



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:33 PM GMT

PDB ID : 1PLG  
Title : EVIDENCE FOR THE EXTENDED HELICAL NATURE OF POLYSACCHARIDE EPITOPES. THE 2.8 ANGSTROMS RESOLUTION STRUCTURE AND THERMODYNAMICS OF LIGAND BINDING OF AN ANTIGEN BINDING FRAGMENT SPECIFIC FOR ALPHA-(2->8)-POLYSIALIC ACID  
Authors : Evans, S.V.; Sigurskjold, B.W.; Jennings, H.J.; Brisson, J.-R.; Tse, W.C.; To, R.; Altman, E.; Frosch, M.; Weisgerber, C.; Kratzin, H.; Klebert, S.; Vaesen, M.; Bitter-Suermann, D.; Rose, D.R.; Young, N.M.; Bundle, D.R.  
Deposited on : 1995-04-24  
Resolution : 2.80 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](mailto: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.

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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

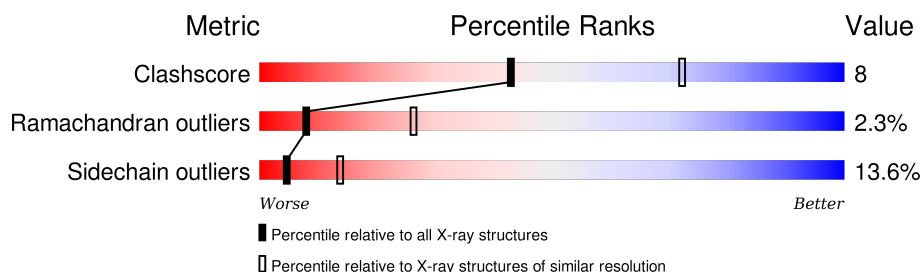
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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  $\geq 3$ , 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	215	
2	H	215	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3325 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 IGG2A=KAPPA=.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	215	Total	C	N	O	S	0	0	0
			1671	1047	283	335	6			

- Molecule 2 is a protein called IGG2A=KAPPA=.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	215	Total	C	N	O	S	0	0	0
			1620	1027	262	324	7			

- Molecule 3 is water.

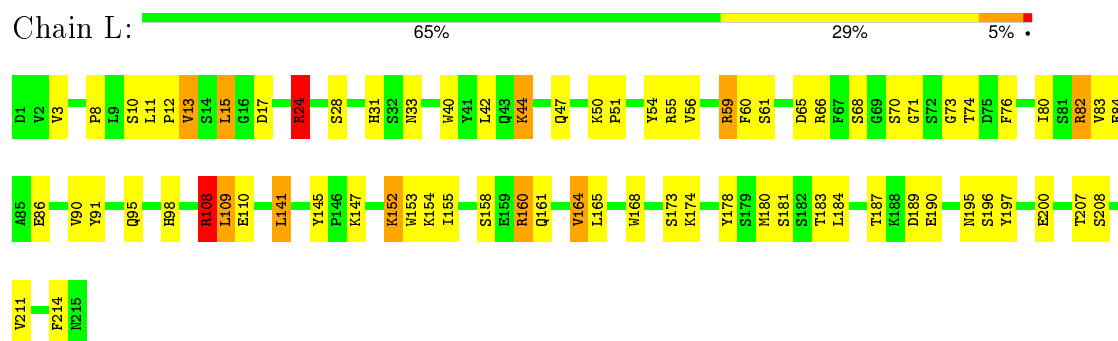
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	22	Total	O	0	0
			22	22		
3	L	12	Total	O	0	0
			12	12		

### 3 Residue-property plots

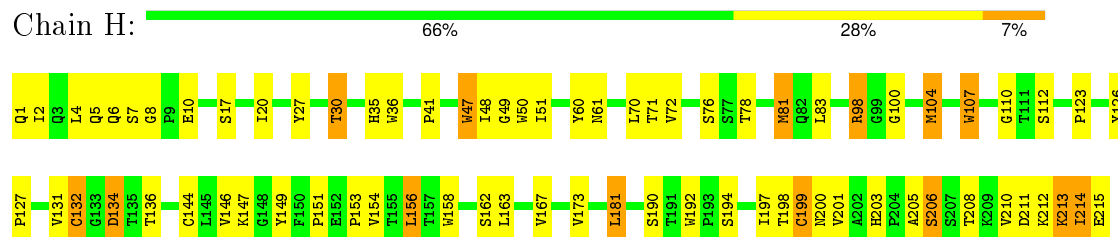
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: IGG2A=KAPPA=



- Molecule 2: IGG2A=KAPPA=



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.14Å 91.21Å 141.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.80)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.164 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3325	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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	0.80	0/1712	1.57	28/2325 (1.2%)
2	H	0.86	0/1663	1.76	41/2269 (1.8%)
All	All	0.83	0/3375	1.67	69/4594 (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	L	0	1

There are no bond length outliers.

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	81	MET	CG-SD-CE	-10.64	83.17	100.20
2	H	27	TYR	CB-CG-CD2	-10.11	114.94	121.00
2	H	36	TRP	CG-CD2-CE3	9.74	142.66	133.90
2	H	192	TRP	CD1-CG-CD2	9.00	113.50	106.30
1	L	153	TRP	CD1-CG-CD2	8.90	113.42	106.30
1	L	40	TRP	CD1-CG-CD2	8.08	112.77	106.30
1	L	160	ARG	NE-CZ-NH1	8.06	124.33	120.30
2	H	47	TRP	CD1-CG-CD2	8.06	112.75	106.30
2	H	36	TRP	CD1-CG-CD2	7.73	112.48	106.30
2	H	36	TRP	CE2-CD2-CG	-7.73	101.12	107.30
2	H	192	TRP	CE2-CD2-CG	-7.71	101.13	107.30
1	L	153	TRP	CE2-CD2-CG	-7.56	101.25	107.30
2	H	47	TRP	CE2-CD2-CG	-7.54	101.27	107.30
1	L	40	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	L	178	TYR	CB-CG-CD1	-7.49	116.51	121.00
2	H	158	TRP	CA-C-N	7.34	133.34	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	50	TRP	CE2-CD2-CG	-7.26	101.49	107.30
2	H	107	TRP	CD1-CG-CD2	7.22	112.08	106.30
1	L	168	TRP	CD1-CG-CD2	7.15	112.02	106.30
1	L	160	ARG	NE-CZ-NH2	-7.11	116.75	120.30
2	H	36	TRP	CB-CG-CD1	-7.07	117.81	127.00
2	H	50	TRP	CB-CG-CD1	-7.07	117.81	127.00
2	H	158	TRP	CD1-CG-CD2	6.98	111.89	106.30
1	L	168	TRP	CE2-CD2-CG	-6.94	101.75	107.30
2	H	107	TRP	CE2-CD2-CG	-6.87	101.80	107.30
1	L	195	ASN	CA-C-N	6.70	131.94	117.20
2	H	158	TRP	CE2-CD2-CG	-6.68	101.95	107.30
1	L	109	LEU	CA-CB-CG	6.63	130.55	115.30
1	L	82	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	L	108	ARG	NE-CZ-NH1	6.56	123.58	120.30
2	H	50	TRP	CD1-CG-CD2	6.55	111.54	106.30
2	H	10	GLU	CA-C-N	6.53	131.57	117.20
1	L	59	ARG	NE-CZ-NH1	6.47	123.53	120.30
2	H	98	ARG	NE-CZ-NH1	6.44	123.52	120.30
2	H	47	TRP	CG-CD2-CE3	6.41	139.67	133.90
2	H	83	LEU	CA-CB-CG	6.37	129.95	115.30
2	H	50	TRP	CG-CD2-CE3	6.36	139.62	133.90
1	L	95	GLN	CA-CB-CG	6.30	127.26	113.40
2	H	136	THR	N-CA-CB	-6.27	98.38	110.30
1	L	24	ARG	NE-CZ-NH1	6.22	123.41	120.30
2	H	47	TRP	CB-CG-CD1	-6.17	118.98	127.00
1	L	141	LEU	CA-CB-CG	6.01	129.11	115.30
2	H	192	TRP	CG-CD1-NE1	-5.97	104.13	110.10
2	H	210	VAL	CG1-CB-CG2	-5.91	101.44	110.90
2	H	158	TRP	CG-CD2-CE3	5.87	139.18	133.90
2	H	30	THR	N-CA-CB	-5.85	99.18	110.30
1	L	153	TRP	CG-CD1-NE1	-5.74	104.36	110.10
1	L	197	TYR	CB-CG-CD2	-5.72	117.57	121.00
1	L	82	ARG	NE-CZ-NH2	-5.68	117.46	120.30
2	H	27	TYR	CB-CG-CD1	5.56	124.34	121.00
1	L	147	LYS	CA-CB-CG	5.55	125.61	113.40
2	H	136	THR	N-CA-C	5.48	125.80	111.00
2	H	208	THR	N-CA-C	5.45	125.72	111.00
1	L	145	TYR	CB-CG-CD2	-5.43	117.74	121.00
2	H	36	TRP	CG-CD1-NE1	-5.43	104.67	110.10
1	L	80	ILE	N-CA-C	-5.41	96.39	111.00
1	L	55	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	L	66	ARG	CA-CB-CG	5.36	125.19	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	3	VAL	CA-CB-CG2	-5.30	102.95	110.90
2	H	158	TRP	O-C-N	-5.26	114.28	122.70
2	H	131	VAL	CA-C-N	5.24	128.72	117.20
2	H	158	TRP	CA-CB-CG	-5.24	103.75	113.70
2	H	4	LEU	CA-CB-CG	5.23	127.33	115.30
2	H	136	THR	CA-C-N	-5.22	105.76	116.20
1	L	195	ASN	CA-C-O	-5.12	109.36	120.10
1	L	40	TRP	CG-CD2-CE3	5.05	138.45	133.90
2	H	107	TRP	CG-CD2-CE3	5.03	138.43	133.90
2	H	104	MET	CA-CB-CG	5.01	121.82	113.30
2	H	158	TRP	CB-CG-CD1	-5.01	120.49	127.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	44	LYS	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	L	1671	0	1605	29	0
2	H	1620	0	1576	25	0
3	H	22	0	0	0	0
3	L	12	0	0	0	0
All	All	3325	0	3181	53	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 8.

All (53) 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:L:50:LYS:HD2	1:L:51:PRO:HD2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:51:ILE:HD13	2:H:72:VAL:HG13	1.73	0.70
1:L:160:ARG:HD3	1:L:184:LEU:HD11	1.76	0.67
2:H:35:HIS:HD2	2:H:47:TRP:HE1	1.44	0.65
2:H:8:GLY:HA3	2:H:20:ILE:HG22	1.78	0.64
1:L:71:GLY:HA3	1:L:76:PHE:HA	1.81	0.63
1:L:155:ILE:HD11	1:L:160:ARG:HH11	1.64	0.62
2:H:6:GLN:NE2	2:H:110:GLY:H	1.99	0.59
2:H:35:HIS:HE1	2:H:100:GLY:O	1.86	0.58
2:H:123:PRO:HB3	2:H:149:TYR:HB3	1.87	0.57
2:H:212:LYS:HE3	2:H:214:ILE:HG23	1.88	0.56
2:H:151:PRO:O	2:H:203:HIS:HE1	1.87	0.56
1:L:155:ILE:HD11	1:L:160:ARG:NH1	2.20	0.55
1:L:31:HIS:HD2	1:L:33:ASN:H	1.54	0.55
2:H:8:GLY:HA3	2:H:20:ILE:HA	1.88	0.55
1:L:28:SER:O	1:L:98:HIS:HE1	1.91	0.54
1:L:165:LEU:HD21	2:H:173:VAL:HB	1.90	0.54
1:L:200:GLU:HB3	1:L:211:VAL:HG22	1.90	0.53
1:L:42:LEU:HD22	1:L:44:LYS:HG3	1.91	0.53
2:H:48:ILE:HG21	2:H:81:MET:HE1	1.91	0.51
1:L:17:ASP:O	1:L:83:VAL:HG13	2.10	0.51
1:L:90:VAL:HG22	1:L:108:ARG:HG3	1.92	0.50
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.47	0.50
2:H:214:ILE:O	2:H:215:GLU:HB2	2.11	0.49
1:L:164:VAL:HA	1:L:183:THR:O	2.12	0.49
1:L:24:ARG:HA	1:L:74:THR:O	2.12	0.48
1:L:152:LYS:NZ	1:L:152:LYS:HB3	2.27	0.48
1:L:154:LYS:HA	1:L:158:SER:O	2.14	0.48
2:H:199:CYS:HB3	2:H:213:LYS:NZ	2.28	0.48
1:L:13:VAL:HG22	1:L:17:ASP:HB2	1.95	0.47
2:H:197:ILE:O	2:H:212:LYS:HG2	2.16	0.46
2:H:156:LEU:HD22	2:H:201:VAL:HG22	1.97	0.46
1:L:8:PRO:HG3	1:L:11:LEU:HD13	1.97	0.46
2:H:199:CYS:HB3	2:H:213:LYS:HZ2	1.81	0.45
1:L:12:PRO:HA	1:L:110:GLU:O	2.17	0.45
1:L:155:ILE:HD13	1:L:155:ILE:HG21	1.72	0.44
2:H:154:VAL:HG21	2:H:181:LEU:HD22	2.00	0.44
1:L:91:TYR:CE2	1:L:109:LEU:HG	2.52	0.44
1:L:15:LEU:HA	1:L:83:VAL:HG23	1.99	0.44
2:H:60:TYR:CE1	2:H:70:LEU:HG	2.53	0.44
2:H:48:ILE:HG21	2:H:81:MET:CE	2.48	0.44
1:L:13:VAL:HG13	1:L:83:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:196:SER:HA	1:L:214:PHE:O	2.19	0.43
2:H:126:TYR:HA	2:H:127:PRO:HD3	1.79	0.43
1:L:90:VAL:HG22	1:L:108:ARG:CG	2.49	0.43
1:L:42:LEU:HG	1:L:91:TYR:CE1	2.54	0.42
2:H:70:LEU:HD21	2:H:81:MET:HE2	2.01	0.42
2:H:107:TRP:N	2:H:107:TRP:CD1	2.89	0.41
1:L:54:TYR:HB3	1:L:60:PHE:CE1	2.55	0.41
2:H:76:SER:OG	2:H:78:THR:HG22	2.20	0.40
1:L:180:MET:HG2	1:L:181:SER:N	2.36	0.40
2:H:198:THR:HG22	2:H:200:ASN:ND2	2.36	0.40
1:L:91:TYR:HE2	1:L:109:LEU:HG	1.86	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	L	213/215 (99%)	201 (94%)	8 (4%)	4 (2%)	10	32
2	H	213/215 (99%)	196 (92%)	11 (5%)	6 (3%)	6	21
All	All	426/430 (99%)	397 (93%)	19 (4%)	10 (2%)	8	26

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	134	ASP
1	L	56	VAL
1	L	190	GLU
2	H	132	CYS
2	H	163	LEU
2	H	206	SER
2	H	7	SER

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Mol	Chain	Res	Type
1	L	61	SER
2	H	205	ALA
1	L	73	GLY

### 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%)	169 (88%)	23 (12%)	6	19
2	H	183/183 (100%)	155 (85%)	28 (15%)	3	10
All	All	375/375 (100%)	324 (86%)	51 (14%)	5	14

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	10	SER
1	L	13	VAL
1	L	15	LEU
1	L	24	ARG
1	L	47	GLN
1	L	59	ARG
1	L	65	ASP
1	L	68	SER
1	L	70	SER
1	L	82	ARG
1	L	84	GLU
1	L	86	GLU
1	L	108	ARG
1	L	141	LEU
1	L	152	LYS
1	L	161	GLN
1	L	164	VAL
1	L	173	SER
1	L	174	LYS
1	L	187	THR

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Mol	Chain	Res	Type
1	L	189	ASP
1	L	207	THR
1	L	208	SER
2	H	1	GLN
2	H	2	ILE
2	H	5	GLN
2	H	17	SER
2	H	30	THR
2	H	41	PRO
2	H	61	ASN
2	H	71	THR
2	H	98	ARG
2	H	104	MET
2	H	112	SER
2	H	132	CYS
2	H	134	ASP
2	H	144	CYS
2	H	146	VAL
2	H	147	LYS
2	H	153	PRO
2	H	156	LEU
2	H	162	SER
2	H	167	VAL
2	H	181	LEU
2	H	190	SER
2	H	194	SER
2	H	199	CYS
2	H	206	SER
2	H	211	ASP
2	H	213	LYS
2	H	214	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	31	HIS
1	L	171	GLN
1	L	215	ASN
2	H	6	GLN
2	H	35	HIS
2	H	61	ASN
2	H	203	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.