



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:51 PM UTC

PDB ID : 1LL1 / pdb_00001ll1
Title : HYDROXO BRIDGE MET FORM HEMOCYANIN FROM LIMULUS
Authors : Liu, S.; Magnus, K.
Deposited on : 1997-03-17
Resolution : 2.55 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

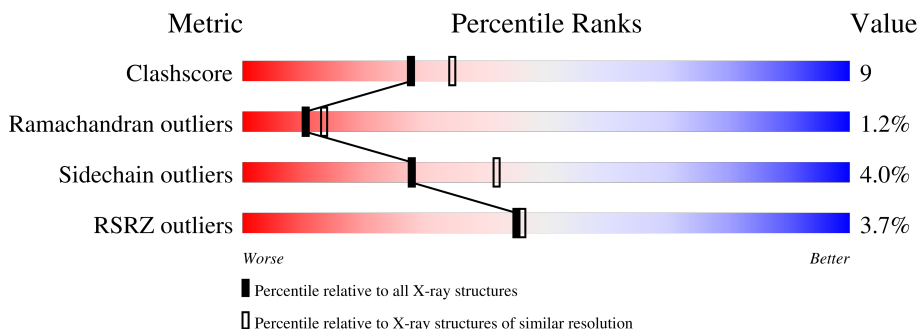
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	4% 74% 18% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4903 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 METCYANIN II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	590	Total	C	N	O	S	0	0	0
			4763	3042	829	870	22			

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

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

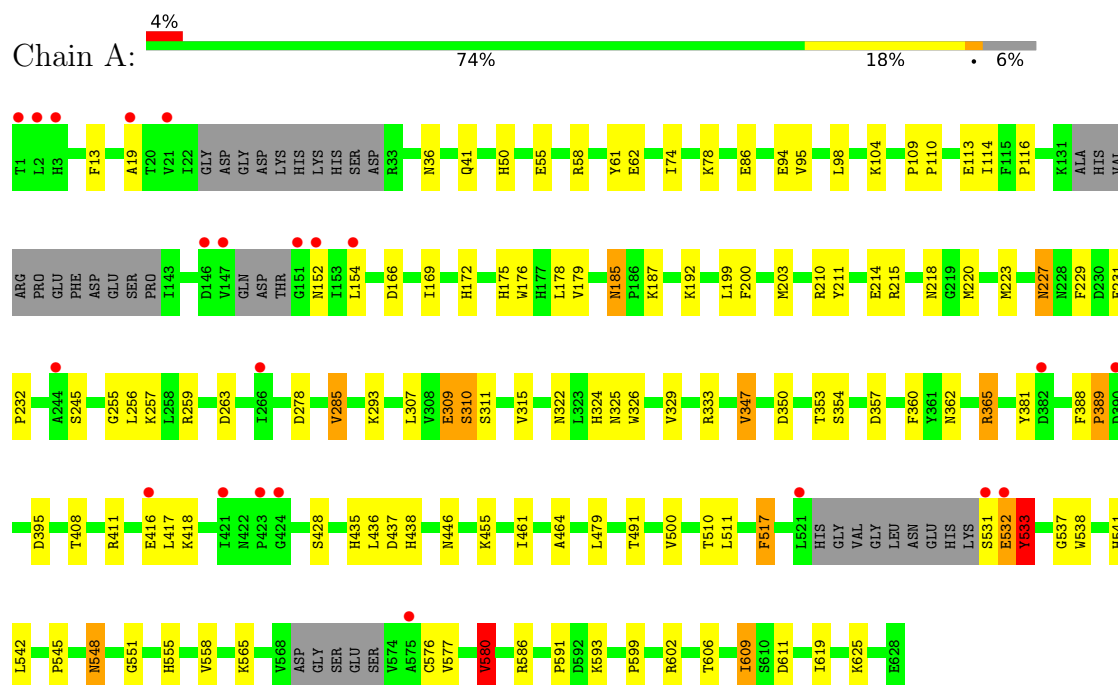
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	137	Total	O	0	0
			137	137		

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: METCYANIN II



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	116.61Å 116.61Å 285.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.00 – 2.55 60.00 – 2.55	Depositor EDS
% Data completeness (in resolution range)	88.6 (60.00-2.55) 90.5 (60.00-2.55)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.45Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.167 , 0.230 0.180 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k +1/3*l 0.000 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/ 3*k+1/3*l 0.001 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+ 1/3*l,-4/3*h+4/3*k+1/3*l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4903	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.41	0/4901	0.91	15/6643 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	GLU	N-CA-C	-9.04	101.37	111.14
1	A	533	TYR	N-CA-C	7.52	126.82	110.80
1	A	388	PHE	CA-C-N	7.18	128.82	119.84
1	A	388	PHE	C-N-CA	7.18	128.82	119.84
1	A	255	GLY	N-CA-C	6.44	124.25	115.30
1	A	311	SER	N-CA-C	-6.07	101.00	110.17
1	A	580	VAL	CB-CA-C	-6.00	104.20	111.88
1	A	50	HIS	CA-C-N	5.71	125.83	119.32
1	A	50	HIS	C-N-CA	5.71	125.83	119.32
1	A	354	SER	N-CA-C	5.70	118.27	111.71
1	A	365	ARG	N-CA-C	-5.44	106.15	112.89
1	A	360	PHE	N-CA-C	-5.23	105.58	111.28
1	A	185	ASN	CA-C-N	5.15	124.77	119.05
1	A	185	ASN	C-N-CA	5.15	124.77	119.05
1	A	580	VAL	N-CA-C	5.11	115.72	110.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4763	0	4482	83	0
2	A	2	0	0	0	0
3	A	1	0	0	1	0
4	A	137	0	0	4	0
All	All	4903	0	4482	83	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 9.

All (83) 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:531:SER:HA	1:A:576:CYS:H	1.41	0.85
1:A:606:THR:HG21	1:A:611:ASP:HB2	1.59	0.82
1:A:531:SER:HA	1:A:576:CYS:N	1.96	0.81
1:A:347:VAL:HG22	1:A:353:THR:HB	1.70	0.74
1:A:381:TYR:CZ	1:A:602:ARG:HD3	2.26	0.71
1:A:172:HIS:HD2	1:A:537:GLY:H	1.40	0.69
1:A:256:LEU:HD22	1:A:259:ARG:HH12	1.58	0.68
1:A:223:MET:HE2	1:A:362:ASN:HD21	1.59	0.67
1:A:609:ILE:HD12	1:A:619:ILE:HD13	1.74	0.67
1:A:555:HIS:CE1	1:A:609:ILE:HD11	2.32	0.65
1:A:551:GLY:HA2	1:A:625:LYS:HG2	1.81	0.62
1:A:511:LEU:HB2	1:A:537:GLY:HA3	1.83	0.60
1:A:416:GLU:HG2	1:A:418:LYS:HZ2	1.67	0.60
1:A:109:PRO:HG2	1:A:114:ILE:HD11	1.82	0.60
1:A:257:LYS:O	1:A:259:ARG:HD3	2.02	0.60
1:A:531:SER:HB3	1:A:577:VAL:H	1.67	0.59
1:A:285:VAL:HG12	1:A:293:LYS:HB3	1.86	0.56
1:A:104:LYS:HG2	1:A:586:ARG:HH22	1.71	0.56
1:A:211:TYR:CE2	1:A:215:ARG:HD2	2.41	0.55
1:A:416:GLU:HG2	1:A:418:LYS:NZ	2.21	0.55
1:A:116:PRO:HB2	1:A:417:LEU:HD22	1.88	0.55
1:A:256:LEU:HD22	1:A:259:ARG:NH1	2.22	0.54
1:A:576:CYS:HB2	1:A:586:ARG:HB2	1.90	0.53
1:A:551:GLY:CA	1:A:625:LYS:HG2	2.38	0.53
1:A:577:VAL:HG12	1:A:577:VAL:O	2.08	0.52
1:A:74:ILE:O	1:A:78:LYS:HG2	2.09	0.52
1:A:329:VAL:HG13	1:A:333:ARG:HE	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:LYS:HE2	1:A:428:SER:OG	2.10	0.52
1:A:609:ILE:HD12	1:A:619:ILE:CD1	2.40	0.52
1:A:310:SER:CB	1:A:322:ASN:HA	2.41	0.51
1:A:285:VAL:CG1	1:A:315:VAL:HG11	2.40	0.51
1:A:310:SER:HB2	1:A:322:ASN:HA	1.93	0.51
1:A:438:HIS:CE1	4:A:713:HOH:O	2.64	0.51
1:A:577:VAL:O	1:A:580:VAL:HG22	2.12	0.50
1:A:176:TRP:CH2	1:A:200:PHE:HA	2.47	0.49
1:A:322:ASN:OD1	1:A:325:ASN:HB2	2.13	0.49
1:A:416:GLU:HB3	1:A:418:LYS:HD2	1.93	0.49
1:A:395:ASP:HB3	1:A:446:ASN:HD22	1.76	0.49
1:A:455:LYS:HE2	4:A:757:HOH:O	2.12	0.49
1:A:285:VAL:HG21	1:A:307:LEU:HD21	1.94	0.48
1:A:416:GLU:HA	1:A:418:LYS:HZ1	1.79	0.48
1:A:94:GLU:HB3	1:A:178:LEU:HD13	1.95	0.47
1:A:166:ASP:O	1:A:169:ILE:HG22	2.15	0.47
1:A:110:PRO:O	1:A:114:ILE:HG13	2.15	0.47
1:A:285:VAL:HG11	1:A:315:VAL:HG11	1.95	0.46
1:A:418:LYS:HD2	1:A:418:LYS:H	1.81	0.46
1:A:350:ASP:HB3	1:A:353:THR:OG1	2.16	0.46
1:A:210:ARG:HD3	1:A:538:TRP:CZ2	2.51	0.45
1:A:214:GLU:OE2	1:A:545:PRO:HA	2.16	0.45
1:A:333:ARG:NH2	3:A:631:CL:CL	2.86	0.45
1:A:309:GLU:HA	1:A:324:HIS:HB3	1.99	0.45
1:A:435:HIS:HD2	1:A:436:LEU:O	1.99	0.45
1:A:218:ASN:HB2	1:A:220:MET:HE3	1.98	0.45
1:A:310:SER:HB3	1:A:322:ASN:OD1	2.16	0.45
1:A:175:HIS:O	1:A:179:VAL:HG23	2.16	0.45
1:A:185:ASN:OD1	1:A:187:LYS:HG2	2.16	0.44
1:A:548:ASN:HD22	1:A:551:GLY:H	1.66	0.44
1:A:464:ALA:HB1	1:A:479:LEU:HD22	1.99	0.44
1:A:94:GLU:O	1:A:98:LEU:HG	2.17	0.44
1:A:172:HIS:HE1	1:A:203:MET:SD	2.41	0.43
1:A:491:THR:HG21	1:A:500:VAL:HG13	2.00	0.43
1:A:293:LYS:HB2	1:A:293:LYS:HE3	1.85	0.43
1:A:541:HIS:CD2	1:A:542:LEU:HD13	2.53	0.43
1:A:555:HIS:HE1	4:A:701:HOH:O	2.01	0.43
1:A:13:PHE:HB2	1:A:109:PRO:HG3	2.00	0.43
1:A:565:LYS:O	1:A:593:LYS:HE2	2.18	0.43
1:A:309:GLU:O	1:A:310:SER:HB3	2.19	0.43
1:A:461:ILE:HG12	1:A:558:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLU:OE1	1:A:517:PHE:HB2	2.20	0.42
1:A:152:ASN:O	1:A:154:LEU:HD22	2.20	0.42
1:A:309:GLU:O	4:A:679:HOH:O	2.21	0.42
1:A:347:VAL:HG12	1:A:357:ASP:HB2	2.02	0.42
1:A:227:ASN:HD22	1:A:227:ASN:H	1.68	0.42
1:A:365:ARG:HA	1:A:365:ARG:HD3	1.75	0.42
1:A:178:LEU:HA	1:A:178:LEU:HD23	1.82	0.42
1:A:229:PHE:N	1:A:229:PHE:CD1	2.88	0.42
1:A:86:GLU:H	1:A:86:GLU:CD	2.28	0.41
1:A:533:TYR:H	1:A:533:TYR:HD1	1.68	0.41
1:A:95:VAL:HG23	1:A:178:LEU:HD22	2.02	0.41
1:A:326:TRP:CE3	1:A:326:TRP:HA	2.56	0.41
1:A:58:ARG:O	1:A:62:GLU:HG3	2.21	0.41
1:A:231:GLU:HA	1:A:232:PRO:HD3	1.87	0.40
1:A:408:THR:HA	1:A:437:ASP:O	2.22	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	578/628 (92%)	556 (96%)	15 (3%)	7 (1%)	10 13

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	533	TYR
1	A	19	ALA
1	A	532	GLU
1	A	245	SER
1	A	310	SER
1	A	389	PRO

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Mol	Chain	Res	Type
1	A	591	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	504/558 (90%)	484 (96%)	20 (4%)	28	42

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	41	GLN
1	A	55	GLU
1	A	61	TYR
1	A	192	LYS
1	A	199	LEU
1	A	227	ASN
1	A	263	ASP
1	A	278	ASP
1	A	285	VAL
1	A	347	VAL
1	A	389	PRO
1	A	411	ARG
1	A	510	THR
1	A	517	PHE
1	A	532	GLU
1	A	548	ASN
1	A	580	VAL
1	A	599	PRO
1	A	609	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	41	GLN
1	A	59	HIS
1	A	172	HIS
1	A	218	ASN
1	A	227	ASN
1	A	316	ASN
1	A	317	HIS
1	A	407	HIS
1	A	419	HIS
1	A	422	ASN
1	A	435	HIS
1	A	438	HIS
1	A	446	ASN
1	A	448	GLN
1	A	513	HIS
1	A	548	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, 3 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	20:THR	C	21:VAL	N	15.45
1	A	130:LYS	C	131:LYS	N	11.03

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	590/628 (93%)	-0.03	22 (3%) 45 46	8, 27, 55, 77	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	147	VAL	5.8
1	A	531	SER	4.9
1	A	416	GLU	3.8
1	A	423	PRO	3.8
1	A	2	LEU	3.7
1	A	424	GLY	3.6
1	A	19	ALA	3.4
1	A	421	ILE	3.3
1	A	575	ALA	3.1
1	A	3	HIS	3.1
1	A	244	ALA	2.9
1	A	146	ASP	2.9
1	A	1	THR	2.7
1	A	21	VAL	2.6
1	A	151	GLY	2.6
1	A	390	ASP	2.6
1	A	532	GLU	2.5
1	A	382	ASP	2.3
1	A	154	LEU	2.1
1	A	521	LEU	2.1
1	A	152	ASN	2.0
1	A	266	ILE	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($\text{\AA}^2$)	Q<0.9
2	CU	A	629	1/1	0.99	0.03	25,25,25,25	0
2	CU	A	630	1/1	0.99	0.02	24,24,24,24	0
3	CL	A	631	1/1	0.99	0.06	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.