



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:21 PM UTC

PDB ID : 1PLG / pdb_00001plg
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
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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

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)	:	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

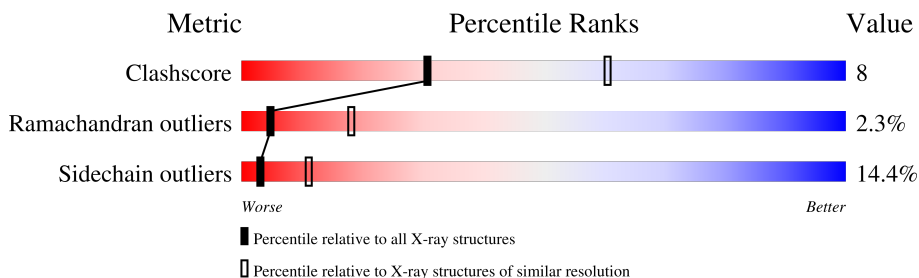
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 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	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	L	12	Total	O	0	0
			12	12		
3	H	22	Total	O	0	0
			22	22		

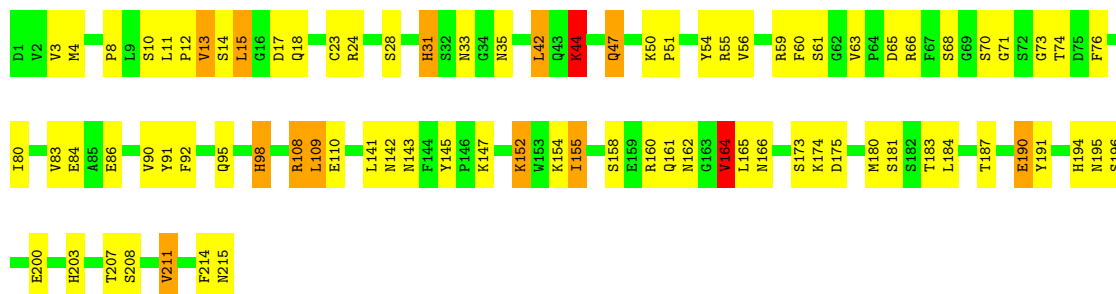
3 Residue-property plots

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.

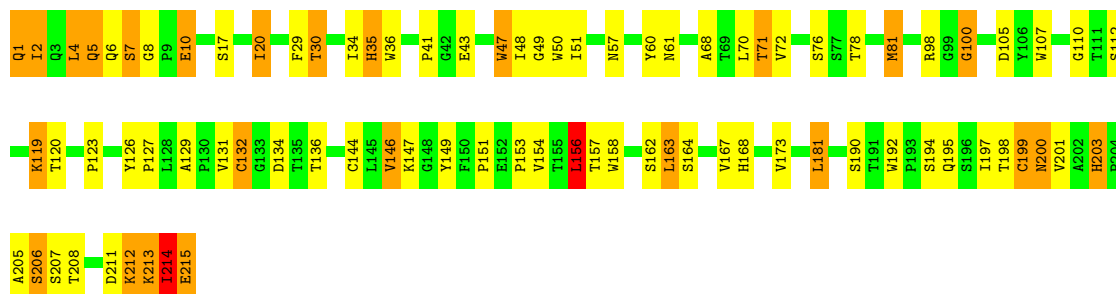
• Molecule 1: IGG2A=KAPPA=

Chain L: 



• Molecule 2: IGG2A=KAPPA=

Chain H: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	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 ²)	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	1.01	6/1712 (0.4%)	1.79	32/2325 (1.4%)
2	H	1.07	5/1663 (0.3%)	1.99	56/2269 (2.5%)
All	All	1.04	11/3375 (0.3%)	1.89	88/4594 (1.9%)

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	203	HIS	CD2-NE2	-7.50	1.29	1.37
2	H	146	VAL	CA-CB	7.11	1.63	1.54
1	L	31	HIS	CD2-NE2	-6.92	1.30	1.37
1	L	98	HIS	CD2-NE2	-6.57	1.30	1.37
2	H	203	HIS	CD2-NE2	-6.53	1.30	1.37
2	H	35	HIS	CD2-NE2	-6.37	1.30	1.37
2	H	168	HIS	CD2-NE2	-6.36	1.30	1.37
1	L	164	VAL	CA-CB	6.34	1.62	1.54
1	L	194	HIS	CD2-NE2	-6.27	1.30	1.37
2	H	2	ILE	CA-CB	5.88	1.61	1.54
1	L	98	HIS	CG-ND1	-5.24	1.32	1.38

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	136	THR	N-CA-C	10.59	125.80	110.24
2	H	208	THR	N-CA-C	9.82	125.72	110.20
1	L	63	VAL	N-CA-C	-8.91	100.97	108.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	36	TRP	CG-CD2-CE3	8.77	142.66	133.90
1	L	143	ASN	N-CA-C	8.54	123.27	111.74
2	H	105	ASP	CA-CB-CG	8.45	121.05	112.60
1	L	80	ILE	N-CA-C	-8.40	96.39	108.48
1	L	175	ASP	CA-CB-CG	8.35	120.95	112.60
2	H	81	MET	CG-SD-CE	-8.06	83.17	100.90
1	L	47	GLN	N-CA-C	7.88	119.61	108.74
1	L	195	ASN	CA-C-O	-7.80	109.36	120.51
2	H	131	VAL	CA-C-O	-7.40	111.53	120.78
2	H	136	THR	N-CA-CB	-7.16	98.38	109.48
2	H	61	ASN	OD1-CG-ND2	-7.01	115.59	122.60
1	L	215	ASN	OD1-CG-ND2	-6.91	115.69	122.60
1	L	203	HIS	CB-CG-CD2	-6.75	122.43	131.20
1	L	142	ASN	OD1-CG-ND2	-6.70	115.90	122.60
2	H	200	ASN	OD1-CG-ND2	-6.69	115.91	122.60
2	H	119	LYS	N-CA-C	-6.68	100.32	110.14
1	L	145	TYR	O-C-N	-6.66	115.27	122.06
1	L	95	GLN	CA-CB-CG	6.58	127.26	114.10
2	H	30	THR	N-CA-CB	-6.55	99.18	110.32
2	H	203	HIS	CB-CG-CD2	-6.53	122.71	131.20
2	H	207	SER	CA-C-N	6.41	130.58	121.42
2	H	207	SER	C-N-CA	6.41	130.58	121.42
2	H	100	GLY	N-CA-C	-6.33	103.89	112.57
1	L	166	ASN	OD1-CG-ND2	-6.30	116.30	122.60
2	H	10	GLU	N-CA-CB	-6.28	102.24	110.59
1	L	92	PHE	CA-CB-CG	6.25	120.05	113.80
2	H	158	TRP	O-C-N	-6.25	114.28	122.59
1	L	194	HIS	CB-CG-CD2	-6.25	123.08	131.20
1	L	35	ASN	CA-CB-CG	6.23	118.83	112.60
2	H	195	GLN	OE1-CD-NE2	-6.21	116.39	122.60
2	H	4	LEU	N-CA-C	-6.12	97.74	108.20
2	H	136	THR	CA-C-O	6.09	127.60	120.96
2	H	36	TRP	CB-CG-CD1	-6.06	117.81	126.90
2	H	50	TRP	CB-CG-CD1	-6.06	117.81	126.90
2	H	57	ASN	OD1-CG-ND2	-5.96	116.64	122.60
1	L	215	ASN	CA-CB-CG	5.94	118.54	112.60
2	H	43	GLU	N-CA-C	5.93	117.23	108.86
2	H	158	TRP	CA-C-O	-5.86	112.13	120.51
2	H	30	THR	N-CA-C	5.84	119.50	112.38
2	H	136	THR	CA-CB-OG1	-5.82	100.87	109.60
2	H	214	ILE	CA-C-N	5.78	132.11	121.70
2	H	214	ILE	C-N-CA	5.78	132.11	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	18	GLN	N-CA-C	-5.78	101.13	110.32
2	H	47	TRP	CG-CD2-CE3	5.77	139.67	133.90
1	L	147	LYS	CA-CB-CG	5.76	125.61	114.10
1	L	44	LYS	CA-C-N	5.74	125.86	119.32
1	L	44	LYS	C-N-CA	5.74	125.86	119.32
2	H	50	TRP	CG-CD2-CE3	5.72	139.62	133.90
2	H	164	SER	N-CA-C	-5.72	106.85	113.88
2	H	7	SER	CA-CB-OG	5.67	122.44	111.10
1	L	190	GLU	CB-CG-CD	5.65	122.21	112.60
1	L	55	ARG	CA-C-N	5.63	132.11	121.97
1	L	55	ARG	C-N-CA	5.63	132.11	121.97
2	H	71	THR	N-CA-CB	-5.59	101.12	111.52
2	H	195	GLN	CG-CD-NE2	5.58	124.78	116.40
1	L	66	ARG	CA-CB-CG	5.55	125.19	114.10
2	H	30	THR	OG1-CB-CG2	5.51	120.33	109.30
2	H	30	THR	CA-CB-OG1	-5.44	101.44	109.60
2	H	1	GLN	CA-C-O	-5.43	111.57	120.80
2	H	10	GLU	O-C-N	-5.43	115.08	122.36
1	L	191	TYR	N-CA-C	-5.40	105.47	111.36
2	H	203	HIS	CB-CG-ND1	5.40	130.80	122.70
1	L	14	SER	N-CA-C	-5.38	100.93	109.96
2	H	129	ALA	CA-C-N	5.37	125.38	119.90
2	H	129	ALA	C-N-CA	5.37	125.38	119.90
1	L	203	HIS	CB-CG-ND1	5.29	130.63	122.70
2	H	158	TRP	CG-CD2-CE3	5.28	139.18	133.90
2	H	47	TRP	CB-CG-CD1	-5.28	118.98	126.90
1	L	31	HIS	CB-CG-CD2	-5.26	124.36	131.20
2	H	156	LEU	N-CA-C	-5.25	100.34	108.90
2	H	10	GLU	CA-C-O	-5.22	113.34	119.24
2	H	158	TRP	CA-CB-CG	-5.19	103.75	113.60
2	H	29	PHE	CA-CB-CG	5.18	118.98	113.80
1	L	155	ILE	CA-CB-CG1	5.17	119.20	110.40
2	H	120	THR	CA-CB-OG1	-5.17	101.84	109.60
1	L	211	VAL	N-CA-C	5.15	115.00	107.37
2	H	163	LEU	N-CA-C	-5.08	99.98	110.80
1	L	162	ASN	N-CA-C	5.07	118.22	110.20
2	H	36	TRP	CE2-CD2-CG	-5.07	101.12	107.20
2	H	192	TRP	CE2-CD2-CG	-5.06	101.13	107.20
1	L	109	LEU	N-CA-CB	5.05	118.49	110.16
2	H	5	GLN	OE1-CD-NE2	-5.04	117.56	122.60
2	H	7	SER	O-C-N	-5.03	115.90	122.59
2	H	34	ILE	N-CA-C	-5.01	101.16	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	5	GLN	CG-CD-NE2	5.00	123.90	116.40

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 [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	L	1671	0	1605	30	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	54	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 (54) 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
2:H:51:ILE:HD13	2:H:72:VAL:HG13	1.73	0.70
1:L:4:MET:HE3	1:L:23:CYS:SG	2.32	0.68
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:48:ILE:HG21	2:H:81:MET:HE1	1.82	0.61
2:H:6:GLN:NE2	2:H:110:GLY:H	1.99	0.59
2:H:70:LEU:HD21	2:H:81:MET:HE3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:68:ALA:HB1	2:H:81:MET:HE2	1.92	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
1:L:164:VAL:HA	1:L:183:THR:O	2.12	0.49
2:H:214:ILE:O	2:H:215:GLU:HB2	2.11	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
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
1:L:13:VAL:HG13	1:L:83:VAL:HG21	2.00	0.43
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:107:TRP:CD1	2:H:107:TRP:N	2.89	0.41
1:L:54:TYR:HB3	1:L:60:PHE:CE1	2.55	0.41
2:H:48:ILE:HG21	2:H:81:MET:CE	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	6	22
2	H	213/215 (99%)	196 (92%)	11 (5%)	6 (3%)	4	14
All	All	426/430 (99%)	397 (93%)	19 (4%)	10 (2%)	5	18

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
1	L	61	SER
2	H	205	ALA
1	L	73	GLY

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	L	192/192 (100%)	170 (88%)	22 (12%)	5	18
2	H	183/183 (100%)	151 (82%)	32 (18%)	2	7
All	All	375/375 (100%)	321 (86%)	54 (14%)	3	11

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	3	VAL
1	L	10	SER
1	L	13	VAL
1	L	15	LEU
1	L	42	LEU
1	L	47	GLN
1	L	59	ARG
1	L	65	ASP
1	L	68	SER
1	L	70	SER
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
1	L	207	THR
1	L	208	SER
2	H	1	GLN
2	H	2	ILE
2	H	4	LEU
2	H	5	GLN
2	H	10	GLU
2	H	17	SER
2	H	20	ILE
2	H	30	THR
2	H	41	PRO
2	H	71	THR
2	H	98	ARG

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Mol	Chain	Res	Type
2	H	112	SER
2	H	119	LYS
2	H	132	CYS
2	H	144	CYS
2	H	146	VAL
2	H	147	LYS
2	H	153	PRO
2	H	156	LEU
2	H	157	THR
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	212	LYS
2	H	213	LYS
2	H	214	ILE
2	H	215	GLU

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

Mol	Chain	Res	Type
1	L	18	GLN
1	L	31	HIS
1	L	171	GLN
2	H	6	GLN
2	H	35	HIS
2	H	61	ASN
2	H	203	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

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 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.