



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 11:32 PM EDT

PDB ID : 1LLA / pdb_00001lla
Title : CRYSTAL STRUCTURE OF DEOXYGENATED LIMULUS POLYPHEMUS SUBUNIT II HEMOCYANIN AT 2.18 ANGSTROMS RESOLUTION: CLUES FOR A MECHANISM FOR ALLOSTERIC REGULATION
Authors : Hazes, B.; Hol, W.G.J.
Deposited on : 1992-09-07
Resolution : 2.18 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
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

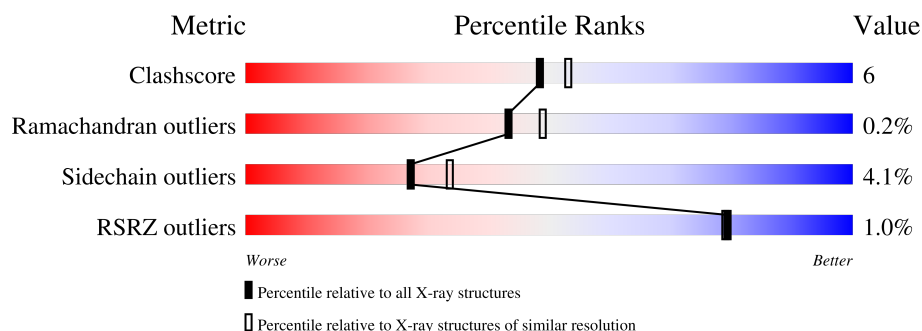
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	71% 21% ...

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5196 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	600	Total	C	N	O	S	0	0	0
			4860	3101	849	888	22			

There are 3 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

- 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 SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

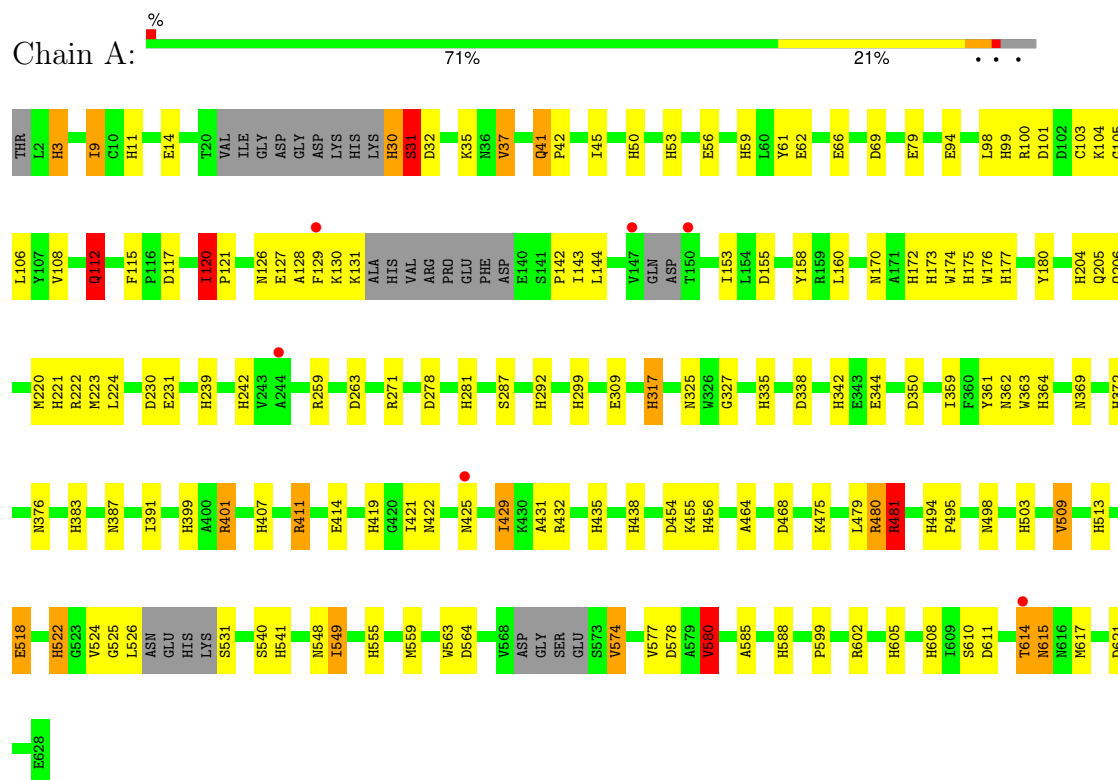
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	332	Total 332	O 332	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: 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)	10.00 – 2.18 10.00 – 2.19	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.18) 94.7 (10.00-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.174 , (Not available) 0.171 , (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)	0.28 , 62.0	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	0.96	EDS
Total number of atoms	5196	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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

5.1 Standard geometry

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

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	1.18	48/5001 (1.0%)	1.70	101/6776 (1.5%)

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	5

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	292	HIS	CD2-NE2	-6.99	1.30	1.37
1	A	419	HIS	CD2-NE2	-6.98	1.30	1.37
1	A	364	HIS	CD2-NE2	-6.94	1.30	1.37
1	A	281	HIS	CD2-NE2	-6.72	1.30	1.37
1	A	172	HIS	CD2-NE2	-6.67	1.30	1.37
1	A	3	HIS	CD2-NE2	-6.55	1.30	1.37
1	A	299	HIS	CD2-NE2	-6.49	1.30	1.37
1	A	173	HIS	CD2-NE2	-6.28	1.30	1.37
1	A	342	HIS	CD2-NE2	-6.25	1.30	1.37
1	A	611	ASP	N-CA	6.24	1.54	1.46
1	A	239	HIS	CD2-NE2	-6.20	1.31	1.37
1	A	456	HIS	CD2-NE2	-6.15	1.31	1.37
1	A	555	HIS	CD2-NE2	-6.14	1.31	1.37
1	A	541	HIS	CD2-NE2	-6.08	1.31	1.37
1	A	59	HIS	CD2-NE2	-6.07	1.31	1.37
1	A	53	HIS	CD2-NE2	-6.06	1.31	1.37
1	A	173	HIS	CG-ND1	-6.05	1.31	1.38
1	A	407	HIS	CD2-NE2	-6.01	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	503	HIS	CD2-NE2	-5.91	1.31	1.37
1	A	494	HIS	CD2-NE2	-5.86	1.31	1.37
1	A	177	HIS	CD2-NE2	-5.82	1.31	1.37
1	A	605	HIS	CD2-NE2	-5.81	1.31	1.37
1	A	383	HIS	CD2-NE2	-5.79	1.31	1.37
1	A	438	HIS	CD2-NE2	-5.74	1.31	1.37
1	A	99	HIS	CD2-NE2	-5.70	1.31	1.37
1	A	610	SER	CA-C	5.65	1.60	1.52
1	A	399	HIS	CD2-NE2	-5.65	1.31	1.37
1	A	50	HIS	CD2-NE2	-5.62	1.31	1.37
1	A	435	HIS	CD2-NE2	-5.55	1.31	1.37
1	A	221	HIS	CD2-NE2	-5.54	1.31	1.37
1	A	610	SER	CA-CB	5.53	1.62	1.53
1	A	588	HIS	CD2-NE2	-5.52	1.31	1.37
1	A	204	HIS	CD2-NE2	-5.49	1.31	1.37
1	A	242	HIS	CD2-NE2	-5.48	1.31	1.37
1	A	522	HIS	CG-CD2	5.45	1.41	1.35
1	A	11	HIS	CD2-NE2	-5.40	1.31	1.37
1	A	563	TRP	CG-CD2	-5.37	1.34	1.43
1	A	509	VAL	CA-CB	5.32	1.61	1.54
1	A	513	HIS	CD2-NE2	-5.32	1.31	1.37
1	A	372	HIS	CD2-NE2	-5.28	1.32	1.37
1	A	175	HIS	CG-ND1	-5.19	1.32	1.38
1	A	317	HIS	CD2-NE2	-5.17	1.32	1.37
1	A	30	HIS	CD2-NE2	-5.13	1.32	1.37
1	A	608	HIS	CD2-NE2	-5.10	1.32	1.37
1	A	541	HIS	CG-ND1	-5.08	1.32	1.38
1	A	281	HIS	CG-ND1	-5.08	1.32	1.38
1	A	335	HIS	CD2-NE2	-5.05	1.32	1.37
1	A	59	HIS	CG-ND1	-5.03	1.32	1.38

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	580	VAL	CB-CA-C	-11.86	96.50	112.04
1	A	325	ASN	OD1-CG-ND2	-9.08	113.52	122.60
1	A	614	THR	N-CA-CB	-8.65	97.45	110.60
1	A	580	VAL	N-CA-CB	8.41	120.98	110.47
1	A	468	ASP	CA-CB-CG	7.86	120.46	112.60
1	A	41	GLN	N-CA-C	7.76	119.49	109.64
1	A	605	HIS	CB-CG-CD2	-7.65	121.25	131.20
1	A	419	HIS	CB-CG-CD2	-7.37	121.62	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	522	HIS	O-C-N	-7.34	112.82	122.59
1	A	126	ASN	OD1-CG-ND2	-7.23	115.37	122.60
1	A	317	HIS	CB-CG-CD2	-6.96	122.15	131.20
1	A	578	ASP	CA-CB-CG	6.83	119.42	112.60
1	A	37	VAL	N-CA-CB	-6.81	99.76	112.36
1	A	338	ASP	CA-CB-CG	6.73	119.33	112.60
1	A	142	PRO	N-CA-CB	6.69	109.56	103.34
1	A	407	HIS	CB-CG-CD2	-6.68	122.52	131.20
1	A	31	SER	N-CA-C	-6.60	96.74	110.80
1	A	376	ASN	OD1-CG-ND2	-6.56	116.04	122.60
1	A	206	GLN	OE1-CD-NE2	-6.54	116.06	122.60
1	A	309	GLU	CA-C-O	-6.47	113.98	120.90
1	A	205	GLN	OE1-CD-NE2	-6.43	116.17	122.60
1	A	11	HIS	CB-CG-CD2	-6.29	123.02	131.20
1	A	387	ASN	OD1-CG-ND2	-6.28	116.32	122.60
1	A	281	HIS	CB-CG-CD2	-6.27	123.05	131.20
1	A	79	GLU	CA-CB-CG	-6.26	101.57	114.10
1	A	555	HIS	CB-CG-CD2	-6.26	123.06	131.20
1	A	299	HIS	CB-CG-CD2	-6.23	123.10	131.20
1	A	456	HIS	CB-CG-CD2	-6.23	123.10	131.20
1	A	69	ASP	CA-CB-CG	6.22	118.83	112.60
1	A	230	ASP	CA-CB-CG	6.13	118.73	112.60
1	A	422	ASN	CA-C-N	6.10	125.81	119.64
1	A	422	ASN	C-N-CA	6.10	125.81	119.64
1	A	50	HIS	CB-CG-CD2	-6.09	123.28	131.20
1	A	9	ILE	CA-CB-CG1	-6.09	100.05	110.40
1	A	3	HIS	CB-CG-CD2	-6.07	123.31	131.20
1	A	615	ASN	OD1-CG-ND2	-6.05	116.55	122.60
1	A	37	VAL	CB-CA-C	6.04	120.52	110.30
1	A	369	ASN	OD1-CG-ND2	-6.03	116.58	122.60
1	A	435	HIS	CB-CG-CD2	-6.02	123.37	131.20
1	A	563	TRP	CE2-CD2-CE3	6.02	124.82	118.80
1	A	117	ASP	CA-CB-CG	5.99	118.58	112.60
1	A	112	GLN	OE1-CD-NE2	-5.98	116.62	122.60
1	A	180	TYR	CA-C-N	5.95	125.89	119.76
1	A	180	TYR	C-N-CA	5.95	125.89	119.76
1	A	155	ASP	CA-CB-CG	5.94	118.54	112.60
1	A	605	HIS	CB-CG-ND1	5.92	131.58	122.70
1	A	230	ASP	CB-CA-C	-5.92	99.36	110.01
1	A	364	HIS	CA-CB-CG	-5.89	107.91	113.80
1	A	615	ASN	CB-CG-ND2	5.86	125.19	116.40
1	A	221	HIS	CB-CG-CD2	-5.82	123.63	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	429	ILE	N-CA-C	-5.81	99.17	107.77
1	A	30	HIS	CB-CG-CD2	-5.78	123.68	131.20
1	A	174	TRP	CG-CD2-CE3	5.77	139.67	133.90
1	A	120	ILE	N-CA-CB	-5.76	103.14	111.21
1	A	309	GLU	O-C-N	-5.74	116.12	122.09
1	A	540	SER	CA-CB-OG	-5.73	99.64	111.10
1	A	350	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	621	ASP	CA-CB-CG	-5.67	106.93	112.60
1	A	480	ARG	N-CA-C	5.55	118.09	111.71
1	A	435	HIS	CA-CB-CG	5.54	119.34	113.80
1	A	383	HIS	CB-CG-CD2	-5.54	124.00	131.20
1	A	503	HIS	CB-CG-CD2	-5.51	124.04	131.20
1	A	204	HIS	CB-CG-CD2	-5.50	124.05	131.20
1	A	172	HIS	CB-CG-CD2	-5.50	124.05	131.20
1	A	608	HIS	CB-CG-CD2	-5.45	124.12	131.20
1	A	425	ASN	OD1-CG-ND2	-5.43	117.17	122.60
1	A	224	LEU	CA-C-N	5.40	125.16	119.76
1	A	224	LEU	C-N-CA	5.40	125.16	119.76
1	A	411	ARG	NE-CZ-NH1	-5.37	116.13	121.50
1	A	548	ASN	CA-CB-CG	5.37	117.97	112.60
1	A	61	TYR	CA-CB-CG	5.35	123.53	113.90
1	A	120	ILE	CA-C-N	5.35	125.35	119.89
1	A	120	ILE	C-N-CA	5.35	125.35	119.89
1	A	498	ASN	CA-CB-CG	5.35	117.95	112.60
1	A	481	ARG	N-CA-C	-5.34	106.60	113.23
1	A	100	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	A	103	CYS	CA-CB-SG	-5.29	102.23	114.40
1	A	56	GLU	N-CA-C	-5.29	105.60	111.36
1	A	481	ARG	NE-CZ-NH1	5.25	126.75	121.50
1	A	342	HIS	CB-CG-CD2	-5.23	124.40	131.20
1	A	419	HIS	CB-CG-ND1	5.23	130.54	122.70
1	A	407	HIS	CB-CG-ND1	5.21	130.52	122.70
1	A	541	HIS	CB-CG-CD2	-5.21	124.43	131.20
1	A	170	ASN	OD1-CG-ND2	-5.20	117.40	122.60
1	A	299	HIS	CA-CB-CG	-5.18	108.62	113.80
1	A	115	PHE	CA-C-N	5.17	125.47	119.47
1	A	115	PHE	C-N-CA	5.17	125.47	119.47
1	A	176	TRP	CG-CD2-CE3	5.15	139.05	133.90
1	A	524	VAL	N-CA-C	-5.15	107.73	112.83
1	A	387	ASN	CB-CG-ND2	5.14	124.11	116.40
1	A	364	HIS	CB-CG-CD2	-5.11	124.56	131.20
1	A	155	ASP	CA-C-N	5.10	124.89	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	ASP	C-N-CA	5.10	124.89	119.28
1	A	126	ASN	N-CA-C	-5.08	105.65	111.14
1	A	456	HIS	CB-CG-ND1	5.04	130.26	122.70
1	A	564	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	350	ASP	O-C-N	-5.03	117.42	123.31
1	A	105	GLY	N-CA-C	-5.01	108.41	114.92
1	A	435	HIS	CB-CG-ND1	5.01	130.21	122.70
1	A	364	HIS	N-CA-C	5.00	117.63	111.82
1	A	292	HIS	CB-CG-CD2	-5.00	124.70	131.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	222	ARG	Sidechain
1	A	271	ARG	Sidechain
1	A	401	ARG	Sidechain
1	A	411	ARG	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	4860	0	4587	52	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	332	0	0	7	0
All	All	5196	0	4587	52	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 (52) 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:9:ILE:HD12	1:A:106:LEU:HD13	1.63	0.81
1:A:112:GLN:HE21	1:A:112:GLN:H	1.30	0.80
1:A:144:LEU:HD21	1:A:432:ARG:NH2	1.97	0.78
1:A:614:THR:OG1	1:A:617:MET:HE3	1.88	0.72
1:A:104:LYS:NZ	1:A:104:LYS:HB3	2.06	0.71
1:A:481:ARG:HG3	1:A:481:ARG:NH1	2.14	0.62
1:A:614:THR:HG1	1:A:617:MET:HE3	1.63	0.62
1:A:104:LYS:HB3	1:A:104:LYS:HZ3	1.65	0.61
1:A:62:GLU:O	1:A:66:GLU:HG2	2.01	0.60
1:A:614:THR:HG1	1:A:617:MET:CE	2.15	0.59
1:A:464:ALA:HB1	1:A:479:LEU:HD22	1.86	0.57
1:A:128:ALA:HB1	1:A:429:ILE:HG21	1.86	0.56
1:A:317:HIS:C	1:A:317:HIS:CD2	2.86	0.54
1:A:112:GLN:HE21	1:A:112:GLN:N	2.03	0.54
1:A:98:LEU:HD23	5:A:914:HOH:O	2.10	0.52
1:A:41:GLN:HA	1:A:41:GLN:OE1	2.10	0.51
1:A:549:ILE:HG23	5:A:930:HOH:O	2.11	0.51
1:A:129:PHE:CZ	1:A:421:ILE:HB	2.46	0.51
1:A:481:ARG:HD2	5:A:767:HOH:O	2.11	0.50
1:A:32:ASP:O	1:A:35:LYS:HG2	2.12	0.50
1:A:3:HIS:NE2	1:A:522:HIS:O	2.45	0.50
1:A:112:GLN:H	1:A:112:GLN:NE2	2.03	0.50
1:A:259:ARG:HG3	5:A:863:HOH:O	2.10	0.50
1:A:45:ILE:HD12	1:A:344:GLU:HB3	1.94	0.49
1:A:327:GLY:HA3	1:A:363:TRP:CZ2	2.48	0.49
1:A:414:GLU:HA	1:A:431:ALA:O	2.14	0.48
1:A:104:LYS:NZ	1:A:104:LYS:CB	2.76	0.48
1:A:615:ASN:HB2	5:A:895:HOH:O	2.14	0.48
1:A:94:GLU:HG3	1:A:108:VAL:HG21	1.96	0.47
1:A:317:HIS:CD2	1:A:317:HIS:O	2.67	0.47
1:A:98:LEU:CD2	5:A:914:HOH:O	2.63	0.47
1:A:143:ILE:HD12	1:A:429:ILE:HG13	1.96	0.46
1:A:577:VAL:O	1:A:580:VAL:HG22	2.16	0.45
1:A:518:GLU:HA	1:A:518:GLU:OE1	2.16	0.44
1:A:481:ARG:HG3	1:A:481:ARG:HH11	1.82	0.44
1:A:127:GLU:O	1:A:131:LYS:HG2	2.17	0.44
1:A:391:ILE:HD11	1:A:455:LYS:HG3	2.00	0.43
1:A:454:ASP:OD1	1:A:495:PRO:HD3	2.19	0.43
1:A:574:VAL:HG11	1:A:585:ALA:HB1	2.00	0.43
1:A:153:ILE:HG12	1:A:158:TYR:CE1	2.54	0.43
1:A:359:ILE:HA	1:A:362:ASN:HD22	1.83	0.42
1:A:480:ARG:HD3	1:A:602:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:PRO:HD3	5:A:802:HOH:O	2.18	0.42
1:A:559:MET:HG3	1:A:617:MET:HG2	2.00	0.42
1:A:223:MET:SD	1:A:361:TYR:HB3	2.60	0.42
1:A:475:LYS:HA	1:A:475:LYS:HD3	1.78	0.41
1:A:30:HIS:O	1:A:31:SER:HB2	2.20	0.41
1:A:559:MET:HE3	1:A:617:MET:HE2	2.02	0.41
1:A:160:LEU:HD21	1:A:220:MET:SD	2.61	0.41
1:A:153:ILE:HG12	1:A:158:TYR:CD1	2.56	0.40
1:A:120:ILE:HA	1:A:121:PRO:HD3	1.96	0.40
1:A:522:HIS:N	1:A:522:HIS:CD2	2.89	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	588/628 (94%)	573 (97%)	14 (2%)	1 (0%)	43	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	SER

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	518/558 (93%)	497 (96%)	21 (4%)	27	33

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	31	SER
1	A	37	VAL
1	A	101	ASP
1	A	112	GLN
1	A	120	ILE
1	A	130	LYS
1	A	231	GLU
1	A	263	ASP
1	A	278	ASP
1	A	287	SER
1	A	401	ARG
1	A	481	ARG
1	A	509	VAL
1	A	518	GLU
1	A	526	LEU
1	A	531	SER
1	A	549	ILE
1	A	574	VAL
1	A	580	VAL
1	A	599	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	15	GLN
1	A	30	HIS
1	A	112	GLN
1	A	317	HIS
1	A	362	ASN
1	A	399	HIS
1	A	425	ASN
1	A	446	ASN
1	A	513	HIS
1	A	522	HIS
1	A	605	HIS

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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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 [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	600/628 (95%)	-0.60	6 (1%) 79 79	4, 19, 38, 48	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	129	PHE	3.3
1	A	244	ALA	2.8
1	A	150	THR	2.5
1	A	614	THR	2.4
1	A	425	ASN	2.0
1	A	147	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CU	A	630	1/1	0.99	0.02	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	A	631	1/1	0.99	0.07	17,17,17,17	0
4	CL	A	632	1/1	0.99	0.02	18,18,18,18	0
2	CU	A	629	1/1	1.00	0.01	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.