



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 11:13 AM GMT

PDB ID : 1AJB  
Title : THREE-DIMENSIONAL STRUCTURE OF THE D153G MUTANT OF E. COLI ALKALINE PHOSPHATASE: A MUTANT WITH WEAKER MAGNESIUM BINDING AND INCREASED CATALYTIC ACTIVITY  
Authors : Dealwis, C.G.; Chen, L.; Abad-Zapatero, C.  
Deposited on : 1995-08-19  
Resolution : 2.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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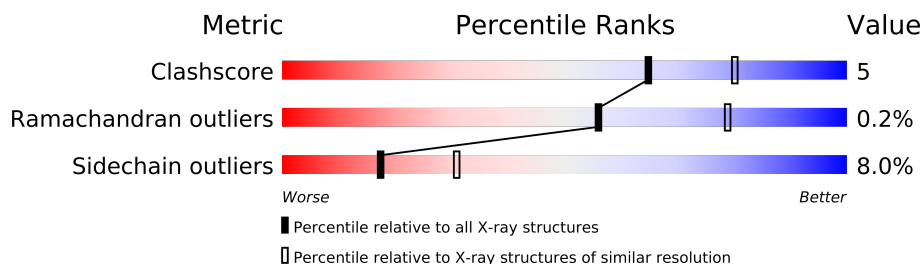
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : NOT EXECUTED  
EDS : NOT EXECUTED  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	449	
1	B	449	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6783 atoms, of which 0 are hydrogen and 0 are deuterium.

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	449	Total	C	N	O	S	0	0	0
			3300	2040	580	668	12			
1	B	449	Total	C	N	O	S	0	0	0
			3300	2040	580	668	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

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

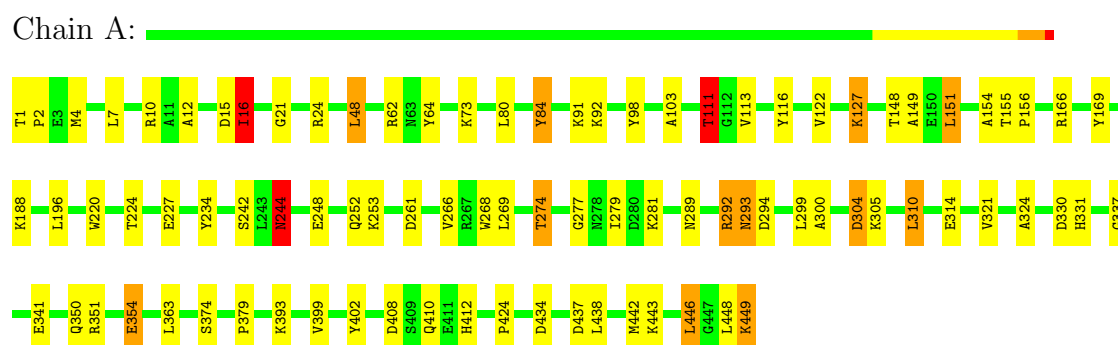
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	103	Total	O	8	0
			103	103		
5	B	64	Total	O	0	0
			64	64		

### 3 Residue-property plots

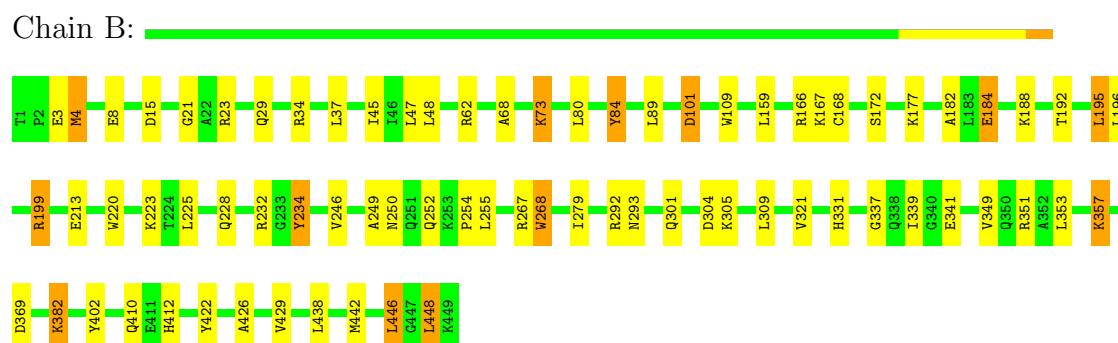
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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



#### • Molecule 1: ALKALINE PHOSPHATASE



## 4 Data and refinement statistics

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, $\alpha$ , $\beta$ , $\gamma$	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	6783	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, SO4

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	0.78	0/3355	1.37	28/4554 (0.6%)
1	B	0.77	0/3355	1.37	29/4554 (0.6%)
All	All	0.78	0/6710	1.37	57/9108 (0.6%)

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	ARG	NE-CZ-NH1	16.22	128.41	120.30
1	A	166	ARG	NE-CZ-NH2	-14.43	113.08	120.30
1	B	84	TYR	CB-CG-CD2	-10.39	114.77	121.00
1	B	267	ARG	NE-CZ-NH2	-9.44	115.58	120.30
1	B	199	ARG	NE-CZ-NH1	9.43	125.02	120.30
1	B	220	TRP	CD1-CG-CD2	8.97	113.48	106.30
1	B	166	ARG	NE-CZ-NH1	8.77	124.69	120.30
1	B	267	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	A	234	TYR	CB-CG-CD2	-8.12	116.13	121.00
1	A	62	ARG	NE-CZ-NH2	-8.03	116.29	120.30
1	B	34	ARG	NE-CZ-NH1	7.75	124.18	120.30
1	A	220	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	B	268	TRP	CD1-CG-CD2	7.68	112.44	106.30
1	B	109	TRP	CD1-CG-CD2	7.46	112.27	106.30
1	A	84	TYR	CB-CG-CD2	-7.46	116.53	121.00
1	B	199	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	B	220	TRP	CE2-CD2-CG	-7.26	101.49	107.30
1	B	268	TRP	CE2-CD2-CG	-7.04	101.67	107.30
1	A	268	TRP	CE2-CD2-CG	-7.03	101.68	107.30
1	B	84	TYR	CB-CG-CD1	6.94	125.16	121.00
1	A	268	TRP	CD1-CG-CD2	6.82	111.76	106.30
1	B	109	TRP	CE2-CD2-CG	-6.82	101.84	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	234	TYR	CB-CG-CD2	-6.69	116.99	121.00
1	A	292	ARG	NE-CZ-NH2	6.57	123.59	120.30
1	A	220	TRP	CE2-CD2-CG	-6.35	102.22	107.30
1	A	84	TYR	CA-CB-CG	6.29	125.35	113.40
1	B	292	ARG	NE-CZ-NH2	6.25	123.42	120.30
1	A	151	LEU	CB-CG-CD2	-6.21	100.45	111.00
1	B	4	MET	CG-SD-CE	6.18	110.08	100.20
1	A	268	TRP	CG-CD2-CE3	6.10	139.39	133.90
1	A	16	ILE	CA-CB-CG1	-5.95	99.70	111.00
1	A	111	THR	N-CA-CB	-5.89	99.11	110.30
1	A	4	MET	CG-SD-CE	5.84	109.54	100.20
1	A	169	TYR	CB-CG-CD2	-5.81	117.52	121.00
1	B	293	ASN	CB-CA-C	-5.78	98.85	110.40
1	B	369	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	16	ILE	CA-CB-CG2	5.68	122.27	110.90
1	B	168	CYS	CA-CB-SG	-5.55	104.01	114.00
1	B	369	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	B	220	TRP	CG-CD1-NE1	-5.51	104.59	110.10
1	B	23	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	24	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	A	10	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	B	3	GLU	O-C-N	5.33	131.23	122.70
1	A	412	HIS	CB-CA-C	-5.32	99.77	110.40
1	A	10	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	A	244	ASN	CA-CB-CG	-5.27	101.81	113.40
1	A	330	ASP	CB-CG-OD1	5.25	123.03	118.30
1	B	422	TYR	CB-CG-CD2	-5.21	117.88	121.00
1	B	166	ARG	NH1-CZ-NH2	-5.16	113.73	119.40
1	A	351	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	A	62	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	62	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	B	351	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	351	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	109	TRP	CG-CD1-NE1	-5.02	105.08	110.10
1	A	310	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

There are no planarity outliers.



## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3300	0	3246	42	0
1	B	3300	0	3246	29	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	103	0	0	0	0
5	B	64	0	0	1	0
All	All	6783	0	6492	69	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (69) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:155:THR:HB	1:A:156:PRO:HD3	1.59	0.82
1:A:111:THR:CG2	1:A:113:VAL:HG12	2.16	0.76
1:A:350:GLN:O	1:A:354:GLU:HG2	1.91	0.69
1:A:111:THR:HG23	1:A:113:VAL:HG12	1.74	0.69
1:A:48:LEU:HD13	1:A:321:VAL:HB	1.75	0.68
1:B:279:ILE:HD11	1:B:382:LYS:HE2	1.76	0.68
1:A:379:PRO:HA	1:A:399:VAL:HG21	1.80	0.64
1:A:155:THR:HB	1:A:156:PRO:CD	2.30	0.60
1:B:48:LEU:HD13	1:B:321:VAL:HB	1.82	0.60
1:B:301:GLN:O	1:B:305:LYS:HG2	2.05	0.56
1:A:292:ARG:O	1:A:293:ASN:HB2	2.05	0.55
1:A:363:LEU:HD13	1:A:424:PRO:O	2.07	0.55
1:A:438:LEU:O	1:A:442:MET:HG3	2.07	0.55
1:A:292:ARG:HG3	1:A:293:ASN:H	1.73	0.54
1:B:337:GLY:O	1:B:341:GLU:HG2	2.08	0.54
1:A:149:ALA:HB2	1:A:324:ALA:HB1	1.89	0.54
1:B:246:VAL:HG11	1:B:255:LEU:HD22	1.90	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:16:ILE:HG23	1:B:89:LEU:HD21	1.91	0.53
1:A:12:ALA:HB1	1:A:16:ILE:HD11	1.91	0.53
1:A:292:ARG:HG3	1:A:293:ASN:N	2.25	0.52
1:A:224:THR:OG1	1:A:227:GLU:HG3	2.11	0.51
1:B:192:THR:O	1:B:195:LEU:HB3	2.09	0.51
1:B:438:LEU:O	1:B:442:MET:HG3	2.11	0.50
1:A:274:THR:HG22	1:A:277:GLY:CA	2.41	0.50
1:B:101:ASP:HA	1:B:412:HIS:CE1	2.47	0.50
1:B:101:ASP:HA	1:B:412:HIS:HE1	1.76	0.49
1:A:331:HIS:ND1	1:A:410:GLN:O	2.45	0.49
1:B:234:TYR:CD2	1:B:254:PRO:HG2	2.48	0.49
1:B:446:LEU:HB3	1:B:448:LEU:HD13	1.95	0.48
1:A:300:ALA:O	1:A:304:ASP:HB2	2.15	0.47
1:A:402:TYR:HB3	1:A:410:GLN:HG3	1.97	0.47
1:A:98:TYR:HE1	1:B:68:ALA:HB2	1.79	0.47
1:B:45:ILE:HD12	1:B:446:LEU:HD22	1.97	0.47
1:A:91:LYS:HE2	1:A:116:TYR:CZ	2.50	0.47
1:A:274:THR:HG22	1:A:277:GLY:HA2	1.98	0.46
1:A:48:LEU:N	1:A:48:LEU:HD22	2.30	0.46
1:A:149:ALA:HB2	1:A:324:ALA:CB	2.46	0.46
1:B:199:ARG:NH2	1:B:232:ARG:O	2.49	0.46
1:A:122:VAL:HA	1:A:127:LYS:O	2.15	0.46
1:A:289:ASN:O	1:A:292:ARG:HG2	2.16	0.46
1:B:331:HIS:ND1	1:B:410:GLN:O	2.49	0.45
1:A:446:LEU:HB3	1:A:448:LEU:HD13	1.99	0.44
1:A:448:LEU:O	1:A:449:LYS:HB2	2.17	0.44
1:A:188:LYS:HB2	1:A:188:LYS:HE3	1.75	0.44
1:B:73:LYS:HD2	5:B:986:HOH:O	2.17	0.44
1:A:12:ALA:CB	1:A:16:ILE:HD11	2.46	0.44
1:B:182:ALA:HB1	1:B:184:GLU:OE2	2.18	0.44
1:B:48:LEU:HG	1:B:349:VAL:HG22	2.00	0.44
1:A:374:SER:HB3	1:A:402:TYR:CE2	2.53	0.44
1:A:337:GLY:O	1:A:341:GLU:HG2	2.18	0.44
1:B:402:TYR:HB3	1:B:410:GLN:HG3	1.99	0.44
1:B:353:LEU:O	1:B:357:LYS:HB3	2.18	0.44
1:A:64:TYR:O	1:A:393:LYS:HB2	2.19	0.42
1:A:244:ASN:HA	1:A:305:LYS:HE2	2.01	0.42
1:A:1:THR:N	1:A:2:PRO:HD3	2.34	0.42
1:B:249:ALA:HB2	1:B:309:LEU:HD13	2.01	0.42
1:A:449:LYS:HA	1:A:449:LYS:HE3	2.01	0.42
1:B:48:LEU:HD22	1:B:48:LEU:N	2.35	0.42
1:B:426:ALA:O	1:B:429:VAL:HG22	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:268:TRP:CZ3	1:B:339:ILE:HG22	2.55	0.42
1:A:379:PRO:HA	1:A:399:VAL:CG2	2.49	0.41
1:B:167:LYS:HB3	1:B:177:LYS:HD3	2.03	0.41
1:B:15:ASP:O	1:B:21:GLY:HA3	2.21	0.41
1:B:228:GLN:O	1:B:232:ARG:HG3	2.20	0.41
1:A:103:ALA:HA	1:A:154:ALA:HB1	2.03	0.41
1:B:80:LEU:HD12	1:B:426:ALA:HB3	2.02	0.41
1:A:148:THR:HG23	1:A:299:LEU:HD13	2.02	0.41
1:A:434:ASP:O	1:A:437:ASP:HB2	2.21	0.40
1:A:15:ASP:O	1:A:21:GLY:HA3	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	447/449 (100%)	439 (98%)	7 (2%)	1 (0%)	56	79
1	B	447/449 (100%)	432 (97%)	14 (3%)	1 (0%)	56	79
All	All	894/898 (100%)	871 (97%)	21 (2%)	2 (0%)	56	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4	MET
1	A	293	ASN

### 5.3.2 Protein sidechains ⓘ

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	339/339 (100%)	308 (91%)	31 (9%)	14	24
1	B	339/339 (100%)	316 (93%)	23 (7%)	22	39
All	All	678/678 (100%)	624 (92%)	54 (8%)	17	31

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	16	ILE
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	151	LEU
1	A	196	LEU
1	A	242	SER
1	A	244	ASN
1	A	248	GLU
1	A	252	GLN
1	A	253	LYS
1	A	261	ASP
1	A	266	VAL
1	A	269	LEU
1	A	274	THR
1	A	279	ILE
1	A	281	LYS
1	A	294	ASP
1	A	304	ASP
1	A	310	LEU
1	A	314	GLU
1	A	354	GLU
1	A	408	ASP
1	A	443	LYS
1	A	446	LEU
1	A	449	LYS
1	B	8	GLU
1	B	29	GLN
1	B	37	LEU
1	B	47	LEU

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Mol	Chain	Res	Type
1	B	73	LYS
1	B	84	TYR
1	B	101	ASP
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	213	GLU
1	B	223	LYS
1	B	225	LEU
1	B	250	ASN
1	B	252	GLN
1	B	304	ASP
1	B	357	LYS
1	B	382	LYS
1	B	446	LEU
1	B	448	LEU

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

Mol	Chain	Res	Type
1	A	252	GLN
1	A	329	GLN
1	A	338	GLN
1	B	244	ASN
1	B	250	ASN
1	B	329	GLN
1	B	338	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	SO4	A	457	-	4,4,4	0.80	0	6,6,6	0.70	0
4	SO4	B	957	-	4,4,4	0.69	0	6,6,6	0.69	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	457	-	-	0/0/0/0	0/0/0/0
4	SO4	B	957	-	-	0/0/0/0	0/0/0/0

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.

## 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.