



# Full wwPDB X-ray Structure Validation Report i

Jun 22, 2024 – 01:29 PM EDT

PDB ID : 6R3T  
Title : Structure of P110 from Mycoplasma Genitalium at 2.7Å  
Authors : Aparicio, D.; Fita, I.  
Deposited on : 2019-03-21  
Resolution : 2.73 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  
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>  
with specific help available everywhere you see the i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 2.37.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

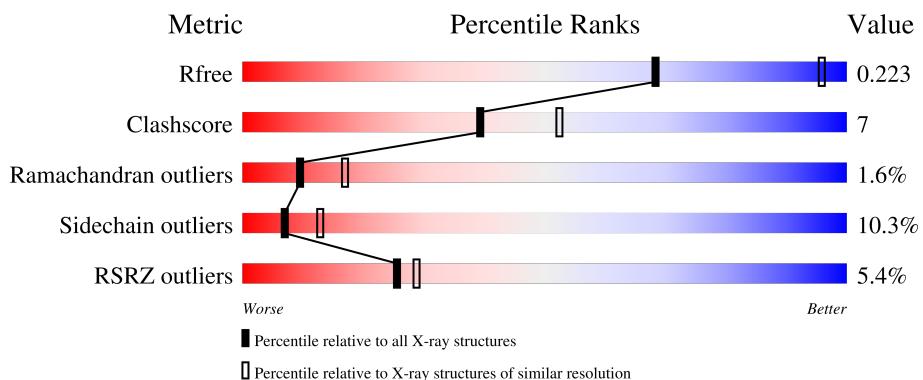
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.73 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))
$R_{free}$	130704	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	916	5%  73% 20% ..

## 2 Entry composition [\(i\)](#)

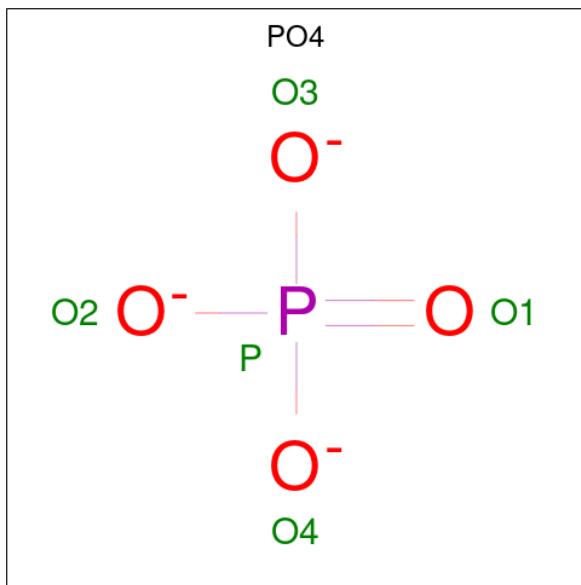
There are 4 unique types of molecules in this entry. The entry contains 6906 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Mgp-operon protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	887	6836	4287	1142	1401	6	0	1	0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	5	4	1	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total K 2 2	0	0

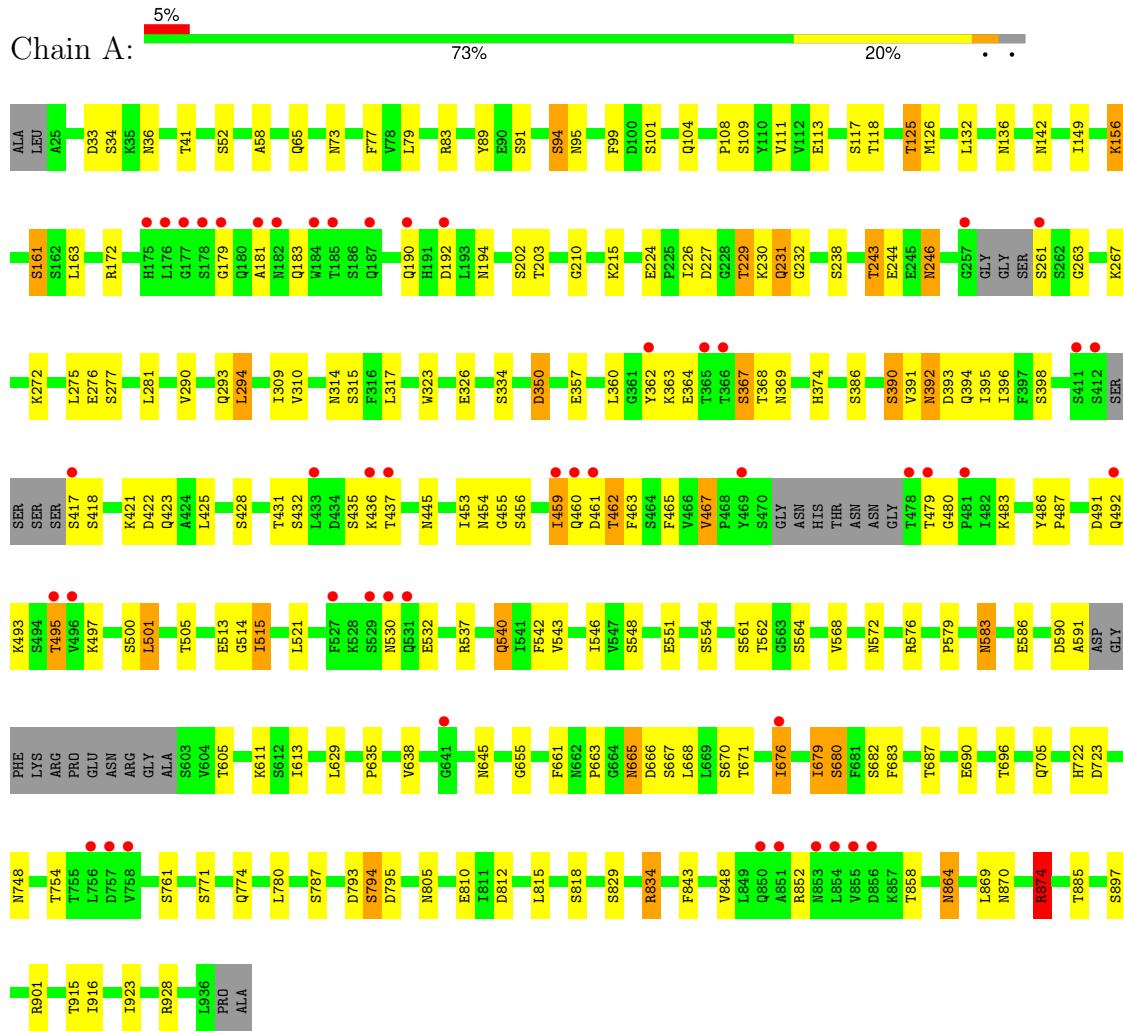
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	63	Total    O 63    63	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 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.

- Molecule 1: Mgp-operon protein 3



## 4 Data and refinement statistics i

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.60Å    152.94Å    172.71Å 90.00°    90.00°    90.00°	Depositor
Resolution (Å)	54.86 – 2.73 54.80 – 2.73	Depositor EDS
% Data completeness (in resolution range)	98.6 (54.86-2.73) 98.6 (54.80-2.73)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	2.30 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
$R$ , $R_{free}$	0.176 , 0.225 0.180 , 0.223	Depositor DCC
$R_{free}$ test set	1930 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	76.8	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 54.6	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.49$ , $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6906	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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  $< |L| >$ ,  $< L^2 >$  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: PO4, K

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	0.81	1/6975 (0.0%)	1.02	6/9486 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	136	ASN	CB-CG	9.46	1.72	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	874	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	392	ASN	CB-CA-C	5.48	121.36	110.40
1	A	314	ASN	CB-CA-C	5.42	121.25	110.40
1	A	923	ILE	C-N-CA	-5.32	111.12	122.30
1	A	109	SER	CB-CA-C	5.27	120.11	110.10
1	A	874	ARG	CB-CA-C	5.11	120.61	110.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243	THR	Peptide
1	A	263	GLY	Peptide
1	A	722	HIS	Peptide
1	A	864	ASN	Peptide

## 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	6836	0	6618	100	0
2	A	5	0	0	0	0
3	A	2	0	0	0	0
4	A	63	0	0	1	0
All	All	6906	0	6618	100	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 7.

All (100) 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:231:GLN:HE21	1:A:231:GLN:N	1.70	0.89
1:A:281:LEU:H	1:A:293:GLN:HE22	1.25	0.85
1:A:77:PHE:CZ	1:A:113:GLU:HG3	2.23	0.73
1:A:210:GLY:H	1:A:232:GLY:HA3	1.52	0.73
1:A:540:GLN:HG2	1:A:579:PRO:HA	1.71	0.71
1:A:231:GLN:HE21	1:A:231:GLN:CA	2.04	0.69
1:A:848:VAL:HG22	1:A:852:ARG:HD3	1.76	0.68
1:A:77:PHE:CE2	1:A:113:GLU:HG3	2.30	0.67
1:A:172:ARG:NE	1:A:181:ALA:HA	2.09	0.67
1:A:554:SER:HB2	1:A:568:VAL:HG13	1.77	0.65
1:A:586:GLU:HG3	1:A:613:ILE:HD13	1.79	0.65
1:A:805:ASN:HB2	4:A:1147:HOH:O	1.97	0.64
1:A:501:LEU:C	1:A:501:LEU:HD12	2.17	0.64
1:A:682:SER:OG	1:A:761:SER:HB3	1.99	0.62
1:A:230:LYS:C	1:A:231:GLN:HE21	2.01	0.62
1:A:41:THR:HG22	1:A:916:ILE:HG21	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:ILE:HD11	1:A:679:ILE:HD12	1.83	0.61
1:A:479:THR:HG22	1:A:480:GLY:N	2.17	0.60
1:A:230:LYS:HB3	1:A:231:GLN:HE22	1.67	0.60
1:A:210:GLY:N	1:A:232:GLY:HA3	2.16	0.60
1:A:687:THR:OG1	1:A:690:GLU:OE1	2.18	0.59
1:A:194:ASN:HD22	1:A:483:LYS:HD3	1.68	0.58
1:A:210:GLY:H	1:A:232:GLY:CA	2.16	0.58
1:A:89:TYR:OH	1:A:142:ASN:ND2	2.37	0.57
1:A:246:ASN:OD1	1:A:246:ASN:N	2.33	0.56
1:A:350:ASP:N	1:A:350:ASP:OD1	2.39	0.56
1:A:495:THR:O	1:A:495:THR:OG1	2.20	0.56
1:A:272:LYS:NZ	1:A:276:GLU:OE1	2.39	0.55
1:A:58:ALA:HA	1:A:126:MET:HE3	1.89	0.54
1:A:548:SER:OG	1:A:551:GLU:HG3	2.06	0.54
1:A:676:ILE:HD11	1:A:679:ILE:CD1	2.37	0.54
1:A:99:PHE:CZ	1:A:108:PRO:HB3	2.43	0.54
1:A:583:ASN:C	1:A:583:ASN:HD22	2.12	0.52
1:A:398:SER:HA	1:A:543:VAL:O	2.09	0.52
1:A:34:SER:HB2	1:A:65:GLN:HG2	1.92	0.52
1:A:117:SER:HB3	1:A:125:THR:HG21	1.91	0.52
1:A:590:ASP:OD1	1:A:591:ALA:N	2.43	0.52
1:A:210:GLY:O	1:A:232:GLY:HA3	2.11	0.51
1:A:104:GLN:NE2	1:A:104:GLN:HA	2.25	0.51
1:A:391:VAL:O	1:A:392:ASN:C	2.49	0.50
1:A:635:PRO:HB3	1:A:705:GLN:O	2.11	0.50
1:A:231:GLN:CA	1:A:231:GLN:NE2	2.75	0.50
1:A:227:ASP:OD1	1:A:229:THR:HB	2.11	0.49
1:A:780:LEU:HD23	1:A:780:LEU:N	2.28	0.49
1:A:655:GLY:HA3	1:A:683:PHE:CE1	2.47	0.49
1:A:396:ILE:HD13	1:A:661:PHE:CZ	2.47	0.49
1:A:36:ASN:HA	1:A:52:SER:O	2.12	0.49
1:A:111:VAL:HG11	1:A:309:ILE:HG21	1.95	0.49
1:A:290:VAL:HG12	1:A:294:LEU:HD22	1.93	0.49
1:A:874:ARG:CG	1:A:874:ARG:HH11	2.26	0.49
1:A:435:SER:HB2	1:A:445:ASN:ND2	2.28	0.48
1:A:231:GLN:OE1	1:A:267:LYS:HE3	2.13	0.48
1:A:390:SER:HA	1:A:394:GLN:O	2.14	0.48
1:A:231:GLN:HG2	1:A:267:LYS:HB3	1.97	0.47
1:A:665:ASN:HD22	1:A:665:ASN:H	1.63	0.47
1:A:771:SER:OG	1:A:774:GLN:HG3	2.13	0.47
1:A:357:GLU:HA	1:A:360:LEU:HG	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:GLN:NE2	1:A:83:ARG:HG3	2.31	0.46
1:A:435:SER:HB2	1:A:445:ASN:HD22	1.79	0.46
1:A:465:PHE:HB3	1:A:515:ILE:HD13	1.98	0.46
1:A:843:PHE:CD2	1:A:928:ARG:HD3	2.50	0.46
1:A:229:THR:HG22	1:A:230:LYS:HG3	1.97	0.45
1:A:243:THR:O	1:A:246:ASN:OD1	2.33	0.45
1:A:230:LYS:C	1:A:231:GLN:NE2	2.68	0.45
1:A:58:ALA:HA	1:A:126:MET:CE	2.47	0.45
1:A:156:LYS:HE2	1:A:696:THR:OG1	2.17	0.45
1:A:638:VAL:CG2	1:A:748:ASN:O	2.64	0.45
1:A:874:ARG:HH11	1:A:874:ARG:HG3	1.81	0.45
1:A:203:THR:O	1:A:425:LEU:HA	2.17	0.44
1:A:398:SER:HB2	1:A:542:PHE:CZ	2.53	0.44
1:A:149:ILE:HD12	1:A:215:LYS:N	2.32	0.44
1:A:94:SER:O	1:A:95:ASN:C	2.55	0.44
1:A:456:SER:HB2	1:A:463:PHE:CZ	2.53	0.43
1:A:834[A]:ARG:HA	1:A:834[A]:ARG:HD2	1.81	0.43
1:A:459:ILE:O	1:A:462:THR:HG23	2.19	0.43
1:A:546:ILE:O	1:A:572:ASN:HB2	2.18	0.43
1:A:897:SER:HA	1:A:928:ARG:O	2.18	0.42
1:A:310:VAL:HG21	1:A:395:ILE:HG13	2.01	0.42
1:A:428:SER:HB3	1:A:454:ASN:HB2	2.01	0.42
1:A:421:LYS:HE2	1:A:422:ASP:OD2	2.20	0.42
1:A:665:ASN:ND2	1:A:667:SER:OG	2.42	0.42
1:A:132:LEU:HB3	1:A:323:TRP:CE2	2.55	0.42
1:A:486:TYR:CD2	1:A:487:PRO:HD2	2.55	0.42
1:A:431:THR:HG22	1:A:432:SER:O	2.20	0.41
1:A:645:ASN:HA	1:A:663:PRO:HG3	2.01	0.41
1:A:161:SER:HB2	1:A:226:ILE:O	2.20	0.41
1:A:465:PHE:CB	1:A:515:ILE:HD13	2.50	0.41
1:A:243:THR:HG22	1:A:244:GLU:N	2.35	0.41
1:A:668:LEU:HB3	1:A:680:SER:HB3	2.02	0.41
1:A:794:SER:OG	1:A:795:ASP:N	2.54	0.41
1:A:203:THR:OG1	1:A:423:GLN:NE2	2.44	0.41
1:A:368:THR:HG23	1:A:368:THR:O	2.21	0.41
1:A:465:PHE:CE1	1:A:514:GLY:HA3	2.56	0.41
1:A:513:GLU:HG3	1:A:515:ILE:HG22	2.04	0.40
1:A:396:ILE:HD13	1:A:661:PHE:CE2	2.57	0.40
1:A:812:ASP:HB3	1:A:815:LEU:HB2	2.03	0.40
1:A:230:LYS:CB	1:A:231:GLN:NE2	2.84	0.40
1:A:362:TYR:OH	1:A:493:LYS:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:ASN:OD1	1:A:467:VAL:HG22	2.21	0.40
1:A:360:LEU:HB2	1:A:374:HIS:HB2	2.02	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	878/916 (96%)	785 (89%)	79 (9%)	14 (2%)	9 17

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	LYS
1	A	491	ASP
1	A	492	GLN
1	A	723	ASP
1	A	73	ASN
1	A	418	SER
1	A	794	SER
1	A	367	SER
1	A	460	GLN
1	A	33	ASP
1	A	666	ASP
1	A	179	GLY
1	A	453	ILE
1	A	455	GLY

### 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	776/795 (98%)	695 (90%)	81 (10%)	7 12

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LEU
1	A	91	SER
1	A	94	SER
1	A	101	SER
1	A	118	THR
1	A	125	THR
1	A	161	SER
1	A	163	LEU
1	A	183	GLN
1	A	190	GLN
1	A	192	ASP
1	A	202	SER
1	A	224	GLU
1	A	229	THR
1	A	231	GLN
1	A	238	SER
1	A	246	ASN
1	A	261	SER
1	A	275	LEU
1	A	277	SER
1	A	294	LEU
1	A	315	SER
1	A	317	LEU
1	A	326	GLU
1	A	334	SER
1	A	350	ASP
1	A	363	LYS
1	A	364	GLU
1	A	367	SER
1	A	369	ASN

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Mol	Chain	Res	Type
1	A	386	SER
1	A	390	SER
1	A	393	ASP
1	A	417	SER
1	A	436	LYS
1	A	437	THR
1	A	459	ILE
1	A	461	ASP
1	A	462	THR
1	A	467	VAL
1	A	495	THR
1	A	497	LYS
1	A	500	SER
1	A	501	LEU
1	A	505	THR
1	A	515	ILE
1	A	521	LEU
1	A	530	ASN
1	A	532	GLU
1	A	537	ARG
1	A	540	GLN
1	A	561	SER
1	A	562	THR
1	A	564	SER
1	A	576	ARG
1	A	583	ASN
1	A	605	THR
1	A	611	LYS
1	A	629	LEU
1	A	665	ASN
1	A	670	SER
1	A	671	THR
1	A	676	ILE
1	A	679	ILE
1	A	680	SER
1	A	754	THR
1	A	787	SER
1	A	793	ASP
1	A	810	GLU
1	A	818	SER
1	A	829	SER
1	A	834[A]	ARG

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Mol	Chain	Res	Type
1	A	834[B]	ARG
1	A	858	THR
1	A	864	ASN
1	A	869	LEU
1	A	870	ASN
1	A	874	ARG
1	A	885	THR
1	A	901	ARG
1	A	915	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	65	GLN
1	A	95	ASN
1	A	96	ASN
1	A	104	GLN
1	A	119	ASN
1	A	142	ASN
1	A	143	GLN
1	A	183	GLN
1	A	187	GLN
1	A	189	ASN
1	A	194	ASN
1	A	231	GLN
1	A	293	GLN
1	A	330	GLN
1	A	359	GLN
1	A	369	ASN
1	A	492	GLN
1	A	508	ASN
1	A	583	ASN
1	A	665	ASN
1	A	674	ASN
1	A	748	ASN
1	A	766	GLN
1	A	850	GLN

### 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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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
2	PO4	A	1001	-	4,4,4	0.84	0	6,6,6	0.50	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

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

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	887/916 (96%)	0.32	48 (5%) 25 29	51, 94, 155, 209	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	182	ASN	5.5
1	A	856	ASP	5.3
1	A	365	THR	5.3
1	A	178	SER	5.1
1	A	527	PHE	4.3
1	A	181	ALA	4.2
1	A	469	TYR	4.0
1	A	855	VAL	3.9
1	A	257	GLY	3.9
1	A	460	GLN	3.8
1	A	184	TRP	3.6
1	A	261	SER	3.6
1	A	459	ILE	3.6
1	A	495	THR	3.5
1	A	676	ILE	3.4
1	A	179	GLY	3.4
1	A	412	SER	3.2
1	A	417	SER	3.1
1	A	481	PRO	3.0
1	A	461	ASP	2.9
1	A	529	SER	2.9
1	A	366	THR	2.9
1	A	362	TYR	2.9
1	A	757	ASP	2.9
1	A	492	GLN	2.8
1	A	530	ASN	2.8
1	A	177	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	479	THR	2.7
1	A	758	VAL	2.6
1	A	496	VAL	2.6
1	A	851	ALA	2.6
1	A	190	GLN	2.5
1	A	854	LEU	2.5
1	A	175	HIS	2.4
1	A	192	ASP	2.4
1	A	411	SER	2.3
1	A	756	LEU	2.3
1	A	433	LEU	2.3
1	A	437	THR	2.3
1	A	850	GLN	2.3
1	A	853	ASN	2.3
1	A	185	THR	2.3
1	A	436	LYS	2.2
1	A	187	GLN	2.2
1	A	478	THR	2.1
1	A	531	GLN	2.1
1	A	641	GLY	2.1
1	A	176	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

## 6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	K	A	1003	1/1	0.82	0.06	118,118,118,118	0
2	PO4	A	1001	5/5	0.94	0.22	75,76,90,95	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	K	A	1002	1/1	0.99	0.26	104,104,104,104	0

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

There are no such residues in this entry.