Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 07:15 PM EDT

PDB ID	:	1DFA
Title	:	CRYSTAL STRUCTURE OF PI-SCEI IN C2 SPACE GROUP
Authors	:	Hu, D.; Crist, M.; Duan, X.; Quiocho, F.A.; Gimble, F.S.
Deposited on	:	1999-11-18
Resolution	:	2.00 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:

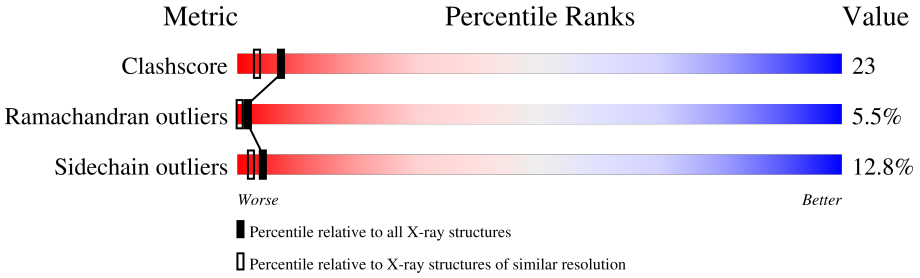
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.00 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	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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	454	50% 31% 7% • 11%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4482 atoms, of which 1113 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 PI-SCEI ENDONUCLEASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	405	3906	2011	729	547	605	14	728	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	O		
2	A	192	576	384	192	384	0

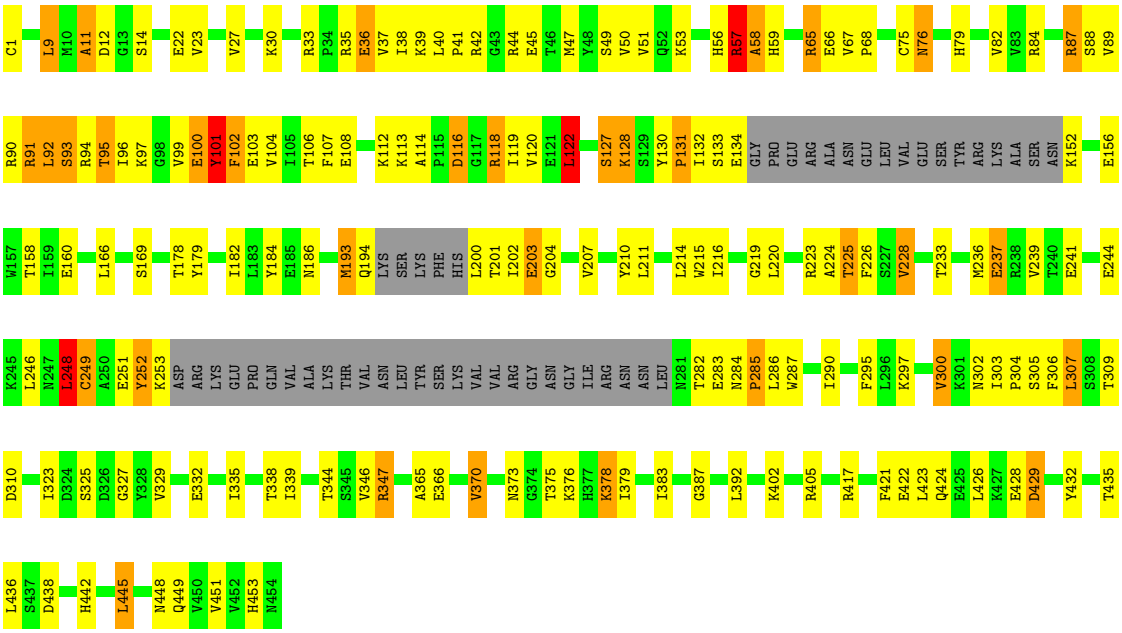
3 Residue-property plots (i)

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: PI-SCEI ENDONUCLEASE

Chain A: 50% 31% 7% • 11%



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	93.60Å 76.00Å 71.40Å 90.00° 111.30° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 98.1	Depositor
R, R_{free}	0.210 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4482	wwPDB-VP
Average B, all atoms (Å^2)	31.0	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	0.65	0/3235	0.90	8/4364 (0.2%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	101	TYR	N-CA-C	6.63	128.89	111.00
1	A	122	LEU	CA-CB-CG	5.99	129.07	115.30
1	A	91	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	A	445	LEU	CA-CB-CG	5.53	128.02	115.30
1	A	57	ARG	N-CA-C	5.39	125.56	111.00
1	A	65	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	347	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	103	GLU	N-CA-C	5.08	124.72	111.00

There are no chirality outliers.

There are no planarity outliers.

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	3177	729	3157	143	0
2	A	192	384	0	8	0
All	All	3369	1113	3157	143	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 23.

All (143) 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:370:VAL:HG13	1:A:373:ASN:HA	1.41	0.98
1:A:84:ARG:NH1	1:A:178:THR:HG21	1.93	0.84
1:A:92:LEU:HD23	1:A:95:THR:HA	1.59	0.84
1:A:91:ARG:NH2	1:A:102:PHE:HB2	1.91	0.84
1:A:297:LYS:HB2	1:A:302:ASN:HB2	1.62	0.81
1:A:92:LEU:HD22	1:A:104:VAL:HG21	1.64	0.80
1:A:116:ASP:HB2	1:A:118:ARG:HH12	1.46	0.79
1:A:202:ILE:HG22	1:A:203:GLU:HG3	1.67	0.77
1:A:1:CYS:HA	1:A:76:ASN:ND2	1.99	0.76
1:A:116:ASP:HB2	1:A:118:ARG:NH1	2.00	0.76
1:A:44:ARG:HA	1:A:429:ASP:O	1.86	0.75
1:A:252:TYR:O	1:A:253:LYS:HG3	1.87	0.75
1:A:57:ARG:HH11	1:A:67:VAL:H	1.33	0.74
1:A:41:PRO:O	1:A:42:ARG:HD3	1.87	0.74
1:A:130:TYR:CD2	1:A:131:PRO:HD2	2.23	0.73
1:A:39:LYS:HB3	1:A:435:THR:HB	1.74	0.70
1:A:49:SER:HB3	1:A:424:GLN:HB2	1.71	0.70
1:A:297:LYS:HB2	1:A:302:ASN:CB	2.22	0.69
1:A:91:ARG:HH21	1:A:102:PHE:HB2	1.57	0.68
1:A:344:THR:HG23	1:A:347:ARG:NH1	2.09	0.67
1:A:92:LEU:HB2	1:A:104:VAL:HG22	1.76	0.67
1:A:228:VAL:HB	1:A:236:MET:SD	2.35	0.67
1:A:76:ASN:H	1:A:76:ASN:HD22	1.40	0.67
1:A:248:LEU:O	1:A:249:CYS:HB2	1.94	0.67
1:A:215:TRP:CD1	1:A:219:GLY:HA3	2.30	0.67
1:A:45:GLU:O	1:A:428:GLU:HA	1.96	0.66
1:A:215:TRP:HB2	1:A:226:PHE:HE2	1.60	0.66
1:A:282:THR:OG1	1:A:284:ASN:HB2	1.96	0.65
1:A:92:LEU:HD22	1:A:104:VAL:CG2	2.27	0.64
1:A:101:TYR:HD2	1:A:128:LYS:HE2	1.61	0.64
1:A:251:GLU:HG3	1:A:252:TYR:CD2	2.33	0.64
1:A:112:LYS:HB2	1:A:122:LEU:HD21	1.80	0.64
1:A:1:CYS:O	1:A:75:CYS:HA	1.97	0.63
1:A:370:VAL:HG13	1:A:373:ASN:CA	2.22	0.63
1:A:57:ARG:NH1	1:A:66:GLU:HA	2.12	0.63
1:A:50:VAL:HG22	1:A:423:LEU:HD11	1.82	0.62
1:A:248:LEU:HD12	1:A:252:TYR:OH	2.00	0.62
1:A:370:VAL:CG1	1:A:373:ASN:HA	2.23	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:THR:HA	1:A:252:TYR:HB3	1.81	0.62
1:A:50:VAL:HG22	1:A:423:LEU:CD1	2.30	0.61
1:A:120:VAL:HG21	1:A:166:LEU:HD12	1.83	0.60
1:A:216:ILE:HD11	1:A:295:PHE:HD2	1.66	0.60
1:A:92:LEU:HD21	1:A:96:ILE:O	2.01	0.60
1:A:35:ARG:HG3	1:A:436:LEU:HD21	1.84	0.60
1:A:207:VAL:O	1:A:211:LEU:HG	2.03	0.59
1:A:224:ALA:O	1:A:252:TYR:HB3	2.03	0.58
1:A:87:ARG:NH2	1:A:88:SER:H	2.01	0.58
1:A:99:VAL:HG12	1:A:100:GLU:HG2	1.86	0.58
1:A:79:HIS:O	1:A:160:GLU:HA	2.03	0.58
1:A:442:HIS:HD2	2:A:502:HOH:O	1.87	0.57
1:A:297:LYS:HB2	1:A:302:ASN:CG	2.24	0.57
1:A:57:ARG:HH11	1:A:67:VAL:N	2.02	0.57
1:A:27:VAL:HG23	1:A:35:ARG:HB2	1.86	0.56
1:A:87:ARG:NH2	1:A:107:PHE:O	2.39	0.56
1:A:182:ILE:HG21	1:A:309:THR:HG22	1.87	0.56
1:A:11:ALA:HB2	1:A:27:VAL:O	2.06	0.55
1:A:297:LYS:CB	1:A:302:ASN:HB2	2.35	0.55
1:A:365:ALA:HB1	1:A:379:ILE:HD11	1.87	0.55
1:A:92:LEU:HG	1:A:96:ILE:H	1.71	0.54
1:A:287:TRP:CE3	1:A:290:ILE:HD12	2.42	0.54
1:A:438:ASP:O	1:A:442:HIS:HE1	1.91	0.54
1:A:84:ARG:HH11	1:A:178:THR:HG21	1.71	0.54
1:A:237:GLU:O	1:A:241:GLU:HB2	2.08	0.54
1:A:53:LYS:HE3	1:A:421:PHE:O	2.09	0.53
1:A:207:VAL:HG23	1:A:246:LEU:HD13	1.91	0.52
1:A:204:GLY:O	1:A:207:VAL:HG22	2.09	0.52
1:A:228:VAL:HG21	1:A:239:VAL:HG21	1.91	0.52
1:A:23:VAL:HG13	1:A:37:VAL:O	2.10	0.52
1:A:304:PRO:HB2	1:A:306:PHE:CE2	2.45	0.51
1:A:210:TYR:CE2	1:A:214:LEU:HD22	2.45	0.51
1:A:286:LEU:O	1:A:290:ILE:HG13	2.10	0.51
1:A:442:HIS:CD2	2:A:502:HOH:O	2.63	0.50
1:A:297:LYS:N	1:A:300:VAL:O	2.44	0.50
1:A:96:ILE:HG22	1:A:97:LYS:N	2.26	0.50
1:A:248:LEU:H	1:A:248:LEU:HD23	1.77	0.49
1:A:448:ASN:O	1:A:449:GLN:HB2	2.12	0.49
1:A:51:VAL:HG13	1:A:422:GLU:HG3	1.93	0.49
1:A:91:ARG:NH2	1:A:102:PHE:CB	2.67	0.49
1:A:120:VAL:HG21	1:A:166:LEU:CD1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:LEU:HD23	1:A:223:ARG:HE	1.78	0.49
1:A:225:THR:HA	1:A:252:TYR:CB	2.43	0.49
1:A:36:GLU:H	1:A:36:GLU:CD	2.17	0.48
1:A:179:TYR:CE2	1:A:417:ARG:HB2	2.49	0.48
1:A:127:SER:OG	1:A:128:LYS:N	2.47	0.47
1:A:193:MET:HG2	1:A:194:GLN:N	2.30	0.47
1:A:303:ILE:HD11	1:A:346:VAL:HG13	1.96	0.47
1:A:36:GLU:CD	1:A:36:GLU:N	2.68	0.46
1:A:1:CYS:HB3	1:A:79:HIS:CD2	2.49	0.46
1:A:57:ARG:HD3	1:A:67:VAL:H	1.80	0.46
1:A:184:TYR:OH	1:A:186:ASN:ND2	2.48	0.46
1:A:297:LYS:HB3	1:A:300:VAL:HG12	1.97	0.46
1:A:35:ARG:HB3	1:A:436:LEU:HG	1.98	0.46
1:A:49:SER:O	1:A:423:LEU:HA	2.16	0.46
1:A:87:ARG:NH1	2:A:560:HOH:O	2.49	0.46
1:A:96:ILE:HG22	1:A:97:LYS:H	1.81	0.46
1:A:252:TYR:C	1:A:253:LYS:HG3	2.35	0.45
1:A:335:ILE:HG22	2:A:615:HOH:O	2.16	0.45
1:A:91:ARG:HH22	1:A:102:PHE:CB	2.28	0.45
1:A:82:VAL:HG23	2:A:521:HOH:O	2.15	0.45
1:A:57:ARG:HD2	1:A:67:VAL:HG22	1.99	0.45
1:A:344:THR:HG23	1:A:347:ARG:CZ	2.46	0.45
1:A:236:MET:HB3	2:A:611:HOH:O	2.15	0.45
1:A:366:GLU:O	1:A:379:ILE:HG13	2.17	0.45
1:A:112:LYS:HB2	1:A:122:LEU:CD2	2.46	0.44
1:A:226:PHE:H	1:A:252:TYR:HB2	1.81	0.44
1:A:233:THR:HG21	2:A:642:HOH:O	2.16	0.44
1:A:99:VAL:HG12	1:A:100:GLU:N	2.32	0.44
1:A:108:GLU:HB2	1:A:134:GLU:HA	2.00	0.44
1:A:23:VAL:HG13	1:A:38:ILE:HA	1.98	0.44
1:A:82:VAL:HG13	1:A:453:HIS:HB2	2.00	0.44
1:A:96:ILE:O	1:A:97:LYS:HG3	2.17	0.44
1:A:202:ILE:O	1:A:203:GLU:HB2	2.18	0.44
1:A:49:SER:HB2	1:A:426:LEU:HD11	1.99	0.44
1:A:92:LEU:HG	1:A:96:ILE:HB	2.00	0.44
1:A:114:ALA:HB1	1:A:116:ASP:OD2	2.18	0.43
1:A:297:LYS:H	1:A:302:ASN:HB2	1.83	0.43
1:A:91:ARG:NH2	2:A:572:HOH:O	2.51	0.43
1:A:108:GLU:HB2	1:A:134:GLU:CA	2.49	0.43
1:A:246:LEU:O	1:A:248:LEU:HD23	2.18	0.43
1:A:102:PHE:CD1	1:A:102:PHE:N	2.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:MET:O	1:A:426:LEU:HB2	2.19	0.42
1:A:90:ARG:O	1:A:91:ARG:HB2	2.19	0.42
1:A:30:LYS:NZ	1:A:451:VAL:HG11	2.35	0.42
1:A:89:VAL:HG22	1:A:90:ARG:N	2.35	0.42
1:A:402:LYS:HG2	1:A:402:LYS:O	2.20	0.42
1:A:130:TYR:HD2	1:A:131:PRO:HD2	1.78	0.42
1:A:370:VAL:HG12	1:A:370:VAL:O	2.20	0.42
1:A:9:LEU:HD23	1:A:9:LEU:HA	1.93	0.42
1:A:56:HIS:ND1	1:A:56:HIS:N	2.68	0.42
1:A:284:ASN:HA	1:A:285:PRO:HD2	1.88	0.41
1:A:327:GLY:HA2	1:A:338:THR:O	2.19	0.41
1:A:104:VAL:O	1:A:127:SER:O	2.39	0.41
1:A:307:LEU:HD12	1:A:307:LEU:HA	1.70	0.41
1:A:65:ARG:HH21	1:A:378:LYS:HG2	1.86	0.41
1:A:120:VAL:H	1:A:120:VAL:HG22	1.64	0.41
1:A:89:VAL:HG23	1:A:106:THR:HG22	2.02	0.41
1:A:202:ILE:HD13	1:A:202:ILE:HA	1.90	0.41
1:A:432:TYR:CD1	1:A:432:TYR:N	2.89	0.41
1:A:41:PRO:C	1:A:42:ARG:HD3	2.41	0.40
1:A:57:ARG:HB3	1:A:58:ALA:H	1.63	0.40
1:A:99:VAL:N	1:A:102:PHE:CZ	2.89	0.40
1:A:323:ILE:HG13	1:A:339:ILE:HD11	2.03	0.40
1:A:93:SER:OG	1:A:96:ILE:HD11	2.21	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	397/454 (87%)	337 (85%)	38 (10%)	22 (6%)	2 0

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	100	GLU
1	A	127	SER
1	A	128	LYS
1	A	131	PRO
1	A	133	SER
1	A	375	THR
1	A	93	SER
1	A	132	ILE
1	A	248	LEU
1	A	370	VAL
1	A	376	LYS
1	A	378	LYS
1	A	101	TYR
1	A	249	CYS
1	A	332	GLU
1	A	58	ALA
1	A	201	THR
1	A	11	ALA
1	A	203	GLU
1	A	285	PRO
1	A	387	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	A	344/392 (88%)	300 (87%)	44 (13%)	4 2

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	12	ASP
1	A	14	SER
1	A	22	GLU
1	A	33	ARG

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Mol	Chain	Res	Type
1	A	36	GLU
1	A	40	LEU
1	A	59	HIS
1	A	68	PRO
1	A	76	ASN
1	A	87	ARG
1	A	92	LEU
1	A	94	ARG
1	A	95	THR
1	A	102	PHE
1	A	113	LYS
1	A	116	ASP
1	A	118	ARG
1	A	119	ILE
1	A	122	LEU
1	A	152	LYS
1	A	156	GLU
1	A	158	THR
1	A	169	SER
1	A	193	MET
1	A	200	LEU
1	A	225	THR
1	A	228	VAL
1	A	237	GLU
1	A	244	GLU
1	A	248	LEU
1	A	252	TYR
1	A	283	GLU
1	A	300	VAL
1	A	305	SER
1	A	307	LEU
1	A	310	ASP
1	A	325	SER
1	A	329	VAL
1	A	383	ILE
1	A	392	LEU
1	A	405	ARG
1	A	429	ASP
1	A	445	LEU

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	76	ASN
1	A	79	HIS
1	A	186	ASN
1	A	188	HIS
1	A	333	HIS
1	A	364	ASN
1	A	442	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 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.