361:TYR:HB3	2.33	0.68
1:A:310:SER:HB2	1:A:322:ASN:HA	1.77	0.67
1:A:359:ILE:HA	1:A:362:ASN:HD22	1.65	0.61
1:A:157:GLU:HG3	1:A:164:ARG:HH12	1.66	0.61
1:A:94:GLU:HB3	1:A:178:LEU:HD13	1.85	0.58
1:A:13:PHE:HB2	4:A:884:HOH:O	2.04	0.57
1:A:6:GLN:HE22	1:A:107:TYR:H	1.53	0.56
1:A:95:VAL:HG23	1:A:178:LEU:HD22	1.88	0.55
1:A:157:GLU:HG3	1:A:164:ARG:NH1	2.22	0.55
1:A:309:GLU:HA	1:A:324:HIS:HB3	1.89	0.55
1:A:275:ARG:HG2	1:A:319:TYR:CZ	2.42	0.55
1:A:559:MET:HG3	1:A:617:MET:HG2	1.88	0.54
1:A:396:VAL:HG22	1:A:445:VAL:HG13	1.89	0.54
1:A:428:SER:O	1:A:429:ILE:HG13	2.08	0.53
1:A:327:GLY:HA3	1:A:363:TRP:CZ2	2.45	0.51
1:A:436:LEU:O	1:A:541:HIS:HB2	2.09	0.51
1:A:429:ILE:HG22	1:A:430:LYS:H	1.75	0.51
1:A:449:ASN:OD1	1:A:451:SER:HB3	2.11	0.51
1:A:577:VAL:O	1:A:580:VAL:HG22	2.11	0.51
1:A:270:VAL:O	1:A:274:GLU:HG2	2.09	0.51
1:A:329:VAL:O	1:A:333:ARG:HG2	2.10	0.51
1:A:347:VAL:HG22	1:A:353:THR:CB	2.38	0.50
1:A:285:VAL:HG13	1:A:315:VAL:HG21	1.94	0.49
1:A:86:GLU:H	1:A:86:GLU:CD	2.20	0.49
1:A:160:LEU:HD11	1:A:215:ARG:HG2	1.96	0.48
1:A:391:ILE:HD11	1:A:455:LYS:HG3	1.97	0.47
1:A:381:TYR:CE2	1:A:602:ARG:HG3	2.50	0.47
1:A:37:VAL:HG13	1:A:84:VAL:HG21	1.97	0.46
1:A:85:ASN:HD22	1:A:88:LEU:H	1.62	0.46
1:A:429:ILE:HG22	1:A:430:LYS:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ASP:O	1:A:169:ILE:HG22	2.16	0.45
1:A:259:ARG:HD2	1:A:259:ARG:HA	1.76	0.45
1:A:176:TRP:HH2	4:A:876:HOH:O	2.00	0.45
1:A:594:LYS:HD3	1:A:598:PHE:CE1	2.52	0.45
1:A:379:LYS:HA	1:A:380:PRO:HD3	1.78	0.45
1:A:532:GLU:HB2	1:A:533:TYR:H	1.59	0.44
1:A:126:ASN:HB2	4:A:789:HOH:O	2.18	0.44
1:A:442:SER:HB3	1:A:503:HIS:HD2	1.83	0.43
1:A:461:ILE:HG12	1:A:558:VAL:HG22	1.99	0.43
1:A:270:VAL:HG13	1:A:273:ARG:NH2	2.33	0.43
1:A:80:ALA:O	1:A:84:VAL:HB	2.19	0.43
1:A:250:SER:HA	1:A:251:PRO:HD3	1.82	0.42
1:A:94:GLU:OE2	1:A:175:HIS:HD2	2.02	0.42
1:A:228:ASN:ND2	1:A:230:ASP:H	2.17	0.42
1:A:109:PRO:HB2	4:A:884:HOH:O	2.19	0.42
1:A:250:SER:HB2	1:A:344:GLU:O	2.20	0.41
1:A:574:VAL:CG2	1:A:585:ALA:HB1	2.51	0.41
1:A:365:ARG:HD2	1:A:365:ARG:HA	1.87	0.41
1:A:153:ILE:O	1:A:153:ILE:HG13	2.21	0.40
1:A:473:GLU:OE2	1:A:608:HIS:HD2	2.04	0.40
1:A:379:LYS:H	1:A:379:LYS:HE3	1.86	0.40
1:A:211:TYR:HD2	1:A:223:MET:HE2	1.86	0.40
1:A:203:MET:HE1	1:A:582:TYR:CD2	2.56	0.40

There are no symmetry-related clashes.

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	561/628 (89%)	535 (95%)	23 (4%)	3 (0%)	24 37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	429	ILE
1	A	152	ASN
1	A	400	ALA

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	499/557 (90%)	454 (91%)	45 (9%)	9 15

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	37	VAL
1	A	39	LYS
1	A	41	GLN
1	A	76	ILE
1	A	79	GLU
1	A	84	VAL
1	A	121	PRO
1	A	127	GLU
1	A	153	ILE
1	A	154	LEU
1	A	187	LYS
1	A	192	LYS
1	A	199	LEU
1	A	227	ASN
1	A	228	ASN
1	A	241	THR
1	A	250	SER
1	A	257	LYS
1	A	278	ASP
1	A	285	VAL
1	A	298	LEU
1	A	310	SER
1	A	333	ARG

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Mol	Chain	Res	Type
1	A	347	VAL
1	A	352	SER
1	A	359	ILE
1	A	379	LYS
1	A	385	VAL
1	A	411	ARG
1	A	428	SER
1	A	436	LEU
1	A	455	LYS
1	A	482	THR
1	A	493	LEU
1	A	513	HIS
1	A	517	PHE
1	A	532	GLU
1	A	542	LEU
1	A	543	LEU
1	A	548	ASN
1	A	549	VAL
1	A	560	LEU
1	A	567	LYS
1	A	580	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	11	HIS
1	A	15	GLN
1	A	59	HIS
1	A	85	ASN
1	A	170	ASN
1	A	172	HIS
1	A	175	HIS
1	A	228	ASN
1	A	299	HIS
1	A	316	ASN
1	A	362	ASN
1	A	392	GLN
1	A	407	HIS
1	A	413	GLN
1	A	446	ASN
1	A	450	ASN

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Mol	Chain	Res	Type
1	A	503	HIS
1	A	513	HIS
1	A	548	ASN
1	A	608	HIS
1	A	615	ASN

5.3.3 RNA [i](#)

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](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z > 2$
3	OXY	A	631	2	1,1,1	0.83	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.

No monomer is involved in short contacts.

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.