



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:23 PM GMT

PDB ID : 1OSP
Title : CRYSTAL STRUCTURE OF OUTER SURFACE PROTEIN A OF BORRELIA BURGDORFERI COMPLEXED WITH A MURINE MONOCLONAL ANTIBODY FAB
Authors : Li, H.; Lawson, C.L.
Deposited on : 1996-11-23
Resolution : 1.95 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

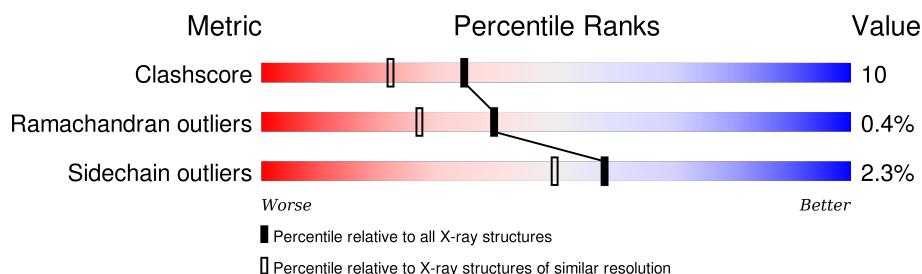
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	214	 77% 22% •
2	H	218	 70% 26% •
3	O	257	 83% 14% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7418 atoms, of which 1881 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 FAB 184.1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	L	214	Total	C	H	N	O	S	29	0	0
			2057	1036	392	278	344	7			

- Molecule 2 is a protein called FAB 184.1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	218	Total	C	H	N	O	S	49	0	0
			2015	1048	364	264	332	7			

- Molecule 3 is a protein called OUTER SURFACE PROTEIN A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	O	251	Total	C	H	N	O	S	0	0	0
			2362	1170	469	313	408	2			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	17	ALA	CYS	CONFLICT	UNP P14013
O	39	LYS	ASN	VARIANT	UNP P14013
O	84	CYS	SER	ENGINEERED	UNP P14013
O	149	GLY	GLU	VARIANT	UNP P14013
O	164	GLY	SER	VARIANT	UNP P14013

- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	99	Total	H	O	0	0
			297	198	99		
4	L	119	Total	H	O	0	0
			357	238	119		

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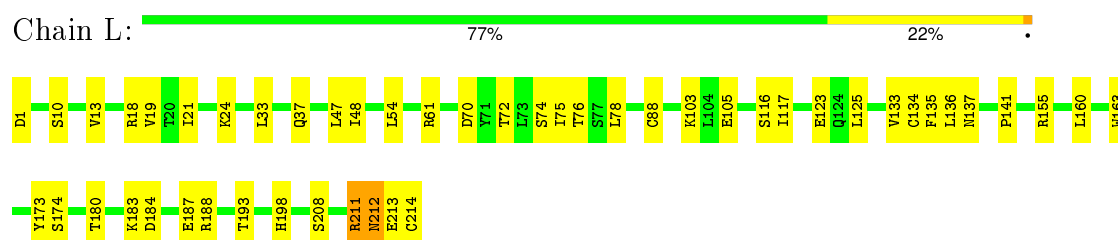
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	O	110	Total	H	O	0	0
			330	220	110		

3 Residue-property plots

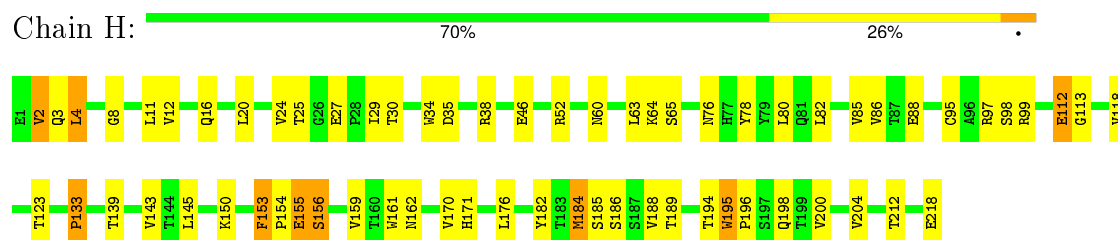
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

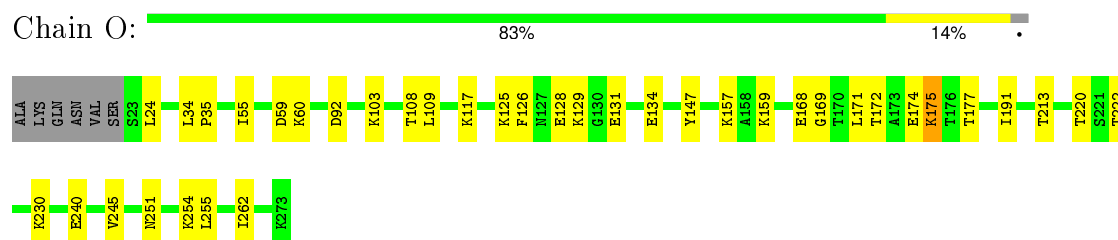
- Molecule 1: FAB 184.1



- Molecule 2: FAB 184.1



- Molecule 3: OUTER SURFACE PROTEIN A



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.10 Å 91.70 Å 100.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 1.95	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-1.95)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.229 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7418	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	L	0.62	3/1704 (0.2%)	0.78	3/2315 (0.1%)
2	H	0.56	1/1698 (0.1%)	0.88	4/2323 (0.2%)
3	O	0.37	0/1902	0.66	0/2550
All	All	0.52	4/5304 (0.1%)	0.78	7/7188 (0.1%)

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	L	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	133	PRO	C-N	14.55	1.59	1.33
1	L	213	GLU	C-N	14.54	1.67	1.34
1	L	211	ARG	C-N	-8.24	1.15	1.34
1	L	212	ASN	C-N	-7.93	1.15	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	133	PRO	O-C-N	15.69	149.87	123.20
2	H	133	PRO	CA-C-N	-13.59	89.02	116.20
1	L	211	ARG	O-C-N	-10.91	105.24	122.70
2	H	4	LEU	CA-CB-CG	6.27	129.73	115.30
2	H	133	PRO	C-N-CA	-6.15	109.39	122.30
1	L	211	ARG	CA-C-N	5.73	129.81	117.20
1	L	212	ASN	O-C-N	-5.28	114.25	122.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	211	ARG	Mainchain
1	L	212	ASN	Mainchain

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	L	1665	392	1589	32	3
2	H	1651	364	1598	49	0
3	O	1893	469	1965	21	6
4	H	99	198	0	2	1
4	L	119	238	0	2	6
4	O	110	220	0	1	0
All	All	5537	1881	5152	98	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 10.

All (98) 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)
2:H:170:VAL:HG22	2:H:188:VAL:HG22	1.39	1.04
3:O:159:LYS:HG2	3:O:168:GLU:HG2	1.53	0.88
1:L:18:ARG:NH2	1:L:76:THR:HG22	1.93	0.84
2:H:2:VAL:HG13	2:H:27:GLU:HB3	1.59	0.84
3:O:24:LEU:HG	3:O:55:ILE:HD12	1.62	0.80
2:H:195:TRP:HZ2	2:H:218:GLU:HB2	1.52	0.74
3:O:220:THR:OG1	3:O:222:THR:HG22	1.87	0.73
1:L:61:ARG:HG3	1:L:75:ILE:HG23	1.69	0.71
1:L:13:VAL:HB	1:L:78:LEU:HD22	1.71	0.70
2:H:24:VAL:HG11	2:H:29:ILE:CG2	2.24	0.67
3:O:129:LYS:NZ	3:O:131:GLU:HB2	2.11	0.66
2:H:20:LEU:HD12	2:H:80:LEU:HD23	1.78	0.66
2:H:195:TRP:CZ2	2:H:218:GLU:HB2	2.32	0.64
3:O:174:GLU:HG3	3:O:175:LYS:HD3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:24:VAL:HG11	2:H:29:ILE:HG23	1.81	0.63
2:H:3:GLN:HB2	2:H:25:THR:OG1	2.00	0.62
1:L:160:LEU:HD11	2:H:176:LEU:HB2	1.81	0.61
2:H:97:ARG:HD2	2:H:98:SER:O	2.03	0.58
1:L:18:ARG:HH12	1:L:74:SER:HB3	1.69	0.58
2:H:65:SER:HB2	2:H:82:LEU:HD11	1.85	0.58
2:H:8:GLY:HA3	2:H:20:LEU:HD23	1.86	0.57
3:O:169:GLY:HA3	3:O:177:THR:O	2.05	0.57
1:L:141:PRO:O	1:L:198:HIS:HE1	1.89	0.56
1:L:117:ILE:HG13	1:L:134:CYS:SG	2.46	0.56
1:L:193:THR:OG1	1:L:208:SER:HB3	2.05	0.55
3:O:129:LYS:HZ2	3:O:131:GLU:HB2	1.71	0.55
2:H:195:TRP:HB3	2:H:196:PRO:HD3	1.89	0.55
2:H:2:VAL:CG1	2:H:27:GLU:HB3	2.34	0.54
3:O:157:LYS:HE2	3:O:159:LYS:HE3	1.89	0.54
3:O:254:LYS:HG2	3:O:255:LEU:N	2.23	0.54
1:L:116:SER:O	1:L:134:CYS:HA	2.09	0.53
2:H:24:VAL:HG13	2:H:76:ASN:ND2	2.23	0.53
1:L:105:GLU:HG3	1:L:173:TYR:OH	2.09	0.53
1:L:125:LEU:HD22	1:L:183:LYS:HG3	1.91	0.53
2:H:161:TRP:CG	2:H:188:VAL:HG21	2.44	0.53
1:L:180:THR:HG21	2:H:150:LYS:NZ	2.24	0.52
2:H:162:ASN:O	2:H:200:VAL:HA	2.10	0.51
1:L:13:VAL:HG11	1:L:19:VAL:HG22	1.92	0.51
3:O:109:LEU:HD13	3:O:126:PHE:CZ	2.45	0.51
2:H:2:VAL:HG13	2:H:27:GLU:CB	2.37	0.51
2:H:159:VAL:HG23	2:H:184:MET:HE1	1.93	0.50
2:H:123:THR:HG23	2:H:154:PRO:HG2	1.93	0.50
2:H:194:THR:O	2:H:198:GLN:HB2	2.12	0.50
1:L:37:GLN:HB2	1:L:47:LEU:HD12	1.94	0.49
2:H:204:VAL:O	2:H:212:THR:HA	2.12	0.49
2:H:34:TRP:CH2	2:H:97:ARG:HG3	2.47	0.49
2:H:133:PRO:HD3	2:H:145:LEU:HD23	1.93	0.49
1:L:21:ILE:O	1:L:72:THR:HA	2.12	0.49
1:L:1:ASP:HA	4:L:278:HOH:O	2.13	0.49
2:H:161:TRP:CE2	2:H:188:VAL:HG23	2.48	0.49
3:O:172:THR:OG1	3:O:174:GLU:HG2	2.13	0.48
3:O:103:LYS:HD2	3:O:108:THR:HB	1.96	0.48
1:L:180:THR:HG21	2:H:150:LYS:HZ3	1.79	0.48
1:L:123:GLU:HB2	4:L:330:HOH:O	2.13	0.47
2:H:11:LEU:HD22	2:H:154:PRO:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:86:VAL:HG23	2:H:88:GLU:H	1.80	0.46
2:H:12:VAL:O	2:H:118:VAL:HA	2.15	0.46
2:H:60:ASN:HB3	2:H:63:LEU:HG	1.97	0.46
2:H:156:SER:HA	4:H:262:HOH:O	2.16	0.46
2:H:112:GLU:HG2	2:H:113:GLY:N	2.30	0.46
1:L:19:VAL:HG21	1:L:78:LEU:HD13	1.98	0.46
1:L:137:ASN:HD22	1:L:174:SER:HB3	1.81	0.46
3:O:129:LYS:HZ1	3:O:131:GLU:HB2	1.81	0.45
1:L:125:LEU:O	1:L:183:LYS:HD2	2.16	0.45
2:H:161:TRP:CD2	2:H:188:VAL:HG21	2.52	0.45
3:O:125:LYS:HB3	3:O:134:GLU:HB2	1.98	0.45
2:H:38:ARG:HD3	2:H:46:GLU:OE1	2.16	0.45
3:O:175:LYS:HB2	3:O:191:ILE:O	2.17	0.45
1:L:48:ILE:HG12	1:L:54:LEU:HD23	1.99	0.45
2:H:155:GLU:O	2:H:156:SER:HB2	2.17	0.45
1:L:18:ARG:HG3	1:L:18:ARG:NH1	2.33	0.44
3:O:240:GLU:HA	4:O:366:HOH:O	2.17	0.44
1:L:33:LEU:HD11	1:L:88:CYS:HB2	1.98	0.44
2:H:82:LEU:HG	2:H:85:VAL:HG12	1.99	0.44
2:H:16:GLN:O	2:H:85:VAL:HG22	2.18	0.44
2:H:184:MET:HG2	2:H:185:SER:N	2.33	0.43
1:L:183:LYS:O	1:L:187:GLU:HG3	2.18	0.43
2:H:133:PRO:HG3	4:H:281:HOH:O	2.18	0.43
1:L:18:ARG:HG3	1:L:18:ARG:HH11	1.83	0.43
2:H:153:PHE:O	2:H:182:TYR:CD2	2.72	0.43
2:H:99:ARG:NH2	3:O:92:ASP:OD2	2.51	0.43
2:H:171:HIS:O	2:H:186:SER:HA	2.19	0.43
2:H:78:TYR:OH	2:H:95:CYS:HB2	2.19	0.43
1:L:10:SER:HA	1:L:103:LYS:O	2.19	0.43
3:O:34:LEU:HB3	3:O:35:PRO:HD2	2.01	0.42
2:H:12:VAL:HG13	2:H:118:VAL:HG22	2.01	0.42
1:L:155:ARG:HH11	1:L:155:ARG:HG3	1.84	0.42
1:L:184:ASP:O	1:L:188:ARG:HG3	2.19	0.42
3:O:59:ASP:O	3:O:60:LYS:HB2	2.19	0.42
2:H:64:LYS:NZ	2:H:86:VAL:HG21	2.35	0.42
3:O:245:VAL:HG21	3:O:262:ILE:HD11	2.02	0.42
2:H:153:PHE:O	2:H:182:TYR:HD2	2.04	0.41
1:L:24:LYS:HG2	1:L:70:ASP:CG	2.41	0.41
1:L:135:PHE:C	1:L:136:LEU:HD12	2.40	0.41
2:H:170:VAL:HG22	2:H:188:VAL:CG2	2.30	0.41
2:H:143:VAL:O	2:H:189:THR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:133:VAL:HG12	1:L:134:CYS:N	2.36	0.40
3:O:147:TYR:CD1	3:O:171:LEU:HD22	2.56	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)
3:O:230:LYS:HZ3	4:L:275:HOH:H1[3_446]	0.65	0.95
3:O:254:LYS:HZ1	4:L:258:HOH:H2[3_446]	0.66	0.94
1:L:188:ARG:HH12	4:L:281:HOH:H1[4_456]	1.09	0.51
1:L:61:ARG:HH22	4:H:306:HOH:H1[4_556]	1.14	0.46
3:O:254:LYS:HZ1	4:L:258:HOH:O[3_446]	1.27	0.33
3:O:230:LYS:HZ3	4:L:275:HOH:O[3_446]	1.55	0.05
1:L:163:TRP:H	3:O:251:ASN:OD1[3_456]	1.57	0.03
3:O:254:LYS:NZ	4:L:258:HOH:O[3_446]	2.17	0.03

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	L	212/214 (99%)	201 (95%)	11 (5%)	0	100	100
2	H	216/218 (99%)	204 (94%)	9 (4%)	3 (1%)	14	4
3	O	249/257 (97%)	245 (98%)	4 (2%)	0	100	100
All	All	677/689 (98%)	650 (96%)	24 (4%)	3 (0%)	39	27

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	153	PHE
2	H	156	SER
2	H	195	TRP

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	L	192/192 (100%)	191 (100%)	1 (0%)	92	91
2	H	190/190 (100%)	181 (95%)	9 (5%)	32	16
3	O	220/225 (98%)	216 (98%)	4 (2%)	66	60
All	All	602/607 (99%)	588 (98%)	14 (2%)	58	50

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	214	CYS
2	H	2	VAL
2	H	4	LEU
2	H	30	THR
2	H	35	ASP
2	H	52	ARG
2	H	112	GLU
2	H	139	THR
2	H	155	GLU
2	H	184	MET
3	O	117	LYS
3	O	128	GLU
3	O	175	LYS
3	O	213	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	137	ASN
1	L	198	HIS
2	H	43	ASN
2	H	171	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.