



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:14 am GMT

PDB ID : 2YOC  
Title : Crystal structure of PulA from *Klebsiella oxytoca*  
Authors : Francetic, O.; Mechaly, A.E.; Tello-Manigne, D.; Buschiazzi, A.; Bernarde, C.; Nadeau, N.; Pugsley, A.P.; Alzari, P.M.  
Deposited on : 2012-10-23  
Resolution : 2.88 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](mailto: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.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

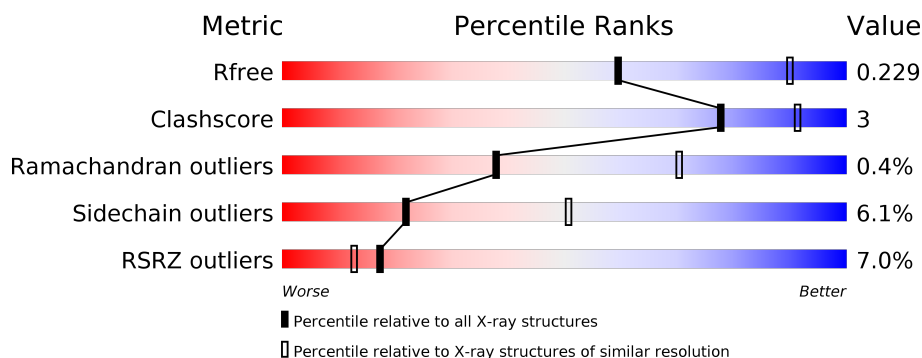
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.88 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))
$R_{free}$	100719	2135 (2.90-2.86)
Clashscore	112137	2400 (2.90-2.86)
Ramachandran outliers	110173	2346 (2.90-2.86)
Sidechain outliers	110143	2349 (2.90-2.86)
RSRZ outliers	101464	2149 (2.90-2.86)

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. 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  $\leq 5\%$ . 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.

Mol	Chain	Length	Quality of chain
1	A	1078	<div> <div>3%</div> <div>85%</div> <div>12%</div> <div>••</div> </div>
1	B	1078	<div> <div>10%</div> <div>85%</div> <div>11%</div> <div>••</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CA	A	2072	-	-	-	X
2	CA	B	2078	-	-	-	X
3	SO4	A	2076	-	-	-	X
3	SO4	A	2078	-	-	-	X
3	SO4	B	2081	-	-	-	X
3	SO4	B	2082	-	-	-	X
3	SO4	B	2083	-	-	-	X
3	SO4	B	2088	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16490 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 PULLULANASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1051	Total	C	N	O	S	Se	0	0	0
			8030	5013	1368	1621	6	22			
1	B	1055	Total	C	N	O	S	Se	0	0	0
			8074	5043	1376	1627	6	22			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	EXPRESSION TAG	UNP P07206
A	1071	TYR	-	EXPRESSION TAG	UNP P07206
A	1072	TYR	-	EXPRESSION TAG	UNP P07206
A	1073	HIS	-	EXPRESSION TAG	UNP P07206
A	1074	HIS	-	EXPRESSION TAG	UNP P07206
A	1075	HIS	-	EXPRESSION TAG	UNP P07206
A	1076	HIS	-	EXPRESSION TAG	UNP P07206
A	1077	HIS	-	EXPRESSION TAG	UNP P07206
A	1078	HIS	-	EXPRESSION TAG	UNP P07206
B	1	MSE	-	EXPRESSION TAG	UNP P07206
B	1071	TYR	-	EXPRESSION TAG	UNP P07206
B	1072	TYR	-	EXPRESSION TAG	UNP P07206
B	1073	HIS	-	EXPRESSION TAG	UNP P07206
B	1074	HIS	-	EXPRESSION TAG	UNP P07206
B	1075	HIS	-	EXPRESSION TAG	UNP P07206
B	1076	HIS	-	EXPRESSION TAG	UNP P07206
B	1077	HIS	-	EXPRESSION TAG	UNP P07206
B	1078	HIS	-	EXPRESSION TAG	UNP P07206

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	4	Total	Ca	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Ca	0	0
			4	4		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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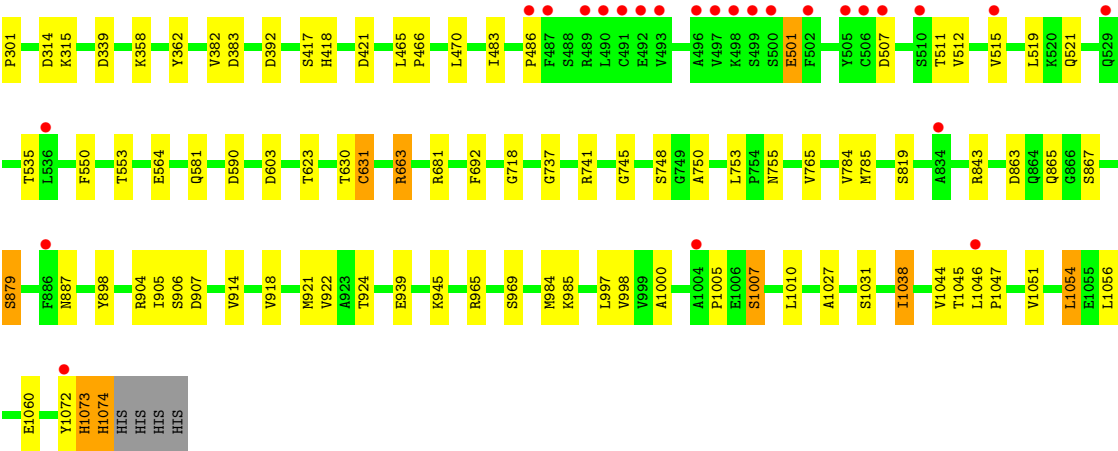
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	145	Total	O	0	0
			145	145		
4	B	163	Total	O	0	0
			163	163		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	179.15Å 179.15Å 334.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.17 – 2.88 58.64 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.5 (42.17-2.88) 99.8 (58.64-2.88)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.15 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, $R_{free}$	0.171 , 0.213 0.187 , 0.229	Depositor DCC
$R_{free}$ test set	3635 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	69.0	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 73.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16490	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: CA, 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	0.50	0/8171	0.74	2/11086 (0.0%)
1	B	0.50	0/8219	0.75	4/11152 (0.0%)
All	All	0.50	0/16390	0.74	6/22238 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	631	CYS	N-CA-C	-5.71	95.59	111.00
1	A	631	CYS	N-CA-C	-5.64	95.76	111.00
1	B	53	THR	C-N-CA	5.59	135.68	121.70
1	B	1073	HIS	C-N-CA	5.31	134.97	121.70
1	A	630	THR	C-N-CA	5.21	134.72	121.70
1	B	630	THR	C-N-CA	5.00	134.20	121.70

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	8030	0	7714	56	0
1	B	8074	0	7746	52	0
2	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4	0	0	0	0
3	A	20	0	0	0	0
3	B	50	0	0	0	0
4	A	145	0	0	0	0
4	B	163	0	0	0	0
All	All	16490	0	15460	106	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 3.

All (106) 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:52:ILE:HD11	1:A:160:PHE:CZ	2.02	0.93
1:A:52:ILE:HD11	1:A:160:PHE:HZ	1.38	0.84
1:A:54:SER:O	1:A:95:LYS:NZ	2.24	0.70
1:B:483:ILE:HA	1:B:512:VAL:HB	1.80	0.63
1:A:483:ILE:HA	1:A:512:VAL:HB	1.81	0.63
1:B:218:GLN:O	1:B:222:MSE:HG2	1.99	0.63
1:A:289:LEU:HD23	1:A:383:ASP:HB2	1.81	0.62
1:B:289:LEU:HD23	1:B:383:ASP:HB2	1.81	0.61
1:B:784:VAL:HG21	1:B:1072:TYR:HB2	1.83	0.61
1:B:843:ARG:HH22	1:B:921:MSE:HE3	1.67	0.60
1:B:104:LEU:HD13	1:B:137:ARG:HH12	1.67	0.59
1:A:843:ARG:HH22	1:A:921:MSE:HE3	1.68	0.58
1:A:315:LYS:NZ	1:A:564:GLU:OE2	2.34	0.58
1:A:745:GLY:H	1:A:748:SER:HB2	1.68	0.57
1:B:315:LYS:NZ	1:B:564:GLU:OE2	2.36	0.56
1:B:745:GLY:H	1:B:748:SER:HB2	1.69	0.56
1:A:218:GLN:O	1:A:222:MSE:HG2	2.05	0.56
1:A:965:ARG:HG2	1:A:1012:GLU:CD	2.26	0.55
1:A:82:ASP:HB3	1:A:85:ASP:HB2	1.90	0.54
1:B:82:ASP:HB3	1:B:85:ASP:HB2	1.89	0.54
1:B:1073:HIS:CG	1:B:1074:HIS:H	2.27	0.53
1:B:1038:ILE:HG23	1:B:1044:VAL:HG22	1.90	0.52
1:A:1038:ILE:HG23	1:A:1044:VAL:HG22	1.91	0.52
1:B:37:ALA:HB2	1:B:43:VAL:HG12	1.91	0.52
1:A:37:ALA:HB2	1:A:43:VAL:HG12	1.92	0.51
1:B:918:VAL:HA	1:B:921:MSE:HG3	1.92	0.51
1:A:164:LEU:HD22	1:A:623:THR:HG22	1.92	0.51
1:B:939:GLU:OE1	1:B:1031:SER:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:753:LEU:HB2	1:B:1005:PRO:HG3	1.92	0.51
1:A:753:LEU:HB2	1:A:1005:PRO:HG3	1.92	0.51
1:B:52:ILE:CG2	1:B:96:TYR:HA	2.42	0.50
1:A:939:GLU:OE1	1:A:1031:SER:HA	2.11	0.50
1:A:918:VAL:HA	1:A:921:MSE:HG3	1.94	0.50
1:B:167:ALA:HB1	1:B:175:LEU:HD21	1.93	0.50
1:B:209:LEU:HD11	1:B:244:LEU:HD21	1.94	0.50
1:A:486:PRO:HA	1:A:511:THR:HA	1.94	0.50
1:A:136:ASP:HB2	1:A:138:THR:HG23	1.94	0.49
1:A:167:ALA:HB1	1:A:175:LEU:HD21	1.93	0.49
1:A:214:THR:OG1	1:B:181:GLN:HG2	2.12	0.49
1:A:299:TRP:CZ2	1:A:301:PRO:HG3	2.48	0.49
1:B:486:PRO:HA	1:B:511:THR:HA	1.95	0.48
1:B:741:ARG:NH2	1:B:755:ASN:HB2	2.28	0.48
1:B:136:ASP:HB2	1:B:138:THR:HG23	1.95	0.48
1:B:104:LEU:HD13	1:B:137:ARG:NH1	2.27	0.48
1:B:535:THR:HG23	1:B:904:ARG:CZ	2.44	0.48
1:B:299:TRP:CZ2	1:B:301:PRO:HG3	2.49	0.48
1:A:879:SER:HB2	1:A:887:ASN:HD21	1.78	0.47
1:A:52:ILE:CG2	1:A:96:TYR:HA	2.44	0.47
1:B:879:SER:HB2	1:B:887:ASN:HD21	1.79	0.47
1:A:741:ARG:NH2	1:A:755:ASN:HB2	2.29	0.47
1:B:164:LEU:HD22	1:B:623:THR:HG22	1.96	0.47
1:A:663:ARG:HA	1:A:692:PHE:O	2.15	0.47
1:B:1010:LEU:HB2	1:B:1044:VAL:HB	1.97	0.47
1:A:22:VAL:HG11	1:A:203:LYS:HD3	1.97	0.46
1:A:209:LEU:HD11	1:A:244:LEU:HD21	1.96	0.46
1:B:260:LEU:HD11	1:B:263:ALA:HB2	1.97	0.46
1:B:663:ARG:HA	1:B:692:PHE:O	2.15	0.46
1:A:1010:LEU:HB2	1:A:1044:VAL:HB	1.97	0.46
1:B:1000:ALA:HB1	1:B:1046:LEU:HD11	1.97	0.45
1:A:1000:ALA:HB1	1:A:1046:LEU:HD11	1.98	0.45
1:B:515:VAL:O	1:B:519:LEU:HG	2.16	0.45
1:A:260:LEU:HD11	1:A:263:ALA:HB2	1.99	0.45
1:B:131:PHE:CD1	1:B:137:ARG:HG2	2.51	0.45
1:B:166:GLU:HB2	1:B:264:THR:HG21	1.98	0.45
1:A:515:VAL:O	1:A:519:LEU:HG	2.16	0.45
1:B:863:ASP:OD2	1:B:867:SER:HB2	2.17	0.45
1:A:38:VAL:HG22	1:A:39:GLU:H	1.83	0.45
1:B:116:ARG:HH11	1:B:119:THR:HA	1.82	0.45
1:A:131:PHE:CD1	1:A:137:ARG:HG2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:HIS:HB3	1:B:421:ASP:HB2	1.98	0.44
1:B:737:GLY:C	1:B:914:VAL:HG21	2.37	0.44
1:B:898:TYR:HB3	1:B:924:THR:HG23	1.99	0.44
1:A:863:ASP:OD2	1:A:867:SER:HB2	2.17	0.44
1:B:998:VAL:HB	1:B:1054:LEU:HB2	1.99	0.44
1:A:186:VAL:HG12	1:A:211:LEU:HB2	2.00	0.44
1:A:965:ARG:HD2	1:A:965:ARG:HA	1.73	0.44
1:B:54:SER:HB3	1:B:55:SER:H	1.58	0.44
1:A:998:VAL:HB	1:A:1054:LEU:HB2	2.00	0.44
1:A:116:ARG:HH11	1:A:119:THR:HA	1.82	0.44
1:A:418:HIS:HB3	1:A:421:ASP:HB2	1.99	0.44
1:A:737:GLY:C	1:A:914:VAL:HG21	2.38	0.43
1:A:1027:ALA:HB3	1:A:1031:SER:HB2	2.00	0.43
1:A:166:GLU:HB2	1:A:264:THR:HG21	2.00	0.43
1:B:177:TRP:O	1:B:231:ALA:HB3	2.19	0.43
1:B:186:VAL:HG12	1:B:211:LEU:HB2	2.00	0.43
1:A:52:ILE:HA	1:A:95:LYS:HE3	2.01	0.43
1:A:898:TYR:HB3	1:A:924:THR:HG23	2.00	0.43
1:B:1027:ALA:HB3	1:B:1031:SER:HB2	2.00	0.43
1:A:68:TRP:HZ3	1:B:82:ASP:OD1	2.01	0.42
1:B:139:VAL:HG13	1:B:148:VAL:HG13	2.01	0.42
1:A:67:LEU:HB3	1:A:76:LEU:CD2	2.50	0.42
1:A:879:SER:HB2	1:A:887:ASN:ND2	2.34	0.42
1:B:211:LEU:HB3	1:B:233:PHE:HB3	2.01	0.42
1:B:879:SER:HB2	1:B:887:ASN:ND2	2.35	0.42
1:B:22:VAL:HG11	1:B:203:LYS:HD3	2.01	0.42
1:A:52:ILE:CD1	1:A:160:PHE:CZ	2.91	0.41
1:A:139:VAL:HG13	1:A:148:VAL:HG13	2.01	0.41
1:B:692:PHE:HA	1:B:718:GLY:O	2.21	0.41
1:B:750:ALA:O	1:B:765:VAL:HG21	2.20	0.41
1:A:211:LEU:HB3	1:A:233:PHE:HB3	2.01	0.41
1:A:575:MSE:HB3	1:A:575:MSE:HE2	2.02	0.41
1:A:170:VAL:HA	1:A:270:GLY:HA3	2.03	0.40
1:A:682:ILE:HG22	1:A:689:ILE:HG21	2.02	0.40
1:A:177:TRP:O	1:A:231:ALA:HB3	2.21	0.40
1:A:618:ARG:HH11	1:A:618:ARG:HD2	1.78	0.40
1:B:1007:SER:HB2	1:B:1047:PRO:HA	2.04	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	1049/1078 (97%)	987 (94%)	58 (6%)	4 (0%)	38	70
1	B	1053/1078 (98%)	986 (94%)	63 (6%)	4 (0%)	38	70
All	All	2102/2156 (98%)	1973 (94%)	121 (6%)	8 (0%)	38	70

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	631	CYS
1	B	631	CYS
1	A	466	PRO
1	B	466	PRO
1	A	501	GLU
1	B	501	GLU
1	B	879	SER
1	A	879	SER

### 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	861/863 (100%)	811 (94%)	50 (6%)	23	53
1	B	865/863 (100%)	809 (94%)	56 (6%)	20	47
All	All	1726/1726 (100%)	1620 (94%)	106 (6%)	22	51

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	40	ASN
1	A	41	GLN
1	A	104	LEU
1	A	105	ASN
1	A	108	SER
1	A	135	THR
1	A	138	THR
1	A	139	VAL
1	A	152	ARG
1	A	162	VAL
1	A	181	GLN
1	A	194	SER
1	A	218	GLN
1	A	219	GLN
1	A	244	LEU
1	A	260	LEU
1	A	262	SER
1	A	314	ASP
1	A	339	ASP
1	A	362	TYR
1	A	392	ASP
1	A	417	SER
1	A	465	LEU
1	A	470	LEU
1	A	501	GLU
1	A	507	ASP
1	A	521	GLN
1	A	550	PHE
1	A	553	THR
1	A	581	GLN
1	A	590	ASP
1	A	632	CYS
1	A	663	ARG
1	A	681	ARG
1	A	785	MSE
1	A	819	SER
1	A	905	ILE
1	A	906	SER
1	A	907	ASP
1	A	922	VAL
1	A	945	LYS
1	A	985	LYS

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Mol	Chain	Res	Type
1	A	997	LEU
1	A	1038	ILE
1	A	1045	THR
1	A	1051	VAL
1	A	1054	LEU
1	A	1056	LEU
1	A	1060	GLU
1	B	40	ASN
1	B	41	GLN
1	B	49	ILE
1	B	56	SER
1	B	104	LEU
1	B	105	ASN
1	B	138	THR
1	B	139	VAL
1	B	152	ARG
1	B	181	GLN
1	B	194	SER
1	B	218	GLN
1	B	219	GLN
1	B	244	LEU
1	B	260	LEU
1	B	262	SER
1	B	314	ASP
1	B	339	ASP
1	B	358	LYS
1	B	362	TYR
1	B	382	VAL
1	B	392	ASP
1	B	417	SER
1	B	465	LEU
1	B	470	LEU
1	B	501	GLU
1	B	507	ASP
1	B	521	GLN
1	B	550	PHE
1	B	553	THR
1	B	581	GLN
1	B	590	ASP
1	B	603	ASP
1	B	663	ARG
1	B	681	ARG

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Mol	Chain	Res	Type
1	B	785	MSE
1	B	819	SER
1	B	865	GLN
1	B	905	ILE
1	B	906	SER
1	B	907	ASP
1	B	922	VAL
1	B	945	LYS
1	B	965	ARG
1	B	969	SER
1	B	984	MSE
1	B	985	LYS
1	B	997	LEU
1	B	1007	SER
1	B	1038	ILE
1	B	1045	THR
1	B	1051	VAL
1	B	1054	LEU
1	B	1056	LEU
1	B	1060	GLU
1	B	1074	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 8 are monoatomic - leaving 14 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	$\# Z  > 2$
3	SO4	A	2075	-	4,4,4	0.55	0	6,6,6	0.34	0
3	SO4	A	2076	-	4,4,4	0.42	0	6,6,6	0.32	0
3	SO4	A	2077	-	4,4,4	0.32	0	6,6,6	0.18	0
3	SO4	A	2078	-	4,4,4	0.45	0	6,6,6	0.15	0
3	SO4	B	2079	-	4,4,4	0.40	0	6,6,6	0.16	0
3	SO4	B	2080	-	4,4,4	0.37	0	6,6,6	0.18	0
3	SO4	B	2081	-	4,4,4	0.53	0	6,6,6	0.23	0
3	SO4	B	2082	-	4,4,4	0.39	0	6,6,6	0.22	0
3	SO4	B	2083	-	4,4,4	0.39	0	6,6,6	0.10	0
3	SO4	B	2084	-	4,4,4	0.43	0	6,6,6	0.23	0
3	SO4	B	2085	-	4,4,4	0.37	0	6,6,6	0.25	0
3	SO4	B	2086	-	4,4,4	0.34	0	6,6,6	0.25	0
3	SO4	B	2087	-	4,4,4	0.39	0	6,6,6	0.20	0
3	SO4	B	2088	-	4,4,4	0.25	0	6,6,6	0.09	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
3	SO4	A	2075	-	-	0/0/0/0	0/0/0/0
3	SO4	A	2076	-	-	0/0/0/0	0/0/0/0
3	SO4	A	2077	-	-	0/0/0/0	0/0/0/0
3	SO4	A	2078	-	-	0/0/0/0	0/0/0/0
3	SO4	B	2079	-	-	0/0/0/0	0/0/0/0
3	SO4	B	2080	-	-	0/0/0/0	0/0/0/0
3	SO4	B	2081	-	-	0/0/0/0	0/0/0/0
3	SO4	B	2082	-	-	0/0/0/0	0/0/0/0
3	SO4	B	2083	-	-	0/0/0/0	0/0/0/0
3	SO4	B	2084	-	-	0/0/0/0	0/0/0/0
3	SO4	B	2085	-	-	0/0/0/0	0/0/0/0
3	SO4	B	2086	-	-	0/0/0/0	0/0/0/0
3	SO4	B	2087	-	-	0/0/0/0	0/0/0/0
3	SO4	B	2088	-	-	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.

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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1029/1078 (95%)	0.17	35 (3%) 46 40	43, 77, 128, 162	0
1	B	1033/1078 (95%)	0.52	110 (10%) 7 4	41, 74, 141, 170	0
All	All	2062/2156 (95%)	0.34	145 (7%) 17 13	41, 76, 136, 170	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	129	VAL	9.5
1	B	131	PHE	6.9
1	B	43	VAL	6.4
1	B	101	VAL	6.4
1	B	108	SER	6.2
1	B	111	ILE	6.1
1	B	75	ALA	6.1
1	B	141	VAL	5.9
1	B	76	LEU	5.6
1	B	135	THR	5.6
1	B	127	LEU	5.5
1	B	134	PHE	5.5
1	B	491	CYS	5.3
1	B	497	VAL	5.3
1	A	1062	GLN	5.2
1	B	37	ALA	5.1
1	B	130	ALA	5.1
1	B	45	HIS	5.0
1	B	38	VAL	4.8
1	B	26	PRO	4.6
1	B	41	GLN	4.6
1	B	44	ILE	4.6
1	B	113	VAL	4.5
1	B	128	ARG	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	109	GLY	4.4
1	A	66	TYR	4.4
1	B	140	SER	4.4
1	B	79	PRO	4.2
1	B	42	ALA	4.2
1	B	91	SER	4.2
1	B	36	THR	4.1
1	A	1063	GLY	4.1
1	B	490	LEU	4.1
1	B	99	TYR	4.0
1	B	100	TRP	3.9
1	A	1013	PHE	3.9
1	B	110	CYS	3.9
1	B	96	TYR	3.9
1	A	1064	ALA	3.9
1	B	160	PHE	3.7
1	B	47	VAL	3.7
1	B	40	ASN	3.7
1	B	506	CYS	3.7
1	B	39	GLU	3.7
1	B	102	ILE	3.7
1	B	67	LEU	3.7
1	B	35	VAL	3.6
1	A	1061	ALA	3.6
1	B	34	ALA	3.6
1	B	153	ALA	3.5
1	B	1072	TYR	3.5
1	B	136	ASP	3.5
1	B	150	ASP	3.4
1	A	980	VAL	3.4
1	B	133	ASP	3.4
1	B	498	LYS	3.3
1	B	107	GLU	3.3
1	B	487	PHE	3.3
1	A	102	ILE	3.2
1	B	149	TYR	3.2
1	B	205	THR	3.2
1	A	995	ASP	3.2
1	B	52	ILE	3.2
1	B	190	TYR	3.2
1	B	510	SER	3.2
1	B	202	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	502	PHE	3.1
1	B	138	THR	3.1
1	B	204	PHE	3.1
1	B	493	VAL	3.1
1	A	986	ALA	3.1
1	B	53	THR	3.1
1	B	27	ASP	3.0
1	B	151	SER	3.0
1	B	83	TRP	3.0
1	A	1066	LEU	2.9
1	A	107	GLU	2.9
1	B	28	VAL	2.9
1	B	115	VAL	2.9
1	B	201	GLU	2.9
1	B	507	ASP	2.9
1	B	137	ARG	2.8
1	B	74	ASP	2.8
1	B	157	ARG	2.8
1	A	112	ASN	2.8
1	A	783	PHE	2.7
1	A	990	LEU	2.7
1	B	104	LEU	2.7
1	B	78	ALA	2.7
1	A	35	VAL	2.7
1	B	486	PRO	2.7
1	B	496	ALA	2.7
1	B	49	ILE	2.6
1	B	203	LYS	2.6
1	B	24	ARG	2.6
1	B	58	ALA	2.6
1	B	189	TYR	2.6
1	B	500	SER	2.6
1	B	106	LYS	2.6
1	B	489	ARG	2.5
1	A	487	PHE	2.5
1	A	949	LEU	2.5
1	B	154	ASP	2.5
1	A	1010	LEU	2.5
1	A	497	VAL	2.5
1	A	490	LEU	2.5
1	B	156	PHE	2.4
1	B	132	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	997	LEU	2.4
1	B	515	VAL	2.4
1	B	886	PHE	2.4
1	A	1058	GLN	2.4
1	B	139	VAL	2.4
1	B	196	VAL	2.4
1	B	152	ARG	2.4
1	B	536	LEU	2.4
1	B	200	GLY	2.4
1	A	1038	ILE	2.4
1	B	23	VAL	2.4
1	B	55	SER	2.4
1	A	790	GLY	2.3
1	A	1059	GLY	2.3
1	B	199	ASP	2.3
1	B	25	LEU	2.3
1	B	834	ALA	2.3
1	A	1060	GLU	2.3
1	B	32	GLY	2.3
1	B	1004	ALA	2.3
1	A	36	THR	2.2
1	A	1054	LEU	2.2
1	B	73	CYS	2.2
1	B	529	GLN	2.2
1	A	134	PHE	2.2
1	B	505	TYR	2.2
1	B	112	ASN	2.1
1	B	499	SER	2.1
1	A	1056	LEU	2.1
1	B	492	GLU	2.1
1	A	506	CYS	2.1
1	B	68	TRP	2.1
1	B	234	LYS	2.0
1	A	104	LEU	2.0
1	A	536	LEU	2.0
1	A	44	ILE	2.0
1	B	1046	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	A	2072	1/1	0.94	0.48	8.92	140,140,140,140	0
3	SO4	B	2081	5/5	0.83	0.32	6.01	145,149,151,151	0
3	SO4	B	2082	5/5	0.86	0.37	5.90	141,145,146,147	0
3	SO4	B	2083	5/5	0.80	0.31	5.85	156,159,161,162	0
3	SO4	A	2076	5/5	0.90	0.26	5.79	130,133,136,137	0
2	CA	B	2078	1/1	0.84	0.43	5.66	106,106,106,106	0
3	SO4	A	2078	5/5	0.83	0.51	5.35	154,158,159,159	0
3	SO4	B	2088	5/5	0.88	0.28	3.21	142,146,147,147	0
2	CA	A	2074	1/1	0.61	0.26	1.79	106,106,106,106	0
3	SO4	A	2077	5/5	0.93	0.17	-0.06	135,139,141,142	0
2	CA	B	2075	1/1	0.95	0.17	-0.18	58,58,58,58	0
3	SO4	A	2075	5/5	0.95	0.15	-0.86	78,82,83,85	0
2	CA	A	2073	1/1	0.89	0.15	-1.75	123,123,123,123	0
2	CA	B	2077	1/1	0.99	0.13	-1.96	78,78,78,78	0
3	SO4	B	2085	5/5	0.95	0.11	-2.46	124,128,130,130	0
2	CA	A	2071	1/1	0.98	0.10	-2.66	51,51,51,51	0
2	CA	B	2076	1/1	0.96	0.12	-5.26	106,106,106,106	0
3	SO4	B	2087	5/5	0.89	0.25	-	131,135,136,137	0
3	SO4	B	2086	5/5	0.73	0.29	-	156,161,162,162	0
3	SO4	B	2084	5/5	0.86	0.20	-	147,152,152,154	0
3	SO4	B	2079	5/5	0.98	0.10	-	106,111,111,112	0
3	SO4	B	2080	5/5	0.90	0.18	-	130,133,135,137	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.