Full wwPDB X-ray Structure Validation Report (i)

Feb 5, 2024 – 04:32 AM EST

PDB ID	:	1SEK
Title	:	THE STRUCTURE OF ACTIVE SERPIN K FROM MANDUCA SEXTA AND A MODEL FOR SERPIN-PROTEASE COMPLEX FORMATION
Authors	:	Li, J.; Wang, Z.; Canagarajah, B.; Jiang, H.; Kanost, M.; Goldsmith, E.J.
Deposited on	:	1998-03-06
Resolution	:	2.10 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:

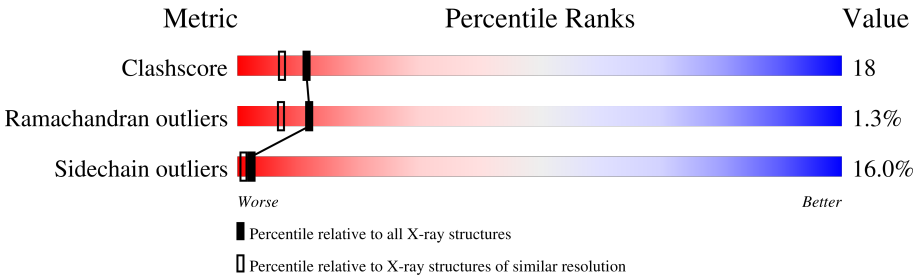
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.10 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	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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	378	61% 30% 9% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3303 atoms, of which 230 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 SERPIN K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	376	2958	1879	497	572	10	0	0	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	189	ASN	VAL	conflict	UNP P14754
A	349	LYS	GLY	conflict	UNP P14754
A	351	THR	VAL	conflict	UNP P14754
A	352	THR	PRO	conflict	UNP P14754
A	353	TYR	ALA	conflict	UNP P14754
A	355	PHE	LEU	conflict	UNP P14754
A	356	HIS	ILE	conflict	UNP P14754
A	357	PHE	LEU	conflict	UNP P14754
A	358	VAL	TYR	conflict	UNP P14754
A	360	LYS	GLU	conflict	UNP P14754
A	362	GLU	HIS	conflict	UNP P14754
A	364	ASN	ASP	conflict	UNP P14754
A	365	LYS	ARG	conflict	UNP P14754
A	368	PHE	TYR	conflict	UNP P14754
A	370	SER	GLU	conflict	UNP P14754
A	373	TYR	ILE	conflict	UNP P14754
A	374	ASN	ASP	conflict	UNP P14754
A	375	ARG	GLY	conflict	UNP P14754
A	376	ASN	ILE	conflict	UNP P14754
A	377	SER	PRO	conflict	UNP P14754
A	380	SER	ASN	conflict	UNP P14754
A	382	VAL	LYS	conflict	UNP P14754
A	383	CYS	VAL	conflict	UNP P14754
A	384	VAL	ILE	conflict	UNP P14754
A	385	GLN	GLU	conflict	UNP P14754

- Molecule 2 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	O		
2	A	115	345	230	115	0	0

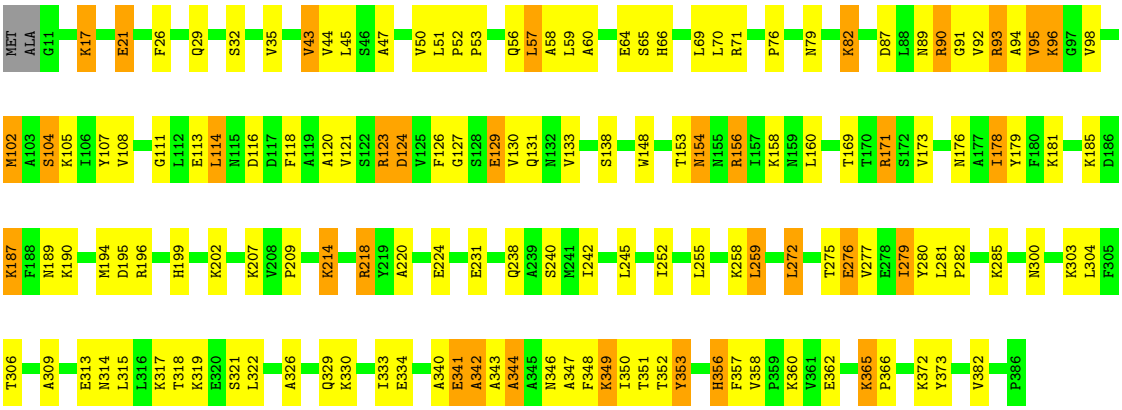
3 Residue-property plots (i)

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: SERPIN K

Chain A: 61% 30% 9%



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	125.96Å 42.05Å 76.05Å 90.00° 117.60° 90.00°	Depositor
Resolution (Å)	8.00 – 2.10	Depositor
% Data completeness (in resolution range)	90.5 (8.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.85	Depositor
R, R_{free}	0.199 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3303	wwPDB-VP
Average B, all atoms (Å^2)	29.0	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	0.44	0/3007	0.77	6/4061 (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	A	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	87	ASP	CB-CG-OD2	-9.53	109.73	118.30
1	A	87	ASP	CB-CG-OD1	7.88	125.39	118.30
1	A	93	ARG	NE-CZ-NH2	7.36	123.98	120.30
1	A	218	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	A	102	MET	CG-SD-CE	5.74	109.39	100.20
1	A	357	PHE	CB-CG-CD1	-5.67	116.83	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	91	GLY	Mainchain

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	2958	0	2984	105	27
2	A	115	230	0	2	10
All	All	3073	230	2984	105	27

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 18.

All (105) 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:94:ALA:O	1:A:95:VAL:HG12	1.12	1.23
1:A:94:ALA:O	1:A:95:VAL:CG1	1.96	1.12
1:A:95:VAL:HG23	1:A:373:TYR:CE1	1.86	1.10
1:A:349:LYS:HE2	1:A:351:THR:HG21	1.31	1.08
1:A:348:PHE:CD1	1:A:348:PHE:O	2.12	1.01
1:A:349:LYS:HE2	1:A:351:THR:CG2	2.03	0.89
1:A:44:VAL:HG21	1:A:333:ILE:HD13	1.58	0.84
1:A:214:LYS:HD3	1:A:358:VAL:HG11	1.61	0.83
1:A:108:VAL:HG21	1:A:114:LEU:HD21	1.60	0.82
1:A:176:ASN:ND2	1:A:329:GLN:HE21	1.81	0.79
1:A:93:ARG:HG3	1:A:94:ALA:H	1.46	0.79
1:A:95:VAL:HG23	1:A:373:TYR:HE1	1.51	0.76
1:A:348:PHE:O	1:A:349:LYS:C	2.25	0.73
1:A:90:ARG:O	1:A:90:ARG:HD3	1.90	0.71
1:A:59:LEU:HD21	1:A:82:LYS:HD2	1.72	0.70
1:A:50:VAL:O	1:A:53:PRO:HD2	1.91	0.70
1:A:245:LEU:HD11	1:A:365:LYS:HG3	1.73	0.69
1:A:120:ALA:HA	1:A:123:ARG:NH1	2.07	0.69
1:A:176:ASN:HD22	1:A:329:GLN:HE21	1.40	0.68
1:A:59:LEU:HD21	1:A:82:LYS:CD	2.24	0.67
1:A:96:LYS:NZ	1:A:238:GLN:OE1	2.25	0.65
1:A:94:ALA:O	1:A:95:VAL:CB	2.45	0.65
1:A:189:ASN:OD1	1:A:343:ALA:HB2	1.97	0.64
1:A:114:LEU:HD11	1:A:130:VAL:HG11	1.80	0.64
1:A:255:LEU:HG	1:A:259:LEU:HD22	1.81	0.63
1:A:60:ALA:HB2	1:A:118:PHE:CZ	2.35	0.62
1:A:153:THR:O	1:A:156:ARG:HB2	2.00	0.62
1:A:306:THR:HB	1:A:309:ALA:HB3	1.79	0.62
1:A:348:PHE:O	1:A:348:PHE:HD1	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:LEU:HD11	1:A:130:VAL:CG1	2.30	0.62
1:A:349:LYS:CE	1:A:351:THR:HG21	2.19	0.61
1:A:95:VAL:CG2	1:A:373:TYR:CE1	2.75	0.60
1:A:93:ARG:HG3	1:A:94:ALA:N	2.16	0.60
1:A:94:ALA:C	1:A:95:VAL:HG12	2.13	0.60
1:A:120:ALA:O	1:A:123:ARG:HG3	2.01	0.60
1:A:156:ARG:HG2	1:A:179:TYR:CZ	2.38	0.59
1:A:26:PHE:HD2	1:A:47:ALA:HB1	1.68	0.58
1:A:123:ARG:O	1:A:127:GLY:HA2	2.03	0.58
1:A:194:MET:HE2	1:A:196:ARG:HH11	1.69	0.57
1:A:347:ALA:O	1:A:348:PHE:HB3	2.04	0.57
1:A:156:ARG:HG3	1:A:156:ARG:HH11	1.69	0.57
1:A:120:ALA:HA	1:A:123:ARG:CZ	2.34	0.57
1:A:58:ALA:O	1:A:66:HIS:HD2	1.88	0.56
1:A:176:ASN:O	1:A:329:GLN:HA	2.06	0.55
1:A:340:ALA:C	1:A:341:GLU:HG2	2.26	0.55
1:A:43:VAL:HG23	1:A:382:VAL:HG22	1.88	0.54
1:A:156:ARG:HG2	1:A:179:TYR:CE1	2.43	0.54
1:A:156:ARG:HG3	1:A:156:ARG:NH1	2.21	0.54
1:A:356:HIS:H	1:A:356:HIS:CD2	2.25	0.53
1:A:214:LYS:CD	1:A:358:VAL:HG11	2.37	0.53
1:A:160:LEU:HD12	1:A:330:LYS:HB3	1.91	0.53
1:A:313:GLU:O	1:A:319:LYS:HG2	2.08	0.52
1:A:53:PRO:HG3	1:A:104:SER:OG	2.09	0.52
1:A:348:PHE:O	1:A:350:ILE:N	2.43	0.52
1:A:348:PHE:CD1	1:A:348:PHE:C	2.79	0.51
1:A:187:LYS:NZ	1:A:342:ALA:HA	2.26	0.51
1:A:280:TYR:HB2	1:A:362:GLU:HA	1.93	0.50
1:A:60:ALA:HA	1:A:314:ASN:HB2	1.92	0.50
1:A:187:LYS:CE	1:A:342:ALA:HA	2.42	0.50
1:A:64:GLU:HB2	1:A:303:LYS:HD3	1.94	0.49
1:A:95:VAL:HG13	1:A:98:VAL:CG2	2.42	0.49
1:A:65:SER:HB2	1:A:303:LYS:HB3	1.94	0.49
1:A:199:HIS:O	1:A:366:PRO:HD3	2.13	0.49
1:A:105:LYS:HG3	1:A:129:GLU:HG3	1.95	0.48
1:A:95:VAL:HG13	1:A:95:VAL:O	2.14	0.48
1:A:105:LYS:HD3	1:A:107:TYR:CZ	2.50	0.47
1:A:93:ARG:CG	1:A:94:ALA:H	2.22	0.47
1:A:218:ARG:HB2	1:A:231:GLU:HB3	1.97	0.47
1:A:275:THR:OG1	1:A:276:GLU:N	2.48	0.47
1:A:231:GLU:OE1	1:A:242:ILE:HD11	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LYS:HZ1	1:A:342:ALA:HA	1.79	0.46
1:A:348:PHE:O	1:A:348:PHE:CG	2.66	0.46
1:A:60:ALA:HB2	1:A:118:PHE:CE1	2.51	0.46
1:A:340:ALA:O	1:A:341:GLU:HG2	2.16	0.46
1:A:209:PRO:HD2	2:A:455:HOH:O	2.14	0.46
1:A:277:VAL:CG2	1:A:279:ILE:HD12	2.46	0.45
1:A:108:VAL:HG21	1:A:114:LEU:CD2	2.39	0.45
1:A:171:ARG:HB3	1:A:322:LEU:HD12	1.98	0.45
1:A:57:LEU:HG	1:A:304:LEU:HD11	2.00	0.44
1:A:43:VAL:HG23	1:A:382:VAL:CG2	2.48	0.44
1:A:57:LEU:HD12	1:A:57:LEU:HA	1.85	0.43
1:A:95:VAL:HG23	1:A:373:TYR:CD1	2.47	0.43
1:A:344:ALA:HA	2:A:512:HOH:O	2.17	0.43
1:A:50:VAL:C	1:A:53:PRO:HD2	2.39	0.43
1:A:69:LEU:HD11	1:A:304:LEU:HD13	2.01	0.43
1:A:108:VAL:CG2	1:A:114:LEU:HD21	2.39	0.42
1:A:173:VAL:HG22	1:A:326:ALA:HB3	2.02	0.42
1:A:154:ASN:HB2	1:A:156:ARG:HD2	2.01	0.42
1:A:187:LYS:HE3	1:A:342:ALA:HA	2.01	0.42
1:A:181:LYS:HG3	1:A:334:GLU:HB3	2.02	0.41
1:A:285:LYS:HA	1:A:333:ILE:O	2.20	0.41
1:A:47:ALA:O	1:A:51:LEU:HG	2.20	0.41
1:A:95:VAL:HG13	1:A:98:VAL:HG23	2.03	0.41
1:A:105:LYS:HB2	1:A:148:TRP:CH2	2.55	0.41
1:A:118:PHE:O	1:A:121:VAL:HG12	2.20	0.41
1:A:281:LEU:HA	1:A:282:PRO:HD3	1.97	0.41
1:A:92:VAL:HG12	1:A:92:VAL:O	2.20	0.41
1:A:102:MET:CE	1:A:178:ILE:HD12	2.51	0.41
1:A:52:PRO:HB2	1:A:53:PRO:HD3	2.02	0.41
1:A:59:LEU:HD22	1:A:126:PHE:CE1	2.56	0.41
1:A:285:LYS:HE3	1:A:285:LYS:HB3	1.89	0.41
1:A:220:ALA:CB	1:A:272:LEU:HD12	2.51	0.41
1:A:17:LYS:HD3	1:A:21:GLU:OE1	2.22	0.40
1:A:347:ALA:O	1:A:348:PHE:CB	2.70	0.40
1:A:44:VAL:HG21	1:A:333:ILE:CD1	2.41	0.40

All (27) 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)
1:A:169:THR:CG2	1:A:195:ASP:OD2[4_546]	0.63	1.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:TYR:OH	1:A:318:THR:O[3_455]	0.87	1.33
1:A:76:PRO:CG	1:A:350:ILE:CD1[2_545]	0.98	1.22
1:A:319:LYS:O	1:A:360:LYS:NZ[3_545]	1.05	1.15
1:A:76:PRO:CB	1:A:350:ILE:CD1[2_545]	1.37	0.83
1:A:169:THR:CB	1:A:195:ASP:OD2[4_546]	1.40	0.80
1:A:224:GLU:OE2	1:A:342:ALA:CB[1_545]	1.55	0.65
1:A:29:GLN:OE1	2:A:497:HOH:O[1_545]	1.66	0.54
1:A:29:GLN:OE1	2:A:497:HOH:H1[1_545]	1.07	0.53
1:A:169:THR:CG2	1:A:195:ASP:CG[4_546]	1.67	0.53
1:A:319:LYS:CE	1:A:358:VAL:O[3_545]	1.67	0.53
1:A:344:ALA:CB	2:A:438:HOH:O[1_565]	1.73	0.47
1:A:76:PRO:CD	1:A:350:ILE:CD1[2_545]	1.74	0.46
1:A:319:LYS:O	1:A:360:LYS:CE[3_545]	1.83	0.37
1:A:258:LYS:CD	2:A:475:HOH:H1[1_545]	1.25	0.35
1:A:258:LYS:CD	2:A:475:HOH:O[1_545]	1.86	0.34
1:A:111:GLY:O	2:A:473:HOH:O[2_656]	1.89	0.31
1:A:258:LYS:CE	2:A:475:HOH:O[1_545]	1.91	0.29
1:A:169:THR:OG1	1:A:195:ASP:OD2[4_546]	1.92	0.28
1:A:76:PRO:CB	1:A:350:ILE:CG1[2_545]	1.94	0.26
1:A:258:LYS:CG	2:A:475:HOH:O[1_545]	2.02	0.18
1:A:111:GLY:O	2:A:473:HOH:H1[2_656]	1.44	0.16
1:A:280:TYR:OH	1:A:318:THR:C[3_455]	2.04	0.16
1:A:124:ASP:OD2	1:A:353:TYR:OH[3_545]	2.07	0.13
1:A:319:LYS:C	1:A:360:LYS:NZ[3_545]	2.12	0.08
1:A:258:LYS:CG	2:A:475:HOH:H2[1_545]	1.56	0.04
1:A:280:TYR:CZ	1:A:318:THR:O[3_455]	2.18	0.02

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	374/378 (99%)	347 (93%)	22 (6%)	5 (1%)	12 7

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	VAL
1	A	341	GLU
1	A	349	LYS
1	A	342	ALA
1	A	344	ALA

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	325/326 (100%)	273 (84%)	52 (16%)	2 1

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	21	GLU
1	A	32	SER
1	A	35	VAL
1	A	43	VAL
1	A	45	LEU
1	A	56	GLN
1	A	57	LEU
1	A	70	LEU
1	A	71	ARG
1	A	79	ASN
1	A	82	LYS
1	A	89	ASN
1	A	90	ARG
1	A	96	LYS
1	A	104	SER
1	A	113	GLU
1	A	114	LEU
1	A	116	ASP
1	A	123	ARG

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Mol	Chain	Res	Type
1	A	124	ASP
1	A	129	GLU
1	A	131	GLN
1	A	133	VAL
1	A	138	SER
1	A	154	ASN
1	A	156	ARG
1	A	158	LYS
1	A	171	ARG
1	A	178	ILE
1	A	185	LYS
1	A	187	LYS
1	A	190	LYS
1	A	202	LYS
1	A	207	LYS
1	A	214	LYS
1	A	240	SER
1	A	252	ILE
1	A	259	LEU
1	A	272	LEU
1	A	276	GLU
1	A	279	ILE
1	A	300	ASN
1	A	315	LEU
1	A	317	LYS
1	A	321	SER
1	A	346	ASN
1	A	352	THR
1	A	353	TYR
1	A	356	HIS
1	A	365	LYS
1	A	372	LYS

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

Mol	Chain	Res	Type
1	A	29	GLN
1	A	56	GLN
1	A	176	ASN
1	A	274	ASN
1	A	346	ASN
1	A	356	HIS

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Mol	Chain	Res	Type
1	A	385	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.