Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 06:42 PM GMT

PDB ID	:	1C28
Title	:	THE CRYSTAL STRUCTURE OF A COMPLMENT-1Q FAMILY PROTEIN SUGGESTS AN EVOLUTIONARY LINK TO TUMOR NECROSIS FACTOR
Authors	:	Shapiro, L.; Scherer, P.
Deposited on	:	1999-07-22
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

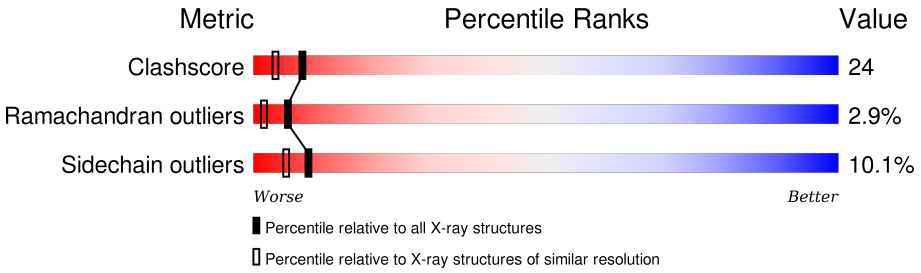
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	135	50% 38% • 7%
1	B	135	46% 27% 7% • 18%
1	C	135	38% 32% 6% 24%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3132 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 PROTEIN (30 KD ADIPOCYTE COMPLEMENT-RELATED PROTEIN PRECURSOR (ACRP30)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	125	Total	C	N	O	S	0	0	0
			1008	656	164	186	2			
1	B	111	Total	C	N	O	S	0	0	0
			910	598	143	167	2			
1	C	102	Total	C	N	O	S	0	0	0
			825	540	134	150	1			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	139	Total	O	0	0
			139	139		
2	B	133	Total	O	0	0
			133	133		
2	C	117	Total	O	0	0
			117	117		

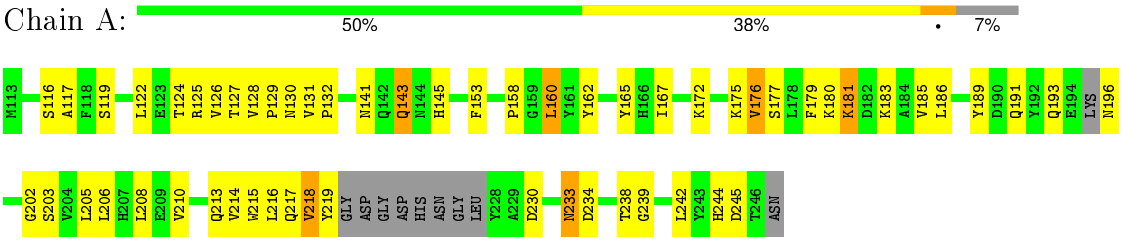
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

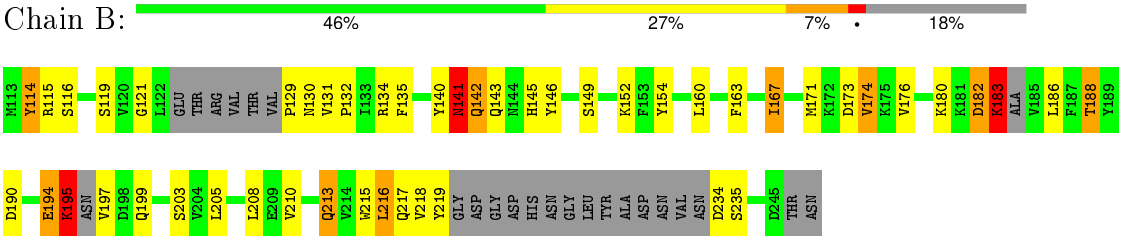
• Molecule 1: PROTEIN (30 KD ADIPOCYTE COMPLEMENT-RELATED PROTEIN PRECURSOR (ACRP30))

Chain A:



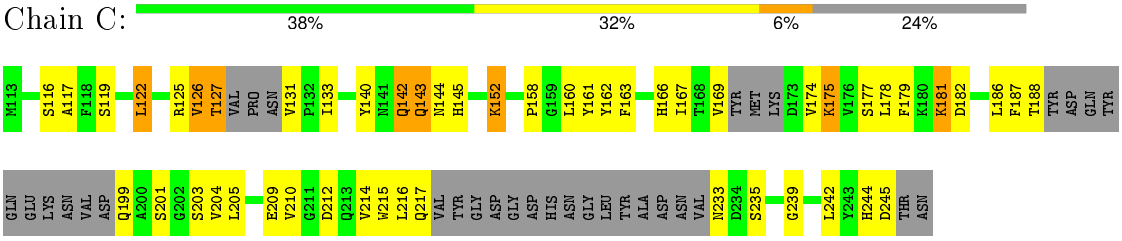
• Molecule 1: PROTEIN (30 KD ADIPOCYTE COMPLEMENT-RELATED PROTEIN PRECURSOR (ACRP30))

Chain B:



• Molecule 1: PROTEIN (30 KD ADIPOCYTE COMPLEMENT-RELATED PROTEIN PRECURSOR (ACRP30))

Chain C:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	112.30Å 112.30Å 71.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.10	Depositor
% Data completeness (in resolution range)	92.8 (8.00-2.10)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.212 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3132	wwPDB-VP
Average B, all atoms (Å^2)	25.0	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	0.65	0/1033	0.86	0/1399
1	B	0.65	0/936	0.94	4/1268 (0.3%)
1	C	0.58	0/844	0.82	0/1139
All	All	0.63	0/2813	0.87	4/3806 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	195	LYS	N-CA-C	8.41	133.71	111.00
1	B	194	GLU	N-CA-C	7.56	131.41	111.00
1	B	183	LYS	N-CA-C	5.39	125.56	111.00
1	B	114	TYR	N-CA-C	5.26	125.21	111.00

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	1008	0	951	60	0
1	B	910	0	853	38	1
1	C	825	0	788	42	0
2	A	139	0	0	12	0
2	B	133	0	0	7	1
2	C	117	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3132	0	2592	129	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 24.

All (129) 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:233:ASN:H	1:A:233:ASN:HD22	1.26	0.79
1:C:122:LEU:HD21	1:C:127:THR:HG21	1.66	0.77
1:B:115:ARG:HD2	2:B:319:HOH:O	1.84	0.77
1:A:175:LYS:HB2	2:A:311:HOH:O	1.86	0.76
1:A:119:SER:HB2	1:B:205:LEU:HB2	1.67	0.75
1:C:209:GLU:HG3	2:C:288:HOH:O	1.87	0.74
1:A:215:TRP:HE1	1:A:217:GLN:HE21	1.33	0.74
1:A:130:ASN:N	2:A:277:HOH:O	2.22	0.71
1:B:116:SER:OG	1:B:145:HIS:HD2	1.74	0.71
1:B:210:VAL:HG13	2:B:360:HOH:O	1.92	0.70
1:C:116:SER:OG	1:C:145:HIS:HD2	1.74	0.69
1:C:175:LYS:HE3	2:C:327:HOH:O	1.92	0.69
1:A:116:SER:OG	1:A:145:HIS:HD2	1.75	0.69
1:A:181:LYS:HA	2:A:279:HOH:O	1.94	0.68
1:A:215:TRP:HE1	1:A:217:GLN:NE2	1.92	0.67
1:B:234:ASP:HB2	1:C:187:PHE:O	1.95	0.67
1:C:127:THR:HB	1:C:169:VAL:HG12	1.78	0.65
1:B:183:LYS:HE3	1:B:219:TYR:CE2	2.31	0.65
1:A:145:HIS:HE1	2:A:249:HOH:O	1.79	0.65
1:C:215:TRP:HE1	1:C:217:GLN:NE2	1.95	0.64
1:A:233:ASN:H	1:A:233:ASN:ND2	1.96	0.64
1:B:140:TYR:CZ	1:B:142:GLN:HB2	2.33	0.64
1:A:122:LEU:HD22	1:A:124:THR:HG22	1.81	0.63
1:C:117:ALA:H	1:C:143:GLN:NE2	1.97	0.62
1:C:181:LYS:HD3	1:C:212:ASP:OD1	1.99	0.62
1:A:205:LEU:HB2	1:C:119:SER:HB2	1.82	0.62
1:B:215:TRP:HE1	1:B:217:GLN:NE2	1.99	0.60
1:B:180:LYS:HD2	1:B:208:LEU:CD2	2.32	0.60
1:C:152:LYS:HE2	2:C:332:HOH:O	2.01	0.60
1:A:219:TYR:HB3	2:A:311:HOH:O	2.02	0.59
1:A:183:LYS:HD3	2:A:381:HOH:O	2.03	0.58
1:B:130:ASN:HA	1:B:219:TYR:O	2.03	0.57
1:A:218:VAL:HB	2:A:255:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:TYR:CZ	1:C:142:GLN:HB2	2.41	0.55
1:A:131:VAL:O	1:A:217:GLN:HG2	2.07	0.55
1:C:215:TRP:HE1	1:C:217:GLN:HE21	1.55	0.54
1:C:144:ASN:HB3	2:C:290:HOH:O	2.07	0.54
1:C:152:LYS:HG3	1:C:215:TRP:HB3	1.88	0.54
1:B:132:PRO:HG2	1:B:152:LYS:HE2	1.90	0.53
1:A:234:ASP:HA	1:B:186:LEU:HD21	1.90	0.53
1:C:127:THR:HA	1:C:133:ILE:HD12	1.91	0.53
1:A:117:ALA:H	1:A:143:GLN:HE21	1.58	0.52
1:C:178:LEU:HD23	1:C:216:LEU:CD2	2.40	0.52
1:A:218:VAL:O	2:A:277:HOH:O	2.19	0.51
1:A:180:LYS:O	1:A:181:LYS:HB2	2.10	0.51
1:C:188:THR:HG21	1:C:201:SER:N	2.26	0.51
1:A:191:GLN:HG2	2:A:318:HOH:O	2.10	0.51
1:A:125:ARG:HD3	1:B:190:ASP:OD2	2.10	0.51
1:B:167:ILE:HA	1:B:235:SER:HB3	1.93	0.51
1:A:160:LEU:HG	1:C:140:TYR:CZ	2.46	0.51
1:B:183:LYS:CE	1:B:219:TYR:CE2	2.93	0.51
1:B:129:PRO:HG3	1:B:171:MET:SD	2.51	0.51
1:C:167:ILE:HA	1:C:235:SER:HB3	1.94	0.50
1:A:238:THR:HG22	2:B:340:HOH:O	2.10	0.50
1:B:130:ASN:HA	1:B:219:TYR:C	2.30	0.50
1:C:163:PHE:O	1:C:203:SER:HA	2.12	0.50
1:A:131:VAL:C	1:A:217:GLN:HG2	2.31	0.50
1:C:152:LYS:CG	1:C:215:TRP:CE3	2.95	0.49
1:A:202:GLY:HA2	2:C:278:HOH:O	2.10	0.49
1:C:152:LYS:HG2	1:C:215:TRP:CE3	2.48	0.49
1:C:152:LYS:NZ	2:C:332:HOH:O	2.45	0.49
1:A:233:ASN:ND2	1:A:233:ASN:N	2.61	0.49
1:A:167:ILE:HG13	1:A:176:VAL:HG11	1.94	0.49
1:C:166:HIS:HB3	2:C:266:HOH:O	2.12	0.49
1:C:152:LYS:CE	2:C:332:HOH:O	2.59	0.49
1:A:189:TYR:HB3	1:C:233:ASN:HB2	1.95	0.48
1:B:180:LYS:NZ	2:B:315:HOH:O	2.46	0.48
1:C:178:LEU:HA	1:C:216:LEU:HD23	1.95	0.48
1:A:180:LYS:HB3	1:A:185:VAL:HG21	1.95	0.48
1:B:180:LYS:C	1:B:182:ASP:N	2.67	0.48
1:A:165:TYR:CD2	1:A:216:LEU:HD21	2.50	0.47
1:B:115:ARG:NH2	2:B:337:HOH:O	2.46	0.47
1:B:195:LYS:HG2	1:B:197:VAL:N	2.29	0.47
1:C:140:TYR:HE2	1:C:143:GLN:HE22	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:TYR:OH	1:A:203:SER:HB2	2.14	0.47
1:A:196:ASN:ND2	1:B:195:LYS:HD2	2.30	0.47
1:C:244:HIS:O	1:C:245:ASP:HB2	2.14	0.47
1:A:233:ASN:O	1:A:234:ASP:HB2	2.15	0.47
1:A:125:ARG:NH2	2:A:357:HOH:O	2.48	0.47
1:B:119:SER:HB2	1:C:205:LEU:HB2	1.97	0.47
1:A:185:VAL:HG11	1:A:206:LEU:HD21	1.96	0.46
1:A:162:TYR:O	1:A:239:GLY:HA2	2.15	0.46
1:A:189:TYR:CE2	1:A:191:GLN:HG3	2.50	0.46
1:B:163:PHE:O	1:B:203:SER:HA	2.16	0.46
1:A:124:THR:HG23	1:A:126:VAL:O	2.17	0.45
1:C:217:GLN:NE2	2:C:310:HOH:O	2.45	0.45
1:C:162:TYR:O	1:C:239:GLY:HA2	2.16	0.45
1:A:153:PHE:O	1:A:213:GLN:HA	2.16	0.45
1:A:132:PRO:HG3	1:A:215:TRP:CD1	2.52	0.45
1:A:117:ALA:H	1:A:143:GLN:NE2	2.14	0.45
1:A:177:SER:HB2	1:A:179:PHE:HE1	1.81	0.45
1:B:173:ASP:OD1	1:B:194:GLU:HB3	2.17	0.45
1:A:125:ARG:NH1	1:A:230:ASP:OD1	2.50	0.45
1:A:177:SER:HB2	1:A:179:PHE:CE1	2.53	0.44
1:A:179:PHE:O	1:A:214:VAL:HB	2.18	0.44
1:A:234:ASP:OD1	1:B:188:THR:HB	2.18	0.44
1:A:116:SER:OG	1:A:145:HIS:CD2	2.64	0.44
1:B:141:ASN:HD21	1:B:146:TYR:H	1.66	0.44
1:A:127:THR:HA	2:A:320:HOH:O	2.18	0.43
1:B:180:LYS:HA	1:B:213:GLN:O	2.18	0.43
1:B:195:LYS:HG2	1:B:197:VAL:H	1.84	0.43
1:A:128:VAL:CA	1:A:129:PRO:N	2.82	0.43
1:C:158:PRO:HG3	1:C:210:VAL:HG23	2.01	0.43
1:C:125:ARG:HB3	1:C:126:VAL:H	1.71	0.43
1:A:172:LYS:HE3	1:A:172:LYS:HB2	1.85	0.43
1:B:135:PHE:HZ	1:B:216:LEU:HD12	1.84	0.42
1:B:174:VAL:HG22	1:B:218:VAL:HG12	2.00	0.42
1:C:177:SER:HA	1:C:186:LEU:O	2.19	0.42
1:A:179:PHE:O	1:A:214:VAL:HA	2.18	0.42
1:A:219:TYR:C	2:A:268:HOH:O	2.58	0.42
1:B:132:PRO:HG3	1:B:215:TRP:NE1	2.35	0.42
1:C:178:LEU:HD23	1:C:216:LEU:HD21	2.01	0.42
1:B:131:VAL:HG22	2:B:308:HOH:O	2.19	0.42
1:A:180:LYS:HZ3	1:A:208:LEU:HD23	1.84	0.42
1:B:134:ARG:HD3	1:B:149:SER:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:HIS:HD2	1:A:245:ASP:O	2.03	0.41
1:C:127:THR:HG23	2:C:251:HOH:O	2.20	0.41
1:C:161:TYR:O	1:C:205:LEU:HA	2.21	0.41
1:C:199:GLN:NE2	2:C:307:HOH:O	2.49	0.41
1:A:158:PRO:HD3	1:A:210:VAL:HG23	2.03	0.41
1:B:167:ILE:HD11	1:B:176:VAL:HG11	2.03	0.40
1:A:196:ASN:HD21	1:B:195:LYS:HE2	1.86	0.40
1:C:179:PHE:O	1:C:214:VAL:HA	2.22	0.40
1:A:167:ILE:HG13	1:A:176:VAL:CG1	2.51	0.40
1:A:165:TYR:HB2	1:A:216:LEU:HD11	2.02	0.40
1:B:121:GLY:HA3	2:B:276:HOH:O	2.21	0.40
1:C:167:ILE:HG22	1:C:169:VAL:HG13	2.02	0.40
1:B:154:TYR:CD1	1:B:154:TYR:N	2.90	0.40
1:A:132:PRO:HG3	1:A:215:TRP:NE1	2.37	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)
1:B:143:GLN:OE1	2:B:250:HOH:O[4_675]	2.12	0.08

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	117/135 (87%)	107 (92%)	8 (7%)	2 (2%)	11 5
1	B	105/135 (78%)	95 (90%)	5 (5%)	5 (5%)	3 0
1	C	92/135 (68%)	83 (90%)	7 (8%)	2 (2%)	8 3
All	All	314/405 (78%)	285 (91%)	20 (6%)	9 (3%)	6 2

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	182	ASP
1	A	141	ASN
1	B	141	ASN
1	B	183	LYS
1	B	195	LYS
1	A	181	LYS
1	C	181	LYS
1	B	114	TYR
1	C	126	VAL

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	109/121 (90%)	101 (93%)	8 (7%)	17 13
1	B	98/121 (81%)	88 (90%)	10 (10%)	9 5
1	C	89/121 (74%)	77 (86%)	12 (14%)	5 2
All	All	296/363 (82%)	266 (90%)	30 (10%)	9 5

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	160	LEU
1	A	176	VAL
1	A	186	LEU
1	A	193	GLN
1	A	218	VAL
1	A	233	ASN
1	A	242	LEU
1	B	141	ASN
1	B	142	GLN
1	B	160	LEU
1	B	167	ILE
1	B	174	VAL
1	B	188	THR

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Mol	Chain	Res	Type
1	B	195	LYS
1	B	199	GLN
1	B	213	GLN
1	B	216	LEU
1	C	122	LEU
1	C	127	THR
1	C	131	VAL
1	C	142	GLN
1	C	143	GLN
1	C	152	LYS
1	C	160	LEU
1	C	174	VAL
1	C	175	LYS
1	C	182	ASP
1	C	204	VAL
1	C	242	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	145	HIS
1	A	196	ASN
1	A	217	GLN
1	A	233	ASN
1	A	244	HIS
1	B	141	ASN
1	B	144	ASN
1	B	145	HIS
1	B	166	HIS
1	B	217	GLN
1	C	143	GLN
1	C	144	ASN
1	C	145	HIS
1	C	166	HIS
1	C	217	GLN

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 carbohydrates 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 will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.