Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2024 – 02:53 PM EDT

PDB ID : 3HLA
Title : HUMAN CLASS I HISTOCOMPATIBILITY ANTIGEN A2.1
Authors : Saper, M.A.; Bjorkman, P.J.; Wiley, D.C.
Deposited on : 1989-10-06
Resolution : 2.60 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:

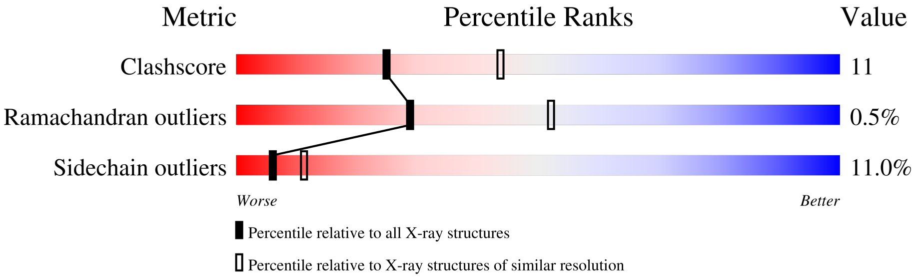
MolProbity : 4.02b-467
Xtriage (Phenix) : NOT EXECUTED
EDS : NOT EXECUTED
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

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 2.60 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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	270	
2	B	99	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3064 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 CLASS I HISTOCOMPATIBILITY ANTIGEN (HLA-A2.1) (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	270	2189	1363	399	418	9	0	0	0

- Molecule 2 is a protein called BETA 2-MICROGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	99	829	528	140	158	3	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	30	30	30	0	0
			Total	O		
3	B	16	16	16	0	0

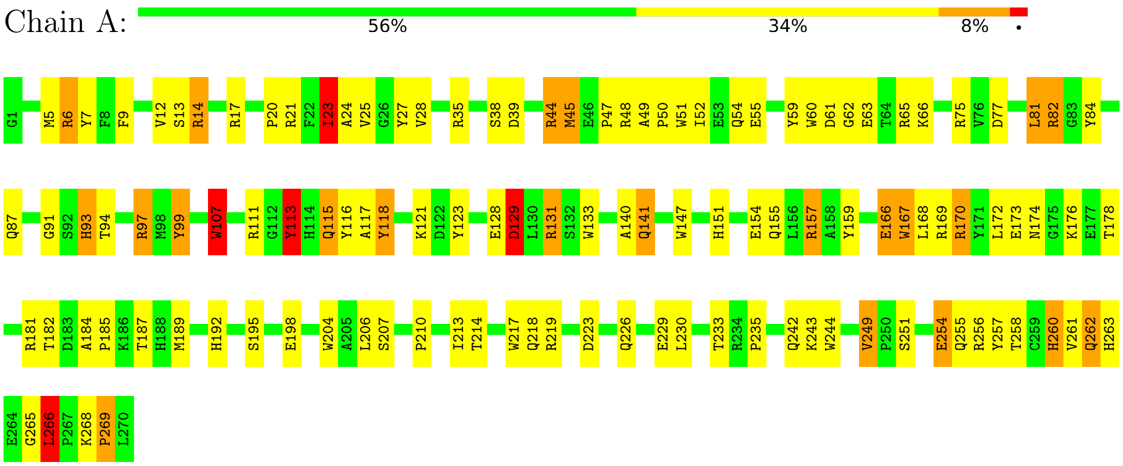
3 Residue-property plots (i)

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. 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.

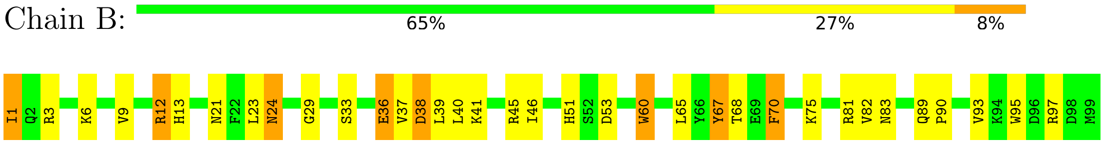
- Molecule 1: CLASS I HISTOCOMPATIBILITY ANTIGEN (HLA-A2.1) (ALPHA CHAIN)

Chain A:



- Molecule 2: BETA 2-MICROGLOBULIN

Chain B:



4 Data and refinement statistics ⓘ

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

Property	**Value**	**Source**
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	60.35Å 80.40Å 56.49Å 90.00° 120.42° 90.00°	Depositor
Resolution (Å)	6.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3064	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	A	1.10	0/2251	1.93	76/3054 (2.5%)
2	B	1.01	0/852	1.70	14/1152 (1.2%)
All	All	1.08	0/3103	1.87	90/4206 (2.1%)

There are no bond length outliers.

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	60	TRP	CD1-CG-CD2	11.09	115.17	106.30
1	A	27	TYR	CB-CG-CD1	-10.82	114.51	121.00
1	A	99	TYR	CB-CG-CD1	-10.82	114.51	121.00
1	A	219	ARG	NE-CZ-NH1	-10.28	115.16	120.30
1	A	97	ARG	NE-CZ-NH2	10.07	125.34	120.30
1	A	133	TRP	CD1-CG-CD2	8.99	113.49	106.30
1	A	75	ARG	NE-CZ-NH2	8.97	124.79	120.30
1	A	60	TRP	CD1-CG-CD2	8.82	113.36	106.30
1	A	217	TRP	CD1-CG-CD2	8.80	113.34	106.30
1	A	244	TRP	CD1-CG-CD2	8.69	113.25	106.30
1	A	21	ARG	NE-CZ-NH2	8.52	124.56	120.30
1	A	113	TYR	CB-CG-CD1	-8.49	115.91	121.00
1	A	35	ARG	NE-CZ-NH1	-8.49	116.06	120.30
1	A	6	ARG	NE-CZ-NH1	-8.38	116.11	120.30
1	A	17	ARG	NE-CZ-NH2	8.10	124.35	120.30
1	A	59	TYR	CB-CG-CD2	-8.08	116.15	121.00
1	A	75	ARG	NE-CZ-NH1	-8.01	116.30	120.30
2	B	60	TRP	CE2-CD2-CG	-7.98	100.92	107.30
1	A	256	ARG	NE-CZ-NH1	-7.94	116.33	120.30
1	A	244	TRP	CE2-CD2-CG	-7.88	101.00	107.30
1	A	51	TRP	CE2-CD2-CG	-7.71	101.13	107.30
2	B	95	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	A	51	TRP	CD1-CG-CD2	7.68	112.45	106.30
2	B	60	TRP	CG-CD1-NE1	-7.62	102.48	110.10
1	A	204	TRP	CD1-CG-CD2	7.54	112.33	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ARG	NE-CZ-NH1	-7.48	116.56	120.30
1	A	269	PRO	N-CA-CB	7.47	112.26	103.30
1	A	14	ARG	NE-CZ-NH1	-7.37	116.61	120.30
1	A	133	TRP	CE2-CD2-CG	-7.30	101.46	107.30
1	A	217	TRP	CE2-CD2-CG	-7.29	101.47	107.30
1	A	39	ASP	CB-CG-OD2	7.29	124.86	118.30
2	B	38	ASP	CA-CB-CG	7.24	129.32	113.40
1	A	157	ARG	NE-CZ-NH1	-7.16	116.72	120.30
1	A	256	ARG	NE-CZ-NH2	7.16	123.88	120.30
1	A	107	TRP	CE2-CD2-CG	-7.10	101.62	107.30
1	A	82	ARG	NE-CZ-NH2	7.08	123.84	120.30
1	A	266	LEU	CA-CB-CG	7.03	131.47	115.30
1	A	167	TRP	CD1-CG-CD2	6.98	111.88	106.30
1	A	60	TRP	CE2-CD2-CG	-6.95	101.74	107.30
2	B	12	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	77	ASP	CB-CG-OD1	6.72	124.35	118.30
1	A	97	ARG	NE-CZ-NH1	-6.68	116.96	120.30
1	A	217	TRP	CG-CD1-NE1	-6.64	103.45	110.10
1	A	244	TRP	CG-CD1-NE1	-6.61	103.49	110.10
1	A	107	TRP	CB-CG-CD1	-6.58	118.45	127.00
1	A	244	TRP	CG-CD2-CE3	6.49	139.74	133.90
1	A	204	TRP	CE2-CD2-CG	-6.43	102.15	107.30
1	A	60	TRP	CG-CD1-NE1	-6.39	103.71	110.10
2	B	89	GLN	CA-CB-CG	6.30	127.26	113.40
2	B	95	TRP	CE2-CD2-CG	-6.30	102.26	107.30
2	B	45	ARG	NE-CZ-NH1	-6.29	117.16	120.30
1	A	131	ARG	NE-CZ-NH1	-6.28	117.16	120.30
1	A	170	ARG	NE-CZ-NH1	-6.24	117.18	120.30
1	A	244	TRP	CB-CG-CD1	-6.21	118.93	127.00
1	A	23	ILE	CG1-CB-CG2	-6.16	97.84	111.40
1	A	27	TYR	CB-CG-CD2	6.16	124.69	121.00
1	A	147	TRP	CD1-CG-CD2	6.14	111.21	106.30
1	A	159	TYR	CB-CG-CD1	6.10	124.66	121.00
1	A	6	ARG	NE-CZ-NH2	5.98	123.29	120.30
2	B	24	ASN	CB-CG-ND2	5.90	130.86	116.70
1	A	111	ARG	CA-CB-CG	5.82	126.20	113.40
1	A	147	TRP	CE2-CD2-CG	-5.81	102.65	107.30
1	A	262	GLN	CA-CB-CG	5.71	125.96	113.40
1	A	244	TRP	CD1-NE1-CE2	5.68	114.11	109.00
2	B	67	TYR	CB-CG-CD1	-5.56	117.66	121.00
1	A	38	SER	CA-CB-OG	-5.55	96.23	111.20
1	A	167	TRP	CE2-CD2-CG	-5.54	102.86	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	PRO	CA-N-CD	-5.47	103.84	111.50
1	A	233	THR	CA-CB-OG1	-5.45	97.55	109.00
1	A	111	ARG	NE-CZ-NH1	-5.43	117.58	120.30
1	A	133	TRP	CG-CD1-NE1	-5.42	104.68	110.10
1	A	107	TRP	CG-CD2-CE3	5.42	138.78	133.90
1	A	25	VAL	CG1-CB-CG2	-5.33	102.38	110.90
1	A	254	GLU	CA-CB-CG	5.32	125.09	113.40
1	A	28	VAL	N-CA-C	-5.28	96.74	111.00
1	A	93	HIS	CA-CB-CG	-5.28	104.62	113.60
2	B	53	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	249	VAL	N-CA-CB	-5.26	99.92	111.50
1	A	118	TYR	CB-CG-CD1	-5.26	117.84	121.00
1	A	107	TRP	NE1-CE2-CZ2	-5.26	124.62	130.40
1	A	181	ARG	O-C-N	5.26	131.11	122.70
1	A	189	MET	CB-CG-SD	-5.22	96.74	112.40
1	A	44	ARG	CA-CB-CG	5.20	124.85	113.40
2	B	97	ARG	CB-CG-CD	-5.18	98.12	111.60
2	B	3	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	A	84	TYR	CB-CG-CD1	-5.13	117.92	121.00
1	A	129	ASP	N-CA-CB	-5.11	101.40	110.60
1	A	260	HIS	CA-CB-CG	-5.04	105.04	113.60
1	A	107	TRP	CA-CB-CG	5.02	123.24	113.70
1	A	7	TYR	CB-CG-CD1	-5.02	117.99	121.00

There are no chirality outliers.

There are no planarity outliers.

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	2189	0	2023	47	0
2	B	829	0	794	18	0
3	A	30	0	0	2	0
3	B	16	0	0	0	0
All	All	3064	0	2817	63	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 11.

All (63) 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:214:THR:HB	1:A:262:GLN:HB2	1.67	0.76
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.68	0.74
1:A:187:THR:HG21	1:A:261:VAL:HG21	1.74	0.70
1:A:218:GLN:HG2	1:A:223:ASP:HA	1.75	0.68
1:A:170:ARG:HH11	1:A:174:ASN:HD21	1.44	0.66
1:A:6:ARG:HD3	1:A:113:TYR:OH	1.97	0.64
1:A:49:ALA:O	1:A:52:ILE:HG22	2.01	0.60
2:B:36:GLU:HG3	2:B:83:ASN:HB3	1.87	0.56
2:B:83:ASN:HB2	2:B:90:PRO:HB3	1.86	0.56
1:A:81:LEU:HD23	1:A:118:TYR:CD1	2.41	0.56
1:A:45:MET:HG2	1:A:63:GLU:HB3	1.88	0.55
1:A:151:HIS:O	1:A:155:GLN:HG2	2.06	0.55
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.88	0.55
1:A:9:PHE:HE1	1:A:99:TYR:CE1	2.25	0.54
1:A:249:VAL:HG22	1:A:257:TYR:CE2	2.43	0.54
1:A:63:GLU:OE2	1:A:66:LYS:NZ	2.43	0.52
1:A:230:LEU:HD11	1:A:243:LYS:HE3	1.92	0.52
1:A:107:TRP:CZ2	1:A:172:LEU:HD13	2.44	0.52
2:B:6:LYS:HE3	2:B:29:GLY:HA3	1.90	0.52
2:B:38:ASP:OD2	2:B:81:ARG:NH2	2.43	0.52
1:A:129:ASP:OD1	1:A:131:ARG:HD2	2.10	0.51
1:A:192:HIS:HB3	3:A:905:HOH:O	2.10	0.51
1:A:82:ARG:HG3	1:A:87:GLN:HB2	1.93	0.51
1:A:167:TRP:CZ3	1:A:170:ARG:HD3	2.46	0.50
1:A:82:ARG:NH1	1:A:91:GLY:O	2.40	0.50
1:A:184:ALA:HB2	1:A:265:GLY:O	2.12	0.50
1:A:206:LEU:HD23	1:A:242:GLN:HB3	1.94	0.49
1:A:185:PRO:HD2	1:A:266:LEU:HD13	1.93	0.49
1:A:12:VAL:HG22	1:A:94:THR:HG23	1.93	0.49
1:A:13:SER:HA	1:A:20:PRO:HB3	1.93	0.48
1:A:6:ARG:NH2	1:A:113:TYR:OH	2.45	0.48
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.48	0.47
1:A:44:ARG:HH12	1:A:61:ASP:CG	2.18	0.46
1:A:182:THR:HG22	1:A:210:PRO:HD3	1.97	0.46
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.51	0.46
1:A:14:ARG:NH1	3:A:926:HOH:O	2.47	0.45
1:A:121:LYS:HE3	1:A:121:LYS:HB2	1.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:LYS:HB2	2:B:46:ILE:HD11	2.00	0.44
1:A:62:GLY:O	1:A:66:LYS:HG3	2.18	0.43
2:B:23:LEU:O	2:B:67:TYR:HA	2.18	0.43
1:A:93:HIS:HB3	1:A:118:TYR:CE1	2.54	0.43
1:A:23:ILE:HG22	1:A:24:ALA:N	2.34	0.42
1:A:206:LEU:CD2	1:A:242:GLN:HB3	2.49	0.42
2:B:12:ARG:HG2	2:B:13:HIS:NE2	2.35	0.42
1:A:218:GLN:HG2	1:A:223:ASP:CA	2.48	0.42
2:B:23:LEU:HD23	2:B:39:LEU:HD22	2.01	0.42
1:A:97:ARG:NH2	1:A:116:TYR:HE1	2.18	0.42
1:A:123:TYR:CZ	1:A:140:ALA:HA	2.55	0.41
1:A:184:ALA:HB1	1:A:266:LEU:HD12	2.02	0.41
2:B:1:ILE:HA	2:B:1:ILE:HD13	1.73	0.41
1:A:166:GLU:OE1	1:A:169:ARG:NH1	2.54	0.41
2:B:36:GLU:H	2:B:36:GLU:HG2	1.74	0.41
1:A:54:GLN:NE2	1:A:174:ASN:HB3	2.36	0.41
1:A:115:GLN:HB2	2:B:60:TRP:HH2	1.86	0.41
1:A:213:ILE:HD12	1:A:263:HIS:HB2	2.03	0.41
2:B:37:VAL:HG13	2:B:82:VAL:HG22	2.03	0.41
2:B:46:ILE:HD13	2:B:46:ILE:HG21	1.74	0.41
1:A:214:THR:HG21	1:A:262:GLN:HE21	1.86	0.40
2:B:9:VAL:HG21	2:B:93:VAL:O	2.21	0.40
1:A:141:GLN:O	1:A:141:GLN:HG3	2.21	0.40
2:B:51:HIS:HA	2:B:65:LEU:O	2.21	0.40
1:A:230:LEU:HD11	1:A:243:LYS:CE	2.52	0.40
1:A:258:THR:HG1	1:A:260:HIS:CE1	2.38	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	268/270 (99%)	250 (93%)	16 (6%)	2 (1%)	22	43
2	B	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
All	All	365/369 (99%)	345 (94%)	18 (5%)	2 (0%)	29	52

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	269	PRO
1	A	268	LYS

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	223/226 (99%)	195 (87%)	28 (13%)	4	8
2	B	94/94 (100%)	87 (93%)	7 (7%)	13	28
All	All	317/320 (99%)	282 (89%)	35 (11%)	6	11

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ILE
1	A	45	MET
1	A	48	ARG
1	A	50	PRO
1	A	55	GLU
1	A	81	LEU
1	A	107	TRP
1	A	113	TYR
1	A	115	GLN
1	A	128	GLU
1	A	129	ASP
1	A	141	GLN
1	A	154	GLU
1	A	157	ARG

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Mol	Chain	Res	Type
1	A	166	GLU
1	A	173	GLU
1	A	176	LYS
1	A	178	THR
1	A	195	SER
1	A	198	GLU
1	A	207	SER
1	A	226	GLN
1	A	229	GLU
1	A	235	PRO
1	A	251	SER
1	A	254	GLU
1	A	255	GLN
1	A	266	LEU
2	B	1	ILE
2	B	33	SER
2	B	36	GLU
2	B	40	LEU
2	B	68	THR
2	B	70	PHE
2	B	75	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	114	HIS
1	A	174	ASN
1	A	262	GLN
1	A	263	HIS
2	B	83	ASN

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.