Full wwPDB X-ray Structure Validation Report (i)

Oct 16, 2021 – 09:37 PM EDT

PDB ID	:	1PIM
Title	:	DITHIONITE REDUCED E. COLI RIBONUCLEOTIDE REDUCTASE R2 SUBUNIT, D84E MUTANT
Authors	:	Voegtli, W.C.; Khidekel, N.; Baldwin, J.; Ley, B.A.; Bollinger Jr., J.M.; Rosenzweig, A.C.
Deposited on	:	2003-05-30
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 following versions of software and data (see references (i)) were used in the production of this report:

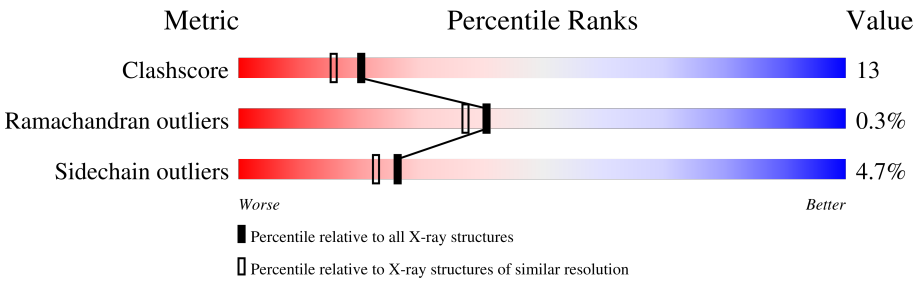
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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	375	68% 21% • 9%
1	B	375	70% 17% • 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5781 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 Ribonucleoside-diphosphate reductase 1 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	340	2784	1782	463	526	13	0	0	0
1	B	340	2784	1782	463	526	13	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	84	GLU	ASP	engineered mutation	UNP P69924
A	326	ASN	GLN	SEE REMARK 999	UNP P69924
B	84	GLU	ASP	engineered mutation	UNP P69924
B	326	ASN	GLN	SEE REMARK 999	UNP P69924

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
2	A	2	2	2	0	0
2	B	2	2	2	0	0

- Molecule 3 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Hg		
3	A	3	3	3	0	0
3	B	4	4	4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	102	102	102	0	0
			Total	O		
4	B	100	100	100	0	0

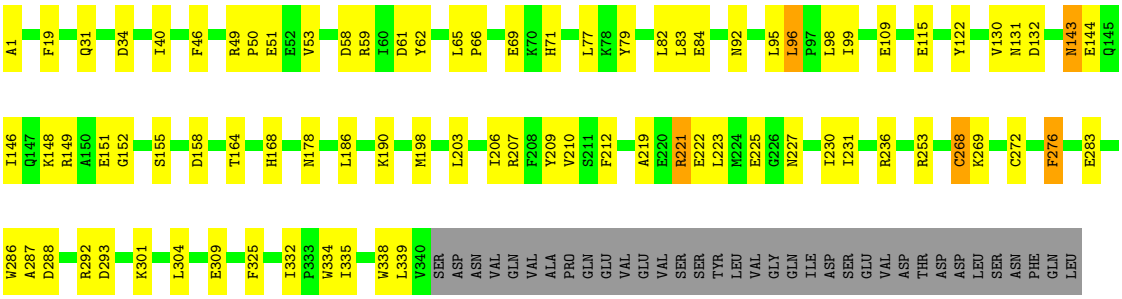
3 Residue-property plots (i)

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.

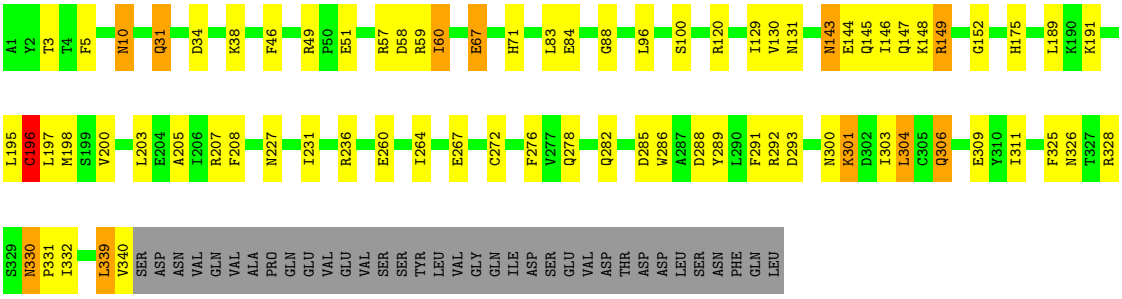
• Molecule 1: Ribonucleoside-diphosphate reductase 1 beta chain

Chain A:



• Molecule 1: Ribonucleoside-diphosphate reductase 1 beta chain

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.10Å 84.60Å 114.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.75 – 2.00	Depositor
% Data completeness (in resolution range)	97.0 (23.75-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.204 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5781	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FE, HG

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	0.34	0/2848	0.53	0/3864
1	B	0.44	1/2848 (0.0%)	0.56	0/3864
All	All	0.39	1/5696 (0.0%)	0.55	0/7728

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	196	CYS	CB-SG	12.35	2.03	1.82

There are no bond angle outliers.

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	2784	0	2727	72	0
1	B	2784	0	2724	71	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	3	0	0	0	0
3	B	4	0	0	0	0
4	A	102	0	0	1	0
4	B	100	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5781	0	5451	137	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 13.

All (137) 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:B:196:CYS:CB	1:B:196:CYS:SG	2.03	1.44
1:A:84:GLU:HG3	1:A:122:TYR:HE2	1.42	0.82
1:A:50:PRO:O	1:A:53:VAL:HG12	1.80	0.81
1:B:236:ARG:HD2	4:B:555:HOH:O	1.82	0.79
1:B:143:ASN:HD22	1:B:146:ILE:H	1.29	0.79
1:A:53:VAL:HG11	1:A:230:ILE:HD11	1.69	0.74
1:B:3:THR:HG22	1:B:5:PHE:H	1.51	0.74
1:B:130:VAL:O	1:B:131:ASN:HB2	1.86	0.73
1:B:148:LYS:O	1:B:149:ARG:HD3	1.87	0.73
1:B:149:ARG:HD2	1:B:282:GLN:HB3	1.71	0.72
1:A:158:ASP:OD2	1:B:3:THR:HG23	1.90	0.71
1:B:143:ASN:ND2	1:B:146:ILE:H	1.88	0.71
1:A:40:ILE:HG21	1:B:120:ARG:HH21	1.58	0.69
1:A:203:LEU:CD1	1:A:207:ARG:HD2	2.26	0.66
1:B:264:ILE:O	1:B:267:GLU:HG3	1.97	0.65
1:A:203:LEU:HD13	1:A:207:ARG:HD2	1.79	0.64
1:B:129:ILE:HG13	1:B:130:VAL:HG13	1.79	0.64
1:A:130:VAL:HG12	1:A:132:ASP:H	1.63	0.63
1:A:221:ARG:O	1:A:223:LEU:HD13	1.99	0.63
1:B:46:PHE:CD2	1:B:236:ARG:HD3	2.35	0.62
1:B:145:GLN:HG2	1:B:289:TYR:CD2	2.35	0.62
1:A:335:ILE:O	1:A:339:LEU:HD23	1.99	0.61
1:A:61:ASP:O	1:A:65:LEU:HD13	2.00	0.61
1:B:49:ARG:HB3	1:B:51:GLU:OE1	2.01	0.61
1:A:144:GLU:O	1:A:148:LYS:HG2	2.01	0.59
1:B:203:LEU:HD13	1:B:207:ARG:HD2	1.84	0.59
1:A:31:GLN:HG3	1:A:34:ASP:HA	1.83	0.59
1:B:34:ASP:O	1:B:38:LYS:HD3	2.02	0.59
1:A:143:ASN:HD22	1:A:146:ILE:HG13	1.68	0.58
1:B:147:GLN:C	1:B:149:ARG:H	2.07	0.58
1:A:65:LEU:HD11	1:A:223:LEU:HD23	1.83	0.58
1:A:143:ASN:ND2	1:A:146:ILE:HG13	2.19	0.58
1:A:79:TYR:CD2	1:A:149:ARG:NH2	2.71	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ARG:HD2	4:A:551:HOH:O	2.03	0.58
1:B:144:GLU:O	1:B:148:LYS:HG3	2.04	0.58
1:B:10:ASN:H	1:B:10:ASN:HD22	1.50	0.57
1:B:152:GLY:HA3	4:B:558:HOH:O	2.04	0.56
1:B:292:ARG:HG3	1:B:293:ASP:OD2	2.06	0.56
1:A:84:GLU:HG3	1:A:122:TYR:CE2	2.32	0.56
1:A:130:VAL:HG12	1:A:132:ASP:N	2.21	0.55
1:B:120:ARG:HG2	1:B:120:ARG:NH1	2.21	0.55
1:A:149:ARG:HD2	1:A:283:GLU:CD	2.28	0.54
1:B:291:PHE:HE2	1:B:304:LEU:HD12	1.73	0.54
1:A:149:ARG:CZ	1:A:286:TRP:CD1	2.91	0.53
1:B:51:GLU:H	1:B:51:GLU:CD	2.11	0.53
1:B:67:GLU:HG2	4:B:540:HOH:O	2.08	0.53
1:B:46:PHE:CG	1:B:236:ARG:HD3	2.43	0.53
1:B:285:ASP:O	1:B:288:ASP:HB3	2.08	0.53
1:B:330:ASN:ND2	1:B:332:ILE:H	2.05	0.53
1:A:66:PRO:HG2	1:A:69:GLU:HB2	1.91	0.53
1:A:292:ARG:HG3	1:A:293:ASP:N	2.23	0.52
1:A:149:ARG:HD2	1:A:283:GLU:OE2	2.08	0.52
1:B:330:ASN:HD22	1:B:331:PRO:N	2.07	0.52
1:A:149:ARG:NH1	1:A:283:GLU:OE1	2.43	0.52
1:B:309:GLU:HG2	1:B:325:PHE:CD2	2.45	0.52
1:B:145:GLN:HG2	1:B:289:TYR:CG	2.45	0.51
1:A:288:ASP:OD1	1:A:301:LYS:HE3	2.10	0.51
1:A:309:GLU:HG2	1:A:325:PHE:CD1	2.46	0.51
1:B:328:ARG:HH11	1:B:328:ARG:HG2	1.74	0.51
1:B:120:ARG:HG2	1:B:120:ARG:HH11	1.75	0.51
1:A:149:ARG:HD3	1:A:286:TRP:CB	2.41	0.50
1:B:198:MET:HG3	1:B:272:CYS:SG	2.52	0.50
1:B:330:ASN:HD22	1:B:330:ASN:C	2.15	0.50
1:A:92:ASN:O	1:A:96:LEU:HB2	2.11	0.49
1:A:149:ARG:HD3	1:A:286:TRP:HB2	1.94	0.49
1:A:334:TRP:CZ3	1:A:335:ILE:HG22	2.47	0.49
1:A:186:LEU:HG	1:A:190:LYS:HE3	1.93	0.49
1:A:332:ILE:HD12	1:A:335:ILE:HG21	1.94	0.49
1:B:143:ASN:HD21	1:B:145:GLN:HB3	1.78	0.49
1:B:260:GLU:O	1:B:264:ILE:HG13	2.13	0.49
1:B:300:ASN:H	1:B:303:ILE:CG2	2.26	0.49
1:A:198:MET:HG2	1:A:272:CYS:HB2	1.95	0.49
1:A:130:VAL:CG1	1:A:132:ASP:H	2.24	0.48
1:B:203:LEU:CD1	1:B:207:ARG:HD2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:LEU:HD22	1:B:203:LEU:HD11	1.96	0.48
1:B:197:LEU:HA	1:B:200:VAL:HG12	1.95	0.48
1:A:152:GLY:O	1:A:155:SER:HB3	2.14	0.47
1:A:292:ARG:HG3	1:A:293:ASP:H	1.78	0.47
1:A:268:CYS:SG	1:A:272:CYS:SG	3.11	0.47
1:B:71:HIS:NE2	1:B:292:ARG:NH1	2.54	0.47
1:A:62:TYR:O	1:A:65:LEU:HB2	2.15	0.47
1:A:79:TYR:CE2	1:A:83:LEU:HD11	2.49	0.47
1:B:191:LYS:O	1:B:195:LEU:HG	2.13	0.47
1:A:71:HIS:NE2	1:A:292:ARG:HG2	2.30	0.47
1:A:227:ASN:O	1:A:231:ILE:HG12	2.14	0.47
1:B:10:ASN:HD22	1:B:10:ASN:N	2.11	0.47
1:A:82:LEU:C	1:A:82:LEU:HD23	2.35	0.47
1:B:31:GLN:HG3	1:B:34:ASP:HA	1.97	0.47
1:A:53:VAL:HG11	1:A:230:ILE:CD1	2.43	0.46
1:B:330:ASN:HD22	1:B:331:PRO:CD	2.28	0.46
1:B:291:PHE:HB3	1:B:301:LYS:HZ2	1.81	0.46
1:B:205:ALA:O	1:B:311:ILE:HD11	2.15	0.46
1:A:339:LEU:HD22	1:A:339:LEU:N	2.31	0.45
1:A:50:PRO:HG2	1:A:51:GLU:OE1	2.16	0.45
1:A:219:ALA:HB1	1:A:338:TRP:CH2	2.51	0.45
1:A:40:ILE:HG21	1:B:120:ARG:NH2	2.30	0.45
1:A:109:GLU:OE2	1:B:88:GLY:O	2.35	0.44
1:A:40:ILE:HG21	1:B:120:ARG:HE	1.81	0.44
1:A:95:LEU:O	1:A:99:ILE:HG13	2.17	0.44
1:A:59:ARG:NH2	1:A:131:ASN:HD22	2.15	0.44
1:A:79:TYR:OH	1:A:149:ARG:HG2	2.17	0.44
1:B:306:GLN:CA	1:B:306:GLN:HE21	2.29	0.44
1:B:339:LEU:HB3	1:B:340:VAL:H	1.54	0.44
1:A:198:MET:SD	1:A:276:PHE:HE2	2.40	0.44
1:B:309:GLU:HG2	1:B:325:PHE:CE2	2.52	0.44
1:A:309:GLU:HG2	1:A:325:PHE:CG	2.52	0.44
1:A:46:PHE:CD2	1:A:236:ARG:HD3	2.51	0.44
1:A:287:ALA:HB2	1:A:304:LEU:HD22	2.00	0.44
1:A:203:LEU:HD12	1:A:207:ARG:HD2	1.97	0.43
1:B:57:ARG:CZ	4:B:581:HOH:O	2.66	0.43
1:B:31:GLN:HE21	1:B:31:GLN:HB3	1.66	0.43
1:B:328:ARG:HG2	1:B:328:ARG:NH1	2.34	0.43
1:A:1:ALA:N	1:A:168:HIS:O	2.49	0.43
1:A:209:TYR:HA	1:A:212:PHE:CD2	2.53	0.43
1:B:83:LEU:HD13	1:B:203:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:LEU:HD21	1:A:164:THR:HG23	2.01	0.42
1:B:60:ILE:O	1:B:60:ILE:HD13	2.20	0.42
1:B:59:ARG:NH1	1:B:131:ASN:ND2	2.68	0.42
1:A:206:ILE:O	1:A:210:VAL:HG23	2.20	0.41
1:A:222:GLU:O	1:A:223:LEU:HD12	2.20	0.41
1:B:301:LYS:CD	1:B:301:LYS:H	2.33	0.41
1:A:19:PHE:CE2	1:A:190:LYS:HG2	2.54	0.41
1:A:288:ASP:CG	1:A:301:LYS:HE3	2.41	0.41
1:B:147:GLN:C	1:B:149:ARG:N	2.72	0.41
1:A:178:ASN:HD21	1:B:175:HIS:CD2	2.38	0.41
1:B:227:ASN:O	1:B:231:ILE:HG12	2.20	0.41
1:B:306:GLN:HE21	1:B:306:GLN:HA	1.86	0.41
1:A:46:PHE:CG	1:A:236:ARG:HD3	2.55	0.41
1:A:115:GLU:HA	1:A:115:GLU:OE1	2.21	0.40
1:B:306:GLN:HA	1:B:306:GLN:NE2	2.36	0.40
1:A:83:LEU:HD13	1:A:203:LEU:HD11	2.03	0.40
1:B:149:ARG:NH2	1:B:286:TRP:CE3	2.89	0.40
1:B:148:LYS:C	1:B:149:ARG:HD3	2.41	0.40
1:B:149:ARG:HG2	1:B:149:ARG:HH11	1.86	0.40
1:A:31:GLN:CG	1:A:34:ASP:HA	2.48	0.40
1:A:148:LYS:O	1:A:151:GLU:HG2	2.22	0.40
1:B:326:ASN:OD1	1:B:328:ARG:NH2	2.55	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	338/375 (90%)	329 (97%)	7 (2%)	2 (1%)	25 19
1	B	338/375 (90%)	331 (98%)	7 (2%)	0	100 100
All	All	676/750 (90%)	660 (98%)	14 (2%)	2 (0%)	41 37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	ASN
1	A	269	LYS

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	306/340 (90%)	297 (97%)	9 (3%)	42	43
1	B	306/340 (90%)	286 (94%)	20 (6%)	17	12
All	All	612/680 (90%)	583 (95%)	29 (5%)	26	22

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	58	ASP
1	A	77	LEU
1	A	96	LEU
1	A	221	ARG
1	A	225	GLU
1	A	253	ARG
1	A	268	CYS
1	A	276	PHE
1	B	10	ASN
1	B	31	GLN
1	B	58	ASP
1	B	60	ILE
1	B	67	GLU
1	B	84	GLU
1	B	96	LEU
1	B	100	SER
1	B	143	ASN
1	B	149	ARG
1	B	189	LEU
1	B	196	CYS

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Mol	Chain	Res	Type
1	B	208	PHE
1	B	276	PHE
1	B	278	GLN
1	B	301	LYS
1	B	304	LEU
1	B	306	GLN
1	B	330	ASN
1	B	339	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	ASN
1	A	143	ASN
1	A	147	GLN
1	A	227	ASN
1	A	278	GLN
1	A	306	GLN
1	A	317	GLN
1	B	10	ASN
1	B	21	GLN
1	B	31	GLN
1	B	63	GLN
1	B	128	ASN
1	B	131	ASN
1	B	143	ASN
1	B	175	HIS
1	B	270	GLN
1	B	306	GLN
1	B	330	ASN
1	B	336	ASN

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)

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.