Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:23 PM GMT

PDB ID	:	1AJA
Title	:	THREE-DIMENSIONAL STRUCTURE OF THE D153G MUTANT OF E. COLI ALKALINE PHOSPHATASE: A MUTANT WITH WEAKER MAGNESIUM BINDING AND INCREASED CATALYTIC ACTIVITY
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Deposited on	:	1995-08-19
Resolution	:	2.50 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 (i) symbol.

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

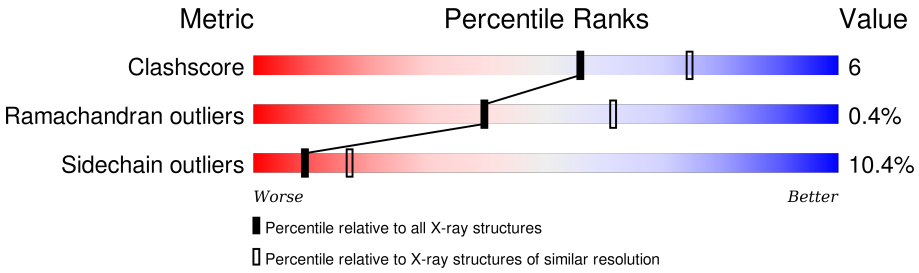
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.50 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	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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	449	77% 17%
1	B	449	76% 16%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6352 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 ALKALINE PHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	0	0
			3184	1975	560	637	12			
1	B	434	Total	C	N	O	S	0	0	0
			3168	1967	556	633	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	GLY	ASP	ENGINEERED	UNP P00634
A	230	GLU	GLN	CONFLICT	UNP P00634
B	153	GLY	ASP	ENGINEERED	UNP P00634
B	230	GLU	GLN	CONFLICT	UNP P00634

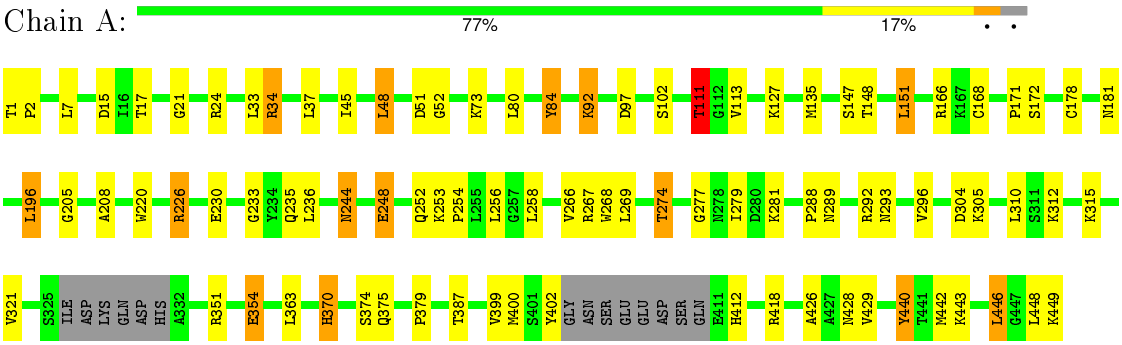
3 Residue-property plots (i)

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.

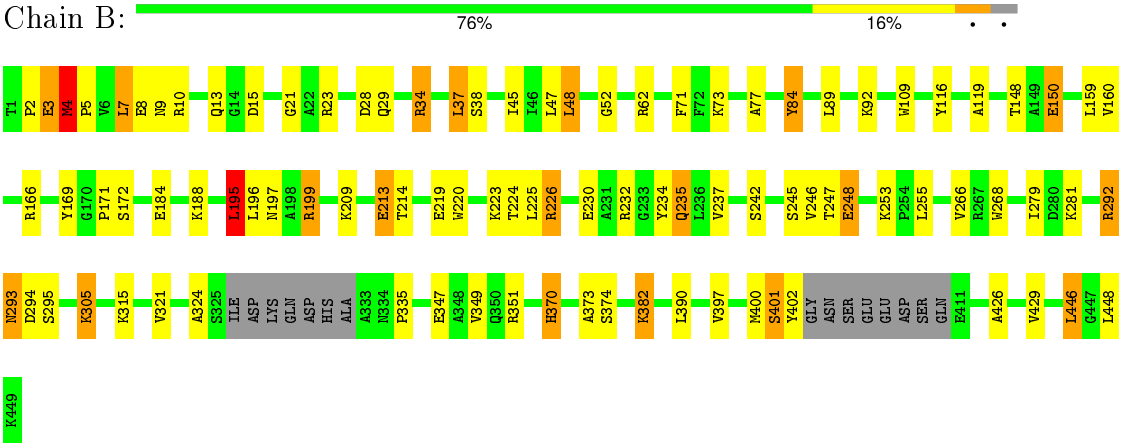
- Molecule 1: ALKALINE PHOSPHATASE

Chain A:



- Molecule 1: ALKALINE PHOSPHATASE

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	195.02Å 166.93Å 76.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.162 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6352	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	0.67	0/3236	1.31	25/4391 (0.6%)
1	B	0.66	0/3219	1.32	34/4369 (0.8%)
All	All	0.66	0/6455	1.31	59/8760 (0.7%)

There are no bond length outliers.

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	418	ARG	NE-CZ-NH2	-11.66	114.47	120.30
1	A	418	ARG	NE-CZ-NH1	10.90	125.75	120.30
1	B	220	TRP	CD1-CG-CD2	9.79	114.13	106.30
1	A	220	TRP	CD1-CG-CD2	9.30	113.74	106.30
1	A	84	TYR	CB-CG-CD2	-8.65	115.81	121.00
1	B	268	TRP	CD1-CG-CD2	8.57	113.16	106.30
1	B	226	ARG	NE-CZ-NH1	8.49	124.55	120.30
1	B	268	TRP	CE2-CD2-CG	-8.44	100.55	107.30
1	B	220	TRP	CE2-CD2-CG	-8.34	100.63	107.30
1	A	268	TRP	CD1-CG-CD2	8.02	112.72	106.30
1	A	220	TRP	CE2-CD2-CG	-8.00	100.90	107.30
1	B	199	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	B	199	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	A	268	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	B	195	LEU	CA-CB-CG	7.15	131.75	115.30
1	A	351	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	B	226	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	B	109	TRP	CD1-CG-CD2	6.93	111.84	106.30
1	B	84	TYR	CB-CG-CD2	-6.86	116.89	121.00
1	B	166	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	B	48	LEU	CA-CB-CG	6.61	130.51	115.30
1	B	268	TRP	CG-CD2-CE3	6.60	139.84	133.90
1	A	84	TYR	CA-CB-CG	6.56	125.87	113.40
1	B	7	LEU	CA-C-N	-6.49	102.93	117.20
1	B	292	ARG	NE-CZ-NH2	-6.26	117.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	34	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	B	292	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	B	34	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	A	351	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	B	293	ASN	CB-CA-C	-6.02	98.35	110.40
1	B	4	MET	CG-SD-CE	6.01	109.82	100.20
1	B	3	GLU	O-C-N	5.98	132.27	122.70
1	B	166	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	97	ASP	N-CA-C	-5.91	95.05	111.00
1	A	220	TRP	CG-CD1-NE1	-5.90	104.20	110.10
1	B	324	ALA	CA-C-N	5.84	130.04	117.20
1	B	109	TRP	CE2-CD2-CG	-5.80	102.66	107.30
1	B	220	TRP	CG-CD1-NE1	-5.80	104.30	110.10
1	A	354	GLU	CA-CB-CG	5.76	126.08	113.40
1	A	34	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	A	111	THR	N-CA-CB	-5.57	99.71	110.30
1	B	169	TYR	CB-CG-CD2	-5.57	117.66	121.00
1	A	24	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	B	34	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	B	62	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	266	VAL	CA-CB-CG2	-5.44	102.74	110.90
1	A	440	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	A	267	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	B	400	MET	CA-CB-CG	-5.36	104.18	113.30
1	B	226	ARG	CB-CG-CD	5.36	125.52	111.60
1	B	220	TRP	CB-CG-CD1	-5.30	120.10	127.00
1	B	84	TYR	CA-CB-CG	5.28	123.44	113.40
1	A	226	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	293	ASN	N-CA-C	5.16	124.93	111.00
1	A	442	MET	CA-CB-CG	-5.16	104.53	113.30
1	A	220	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	A	220	TRP	CG-CD2-CE3	5.07	138.46	133.90
1	A	168	CYS	CA-CB-SG	-5.06	104.89	114.00
1	B	219	GLU	CA-CB-CG	5.03	124.46	113.40

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	3184	0	3147	43	0
1	B	3168	0	3133	41	0
All	All	6352	0	6280	78	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 6.

All (78) 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:293:ASN:HB3	1:A:296:VAL:H	1.53	0.73
1:A:315:LYS:HE2	1:A:315:LYS:HA	1.76	0.68
1:B:45:ILE:HD12	1:B:446:LEU:HD22	1.76	0.66
1:A:111:THR:HG22	1:A:113:VAL:H	1.60	0.66
1:A:293:ASN:HB2	1:A:296:VAL:HG23	1.79	0.65
1:A:379:PRO:HA	1:A:399:VAL:HG21	1.79	0.65
1:A:293:ASN:CB	1:A:296:VAL:HG23	2.26	0.64
1:A:102:SER:HB3	1:A:166:ARG:HH12	1.64	0.62
1:A:248:GLU:HG2	1:A:312:LYS:HE2	1.80	0.62
1:B:426:ALA:O	1:B:429:VAL:HG22	2.01	0.61
1:A:111:THR:CG2	1:A:113:VAL:HG12	2.31	0.61
1:B:48:LEU:HD13	1:B:321:VAL:HB	1.85	0.59
1:B:293:ASN:HB3	1:B:295:SER:H	1.67	0.58
1:B:248:GLU:HG3	1:B:253:LYS:NZ	2.19	0.58
1:B:160:VAL:HG21	1:B:195:LEU:HD22	1.85	0.57
1:B:171:PRO:HD2	1:B:213:GLU:HG2	1.87	0.57
1:A:289:ASN:O	1:A:292:ARG:HG2	2.05	0.56
1:B:52:GLY:HA2	1:B:370:HIS:O	2.05	0.56
1:A:52:GLY:HA2	1:A:370:HIS:O	2.05	0.56
1:B:8:GLU:HG3	1:B:9:ASN:H	1.70	0.56
1:A:293:ASN:HB2	1:A:296:VAL:CG2	2.36	0.56
1:B:48:LEU:HG	1:B:349:VAL:HG22	1.90	0.54
1:A:17:THR:HG22	1:B:89:LEU:HD13	1.89	0.54
1:B:4:MET:HE3	1:B:38:SER:HB2	1.90	0.53
1:A:292:ARG:O	1:A:296:VAL:HB	2.09	0.53
1:B:374:SER:HA	1:B:401:SER:O	2.10	0.52
1:A:92:LYS:HA	1:A:92:LYS:HE3	1.91	0.52
1:B:197:ASN:HA	1:B:232:ARG:NH2	2.24	0.52
1:B:10:ARG:HB2	1:B:71:PHE:CD1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:ALA:O	1:A:429:VAL:HG22	2.11	0.51
1:B:197:ASN:HA	1:B:232:ARG:HH22	1.77	0.50
1:B:248:GLU:HG3	1:B:253:LYS:HZ1	1.77	0.49
1:B:279:ILE:HD11	1:B:382:LYS:HE2	1.93	0.49
1:A:1:THR:N	1:A:2:PRO:HD3	2.27	0.49
1:A:33:LEU:HD23	1:B:37:LEU:HD11	1.94	0.49
1:B:7:LEU:HB2	1:B:77:ALA:HA	1.95	0.49
1:B:235:GLN:HG3	1:B:255:LEU:HA	1.96	0.48
1:A:374:SER:HB3	1:A:402:TYR:CE1	2.48	0.48
1:B:226:ARG:O	1:B:230:GLU:HG3	2.14	0.48
1:B:92:LYS:HA	1:B:92:LYS:HD2	1.62	0.48
1:B:15:ASP:O	1:B:21:GLY:HA3	2.15	0.47
1:A:48:LEU:HD13	1:A:321:VAL:HB	1.95	0.47
1:A:375:GLN:HE22	1:B:373:ALA:HA	1.80	0.47
1:A:226:ARG:O	1:A:230:GLU:HG3	2.15	0.47
1:B:237:VAL:HG22	1:B:242:SER:HB2	1.96	0.46
1:A:440:TYR:CE2	1:B:23:ARG:HD2	2.50	0.46
1:B:199:ARG:HA	1:B:234:TYR:OH	2.15	0.46
1:B:4:MET:HE3	1:B:38:SER:CB	2.45	0.46
1:A:45:ILE:HD12	1:A:446:LEU:HD22	1.97	0.46
1:A:379:PRO:HA	1:A:399:VAL:CG2	2.45	0.46
1:A:135:MET:HB3	1:A:135:MET:HE2	1.89	0.46
1:B:214:THR:HA	1:B:224:THR:HA	1.97	0.45
1:A:45:ILE:HG12	1:A:363:LEU:HB3	1.98	0.45
1:A:15:ASP:O	1:A:21:GLY:HA3	2.17	0.44
1:A:292:ARG:HG3	1:A:293:ASN:N	2.32	0.44
1:A:387:THR:HA	1:A:400:MET:O	2.17	0.44
1:B:116:TYR:CZ	1:B:119:ALA:HB2	2.53	0.44
1:A:111:THR:HG21	1:A:113:VAL:HG12	2.00	0.43
1:A:428:ASN:OD1	1:B:28:ASP:HA	2.19	0.43
1:B:4:MET:HA	1:B:5:PRO:HD2	1.83	0.43
1:A:208:ALA:HB2	1:A:258:LEU:HB3	2.02	0.42
1:B:390:LEU:O	1:B:397:VAL:HA	2.18	0.42
1:A:274:THR:HG22	1:A:277:GLY:CA	2.50	0.42
1:A:37:LEU:HD13	1:B:34:ARG:HG3	2.02	0.41
1:B:292:ARG:O	1:B:293:ASN:HB2	2.19	0.41
1:A:244:ASN:HA	1:A:305:LYS:HE2	2.02	0.41
1:A:48:LEU:CD1	1:A:321:VAL:HB	2.51	0.41
1:A:233:GLY:O	1:A:254:PRO:HD2	2.21	0.41
1:B:150:GLU:HG2	1:B:150:GLU:H	1.62	0.41
1:A:151:LEU:HA	1:A:151:LEU:HD12	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:SER:O	1:A:205:GLY:HA2	2.20	0.41
1:A:178:CYS:HB3	1:A:181:ASN:OD1	2.20	0.41
1:B:347:GLU:O	1:B:351:ARG:HG2	2.21	0.41
1:B:335:PRO:HG3	1:B:402:TYR:CE2	2.56	0.41
1:B:305:LYS:HD3	1:B:305:LYS:HA	1.90	0.41
1:A:236:LEU:HA	1:A:256:LEU:O	2.21	0.41
1:B:242:SER:O	1:B:246:VAL:HG23	2.21	0.40
1:A:196:LEU:HA	1:A:196:LEU:HD12	1.97	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	429/449 (96%)	415 (97%)	13 (3%)	1 (0%)	52	75
1	B	428/449 (95%)	407 (95%)	19 (4%)	2 (0%)	34	55
All	All	857/898 (95%)	822 (96%)	32 (4%)	3 (0%)	39	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4	MET
1	A	51	ASP
1	B	2	PRO

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	325/339 (96%)	292 (90%)	33 (10%)	9 17
1	B	322/339 (95%)	288 (89%)	34 (11%)	8 16
All	All	647/678 (95%)	580 (90%)	67 (10%)	9 16

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	34	ARG
1	A	48	LEU
1	A	73	LYS
1	A	80	LEU
1	A	84	TYR
1	A	92	LYS
1	A	111	THR
1	A	127	LYS
1	A	148	THR
1	A	151	LEU
1	A	171	PRO
1	A	172	SER
1	A	196	LEU
1	A	235	GLN
1	A	244	ASN
1	A	248	GLU
1	A	252	GLN
1	A	253	LYS
1	A	269	LEU
1	A	274	THR
1	A	279	ILE
1	A	281	LYS
1	A	288	PRO
1	A	304	ASP
1	A	310	LEU
1	A	354	GLU
1	A	370	HIS
1	A	412	HIS
1	A	443	LYS
1	A	446	LEU
1	A	448	LEU
1	A	449	LYS

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Mol	Chain	Res	Type
1	B	3	GLU
1	B	4	MET
1	B	13	GLN
1	B	29	GLN
1	B	37	LEU
1	B	47	LEU
1	B	73	LYS
1	B	84	TYR
1	B	148	THR
1	B	150	GLU
1	B	159	LEU
1	B	172	SER
1	B	184	GLU
1	B	188	LYS
1	B	195	LEU
1	B	196	LEU
1	B	209	LYS
1	B	213	GLU
1	B	223	LYS
1	B	225	LEU
1	B	235	GLN
1	B	245	SER
1	B	247	THR
1	B	248	GLU
1	B	266	VAL
1	B	281	LYS
1	B	294	ASP
1	B	305	LYS
1	B	315	LYS
1	B	370	HIS
1	B	382	LYS
1	B	401	SER
1	B	446	LEU
1	B	448	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	252	GLN
1	A	338	GLN
1	A	375	GLN
1	A	391	ASN

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Mol	Chain	Res	Type
1	B	9	ASN
1	B	13	GLN
1	B	29	GLN
1	B	235	GLN
1	B	334	ASN
1	B	338	GLN
1	B	370	HIS

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.