Full wwPDB X-ray Structure Validation Report (i)

Aug 3, 2023 – 01:55 AM EDT

PDB ID	:	1I5K
Title	:	STRUCTURE AND BINDING DETERMINANTS OF THE RECOMBINANT KRINGLE-2 DOMAIN OF HUMAN PLASMINOGEN TO AN INTERNAL PEPTIDE FROM A GROUP A STREPTOCOCCAL SURFACE PROTEIN
Authors	:	Rios-Steiner, J.L.; Schenone, M.; Mochalkin, I.; Tulinsky, A.; Castellino, F.J.
Deposited on	:	2001-02-27
Resolution	:	2.70 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 (i) 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 (i)) were used in the production of this report:

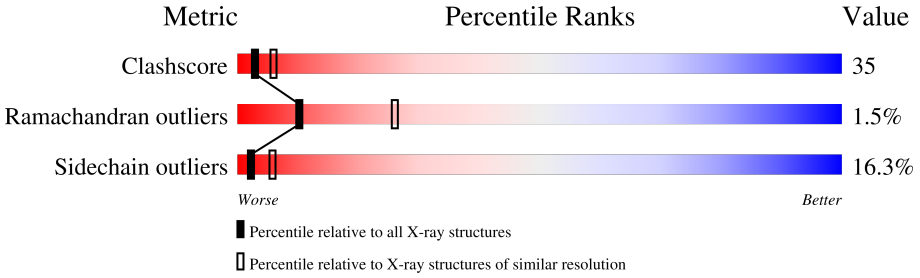
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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	84	35% 52% 5% • 6%
1	B	84	39% 45% 11% 5%
2	C	30	40% 37% 10% 13%
2	D	30	43% 37% • • 13%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1870 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 PLASMINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	79	646	400	118	120	8	0	0	0
1	B	80	651	403	119	121	8	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	PHE	-	cloning artifact	UNP P00747
A	-2	SER	-	cloning artifact	UNP P00747
A	-1	GLU	-	cloning artifact	UNP P00747
A	4	GLY	CYS	engineered mutation	UNP P00747
A	56	ASP	GLU	engineered mutation	UNP P00747
A	72	TYR	LEU	engineered mutation	UNP P00747
A	79	ALA	THR	conflict	UNP P00747
A	80	ALA	THR	conflict	UNP P00747
B	97	PHE	-	cloning artifact	UNP P00747
B	98	SER	-	cloning artifact	UNP P00747
B	99	GLU	-	cloning artifact	UNP P00747
B	104	GLY	CYS	engineered mutation	UNP P00747
B	156	ASP	GLU	engineered mutation	UNP P00747
B	172	TYR	LEU	engineered mutation	UNP P00747
B	179	ALA	THR	conflict	UNP P00747
B	180	ALA	THR	conflict	UNP P00747

- Molecule 2 is a protein called M PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	26	220	133	42	45	0	0	0
2	D	26	220	133	42	45	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	330	TYR	ARG	conflict	UNP P49054
D	430	TYR	ARG	conflict	UNP P49054

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	50	50	50	0	0
			Total	O		
3	B	39	39	39	0	0
			Total	O		
3	C	18	18	18	0	0
			Total	O		
3	D	26	26	26	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.

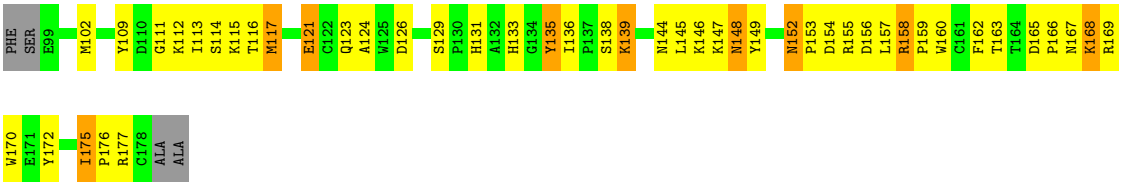
Note EDS was not executed.

• Molecule 1: PLASMINOGEN

Chain A: 35% 52% 5% • 6%

• Molecule 1: PLASMINOGEN

Chain B: 39% 45% 11% 5%



• Molecule 2: M PROTEIN

Chain C: 40% 37% 10% 13%

• Molecule 2: M PROTEIN

Chain D: 43% 37% • • 13%

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	91.98Å 91.98Å 151.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.70	Depositor
% Data completeness (in resolution range)	87.2 (8.00-2.70)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.195 , 0.262	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1870	wwPDB-VP
Average B, all atoms (Å^2)	40.0	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	A	1.16	3/667 (0.4%)	1.15	0/901
1	B	1.07	1/672 (0.1%)	1.11	4/908 (0.4%)
2	C	1.16	0/220	1.11	2/291 (0.7%)
2	D	1.27	1/220 (0.5%)	1.08	0/291
All	All	1.14	5/1779 (0.3%)	1.12	6/2391 (0.3%)

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	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	424	GLU	CG-CD	6.05	1.61	1.51
1	A	46	LYS	CD-CE	5.41	1.64	1.51
1	A	7	GLU	CB-CG	5.38	1.62	1.52
1	B	135	TYR	CE1-CZ	5.25	1.45	1.38
1	A	7	GLU	CG-CD	5.06	1.59	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	155	ARG	NE-CZ-NH1	-6.41	117.10	120.30
2	C	317	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	B	123	GLN	N-CA-C	-5.59	95.90	111.00
2	C	310	LEU	CA-CB-CG	-5.54	102.56	115.30
1	B	177	ARG	N-CA-C	-5.48	96.21	111.00
1	B	177	ARG	C-N-CA	-5.07	109.03	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3	HIS	Sidechain

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	646	0	596	59	0
1	B	651	0	595	46	0
2	C	220	0	221	10	0
2	D	220	0	221	19	0
3	A	50	0	0	1	0
3	B	39	0	0	0	0
3	C	18	0	0	0	1
3	D	26	0	0	1	0
All	All	1870	0	1633	118	1

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 35.

All (118) 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:36:ILE:HG23	2:D:402:GLU:OE1	1.42	1.18
1:A:63:THR:HG22	1:A:65:ASP:H	1.16	1.10
2:D:426:LEU:O	2:D:427:LYS:HB2	1.62	0.96
1:A:63:THR:HG22	1:A:65:ASP:N	1.80	0.96
1:B:157:LEU:O	1:B:158:ARG:HD3	1.64	0.96
1:A:58:ARG:HH11	1:A:58:ARG:HB2	1.32	0.93
1:A:58:ARG:HB2	1:A:58:ARG:NH1	1.86	0.89
1:A:63:THR:CG2	1:A:65:ASP:H	1.90	0.84
1:A:16:THR:HG21	1:A:71:GLU:HB3	1.60	0.83
1:A:63:THR:HB	1:A:68:LYS:O	1.83	0.79
1:A:17:MET:HG2	1:A:72:TYR:O	1.83	0.78
1:A:16:THR:CG2	1:A:71:GLU:HB3	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:HIS:HD2	1:A:35:TYR:H	1.33	0.76
1:A:3:HIS:H	1:A:3:HIS:HD1	1.31	0.76
1:B:158:ARG:HH21	1:B:158:ARG:HG2	1.51	0.76
1:A:16:THR:HG21	1:A:71:GLU:CB	2.17	0.75
2:C:326:LEU:O	2:C:327:LYS:C	2.26	0.74
1:A:9:TYR:OH	1:A:13:ILE:HG12	1.89	0.73
1:A:33:HIS:CD2	1:A:35:TYR:H	2.06	0.72
1:B:115:LYS:HZ1	1:B:121:GLU:HG3	1.55	0.72
1:B:163:THR:HG22	1:B:165:ASP:H	1.55	0.72
1:A:36:ILE:HD12	2:D:402:GLU:OE1	1.91	0.70
2:D:412:ARG:O	2:D:416:GLU:HG3	1.91	0.70
1:B:163:THR:CG2	1:B:165:ASP:H	2.05	0.69
1:B:152:ASN:C	1:B:152:ASN:HD22	1.96	0.68
1:A:30:PRO:HG2	1:A:31:HIS:ND1	2.08	0.68
1:B:133:HIS:CD2	1:B:135:TYR:H	2.11	0.68
2:D:414:LYS:HA	2:D:417:ARG:NH2	2.11	0.66
1:A:63:THR:HG21	1:A:65:ASP:HB3	1.78	0.66
2:D:424:GLU:O	2:D:427:LYS:N	2.28	0.66
2:C:316:GLU:O	2:C:320:GLU:HG3	1.97	0.64
1:B:115:LYS:NZ	1:B:121:GLU:HG3	2.12	0.64
2:C:320:GLU:O	2:C:324:GLU:HG3	1.99	0.63
1:A:20:LEU:HD12	1:A:71:GLU:OE2	1.99	0.62
1:B:109:TYR:CZ	1:B:111:GLY:HA3	2.35	0.61
1:B:133:HIS:HD2	1:B:135:TYR:H	1.46	0.61
1:A:21:GLU:OE2	1:A:21:GLU:HA	1.99	0.61
1:B:163:THR:HB	1:B:168:LYS:O	2.02	0.59
1:A:68:LYS:HE2	1:A:71:GLU:HG3	1.85	0.58
1:B:152:ASN:C	1:B:152:ASN:ND2	2.54	0.58
1:A:48:ASN:HD22	1:A:48:ASN:H	1.51	0.58
1:B:131:HIS:CE1	1:B:169:ARG:HA	2.39	0.57
1:B:144:ASN:HB3	1:B:146:LYS:HE3	1.86	0.57
1:B:152:ASN:HD21	1:B:156:ASP:H	1.54	0.56
1:B:139:LYS:HE3	2:D:409:GLU:OE1	2.07	0.55
1:B:163:THR:HG22	1:B:165:ASP:N	2.21	0.54
1:A:9:TYR:HH	1:A:13:ILE:HG12	1.71	0.54
1:A:63:THR:CG2	1:A:65:ASP:HB3	2.37	0.54
1:B:170:TRP:CD1	2:D:417:ARG:HG2	2.43	0.54
1:A:12:LYS:HG2	1:A:49:TYR:CZ	2.42	0.53
1:B:117:MET:HG2	1:B:172:TYR:O	2.07	0.53
1:A:36:ILE:HD11	2:D:412:ARG:CD	2.39	0.53
1:B:169:ARG:NH1	2:C:319:GLU:OE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:LEU:C	1:B:158:ARG:HD3	2.27	0.53
1:A:30:PRO:HG2	1:A:31:HIS:CE1	2.44	0.52
1:A:16:THR:HB	1:A:71:GLU:OE1	2.09	0.52
1:A:36:ILE:HD11	2:D:412:ARG:HD3	1.91	0.52
2:D:423:LEU:O	2:D:427:LYS:N	2.41	0.52
2:C:314:LYS:HG3	2:C:317:ARG:NH2	2.26	0.51
1:B:115:LYS:NZ	1:B:121:GLU:CG	2.74	0.51
1:A:48:ASN:HD22	1:A:48:ASN:N	2.09	0.51
2:D:418:HIS:O	2:D:422:GLU:HG3	2.11	0.50
1:B:102:MET:HB2	1:B:175:ILE:CG2	2.42	0.50
1:A:9:TYR:CZ	1:A:11:GLY:HA3	2.47	0.50
1:A:40:PHE:HZ	2:C:309:GLU:HG2	1.77	0.50
1:A:54:ASP:OD2	1:A:60:TRP:HZ2	1.95	0.49
1:B:112:LYS:HG2	1:B:149:TYR:CZ	2.48	0.49
1:B:158:ARG:HH21	1:B:158:ARG:CG	2.22	0.49
1:A:0:GLU:N	3:A:580:HOH:O	2.45	0.49
1:A:31:HIS:CE1	1:A:63:THR:O	2.66	0.48
1:B:112:LYS:O	1:B:113:ILE:C	2.52	0.48
1:A:10:ASP:OD2	1:A:44:ASN:ND2	2.47	0.48
1:B:136:ILE:HB	1:B:139:LYS:HG3	1.96	0.48
1:A:40:PHE:CZ	2:C:309:GLU:HG2	2.49	0.47
1:A:5:SER:O	1:A:59:PRO:HD3	2.15	0.47
1:A:0:GLU:HA	1:A:0:GLU:OE2	2.12	0.47
1:B:117:MET:CG	1:B:172:TYR:O	2.63	0.47
1:B:116:THR:O	1:B:117:MET:C	2.52	0.47
1:B:152:ASN:ND2	1:B:152:ASN:O	2.47	0.46
1:A:44:ASN:C	1:A:46:LYS:N	2.68	0.46
1:A:16:THR:HG21	1:A:71:GLU:HB2	1.95	0.46
1:A:27:SER:O	1:A:33:HIS:HE1	1.98	0.46
1:B:165:ASP:OD1	1:B:165:ASP:C	2.54	0.46
1:A:44:ASN:O	1:A:46:LYS:N	2.41	0.46
1:B:109:TYR:CE1	1:B:111:GLY:HA3	2.50	0.46
2:D:412:ARG:NH1	3:D:576:HOH:O	2.47	0.45
1:B:162:PHE:HA	1:B:169:ARG:O	2.17	0.45
1:B:165:ASP:OD1	1:B:166:PRO:HD2	2.15	0.45
1:B:135:TYR:CZ	2:D:413:LEU:HB3	2.52	0.45
1:A:1:CYS:HA	1:A:76:PRO:O	2.17	0.45
1:B:124:ALA:HB1	1:B:147:LYS:O	2.17	0.44
1:A:61:CYS:O	1:A:70:TRP:HB2	2.16	0.44
1:B:136:ILE:O	1:B:139:LYS:HB2	2.17	0.44
1:A:3:HIS:CG	1:A:4:GLY:H	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ASP:OD2	2:D:417:ARG:NH2	2.50	0.44
1:A:36:ILE:CD1	2:D:402:GLU:OE1	2.65	0.44
1:B:175:ILE:CD1	1:B:175:ILE:N	2.81	0.44
1:A:24:ALA:HA	1:A:48:ASN:HB3	2.00	0.44
1:B:148:ASN:HD22	1:B:148:ASN:N	2.16	0.43
1:A:44:ASN:C	1:A:46:LYS:H	2.19	0.43
1:B:160:TRP:CZ3	2:D:417:ARG:HD2	2.54	0.43
2:C:310:LEU:HD23	2:C:310:LEU:HA	1.86	0.43
1:A:58:ARG:HH22	1:A:75:ILE:H	1.67	0.43
1:A:36:ILE:CG2	2:D:402:GLU:OE1	2.37	0.43
1:A:16:THR:C	1:A:18:SER:N	2.72	0.42
1:A:20:LEU:HD22	1:A:65:ASP:HB2	1.99	0.42
1:B:131:HIS:HD2	2:C:319:GLU:OE2	2.02	0.42
1:A:16:THR:C	1:A:18:SER:H	2.22	0.42
1:A:32:ALA:O	1:A:69:ARG:NH2	2.48	0.42
1:B:165:ASP:OD1	1:B:166:PRO:CD	2.68	0.42
2:D:426:LEU:O	2:D:426:LEU:HD22	2.20	0.41
1:B:114:SER:HB3	1:B:148:ASN:OD1	2.21	0.41
1:A:1:CYS:CA	1:A:76:PRO:O	2.69	0.41
1:B:166:PRO:HG2	1:B:167:ASN:H	1.86	0.41
1:B:163:THR:CG2	1:B:165:ASP:HB3	2.51	0.40
1:A:35:TYR:CZ	2:C:313:LEU:HB3	2.56	0.40
1:A:3:HIS:CD2	1:A:6:GLY:H	2.39	0.40
1:A:58:ARG:O	1:A:59:PRO:C	2.58	0.40

All (1) 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:C:554:HOH:O	3:C:554:HOH:O[12_555]	1.81	0.39

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	77/84 (92%)	70 (91%)	5 (6%)	2 (3%)	5 13
1	B	78/84 (93%)	74 (95%)	4 (5%)	0	100 100
2	C	24/30 (80%)	22 (92%)	2 (8%)	0	100 100
2	D	24/30 (80%)	21 (88%)	2 (8%)	1 (4%)	3 5
All	All	203/228 (89%)	187 (92%)	13 (6%)	3 (2%)	10 26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	LYS
2	D	424	GLU
1	A	3	HIS

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	A	72/75 (96%)	61 (85%)	11 (15%)	2 7
1	B	72/75 (96%)	57 (79%)	15 (21%)	1 3
2	C	23/27 (85%)	19 (83%)	4 (17%)	2 5
2	D	23/27 (85%)	22 (96%)	1 (4%)	29 57
All	All	190/204 (93%)	159 (84%)	31 (16%)	2 6

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	MET
1	A	3	HIS
1	A	5	SER
1	A	26	ASP
1	A	38	SER
1	A	39	LYS

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Mol	Chain	Res	Type
1	A	45	LEU
1	A	46	LYS
1	A	48	ASN
1	A	58	ARG
1	A	59	PRO
1	B	117	MET
1	B	121	GLU
1	B	126	ASP
1	B	129	SER
1	B	138	SER
1	B	139	LYS
1	B	145	LEU
1	B	148	ASN
1	B	152	ASN
1	B	153	PRO
1	B	158	ARG
1	B	159	PRO
1	B	168	LYS
1	B	175	ILE
1	B	176	PRO
2	C	303	LYS
2	C	307	ASP
2	C	309	GLU
2	C	318	HIS
2	D	426	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	44	ASN
1	A	48	ASN
1	B	103	HIS
1	B	108	ASN
1	B	133	HIS
1	B	148	ASN
1	B	152	ASN
2	D	411	GLN

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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.