



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:31 pm GMT

PDB ID : 4DKI  
Title : Structural Insights into the Anti- Methicillin-Resistant Staphylococcus aureus (MRSA) Activity of Ceftobiprole  
Authors : Lovering, A.L.; Gretes, M.C.; Strynadka, N.C.J.  
Deposited on : 2012-02-03  
Resolution : 2.90 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

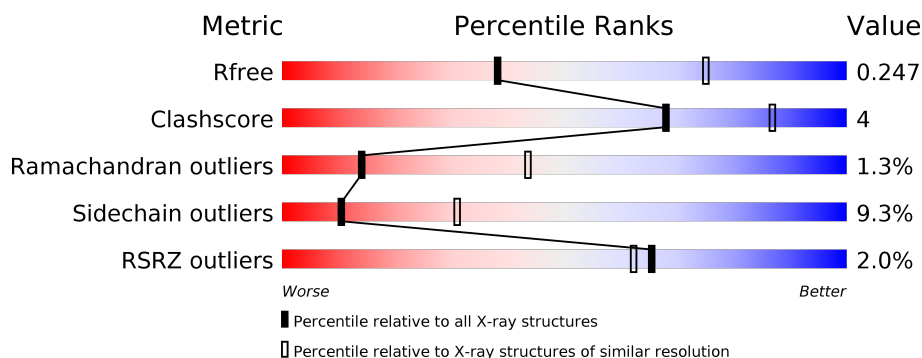
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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	646	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>••</div> </div> </div>
1	B	646	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>16%</div> <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
3	BCT	A	702	-	-	-	X



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.

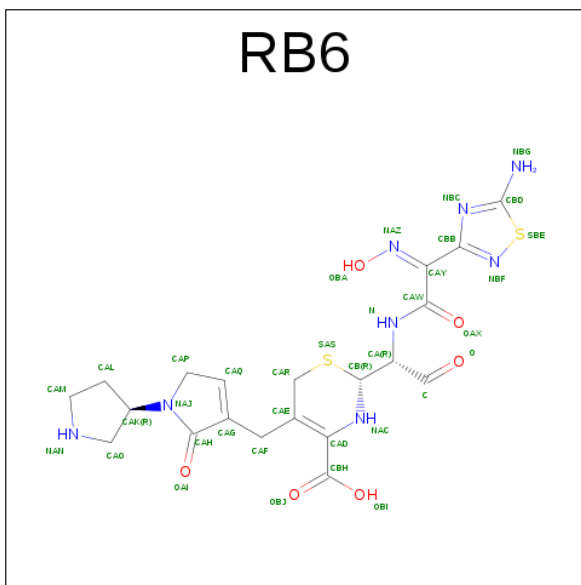
- Molecule 1 is a protein called Penicillin-binding protein 2'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	641	Total 5152	C 3247	N 868	O 1021	S 16	0	0	0
1	B	632	Total 5058	C 3192	N 849	O 1003	S 14	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

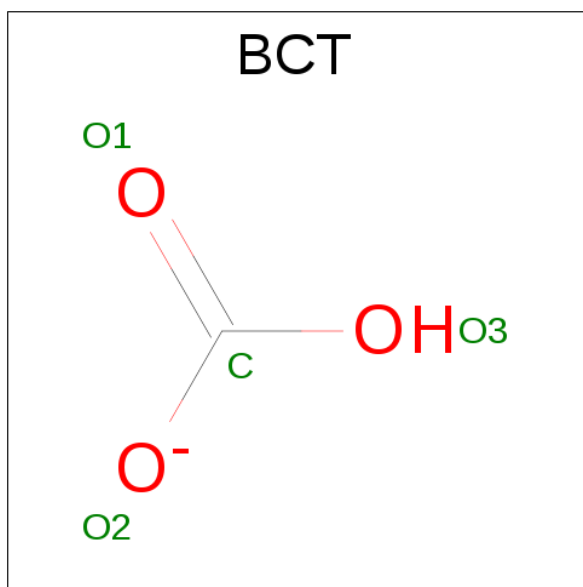
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	EXPRESSION TAG	UNP Q5HJW3
B	23	MET	-	EXPRESSION TAG	UNP Q5HJW3

- Molecule 2 is (2R)-2-[(1R)-1-{[(2Z)-2-(5-AMINO-1,2,4-THIADIAZOL-3-YL)-2-(HYDROXYIMINO)ACETYL]AMINO}-2-OXOETHYL]-5-({2-OXO-1-[(3R)-PYRROLIDIN-3-YL]-2,5-DIHYDRO-1H-PYRROL-3-YL}METHYL)-3,6-DIHYDRO-2H-1,3-THIAZINE-4-CARBOXYLIC ACID (three-letter code: RB6) (formula: C<sub>20</sub>H<sub>24</sub>N<sub>8</sub>O<sub>6</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	1
			45	23	12	7	3		
2	B	1	Total	C	N	O	S	0	0
			36	20	8	6	2		

- Molecule 3 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



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

- Molecule 4 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Cl	0	0
			2	2		
5	A	2	Total	Cl	0	0
			2	2		

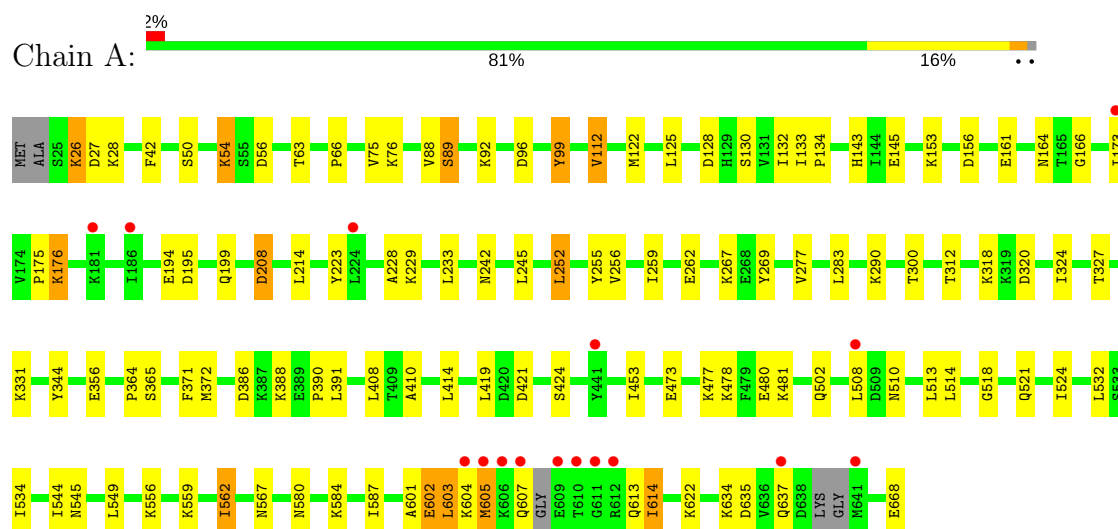
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	18	Total	O	0	0
			18	18		
6	B	21	Total	O	0	0
			21	21		

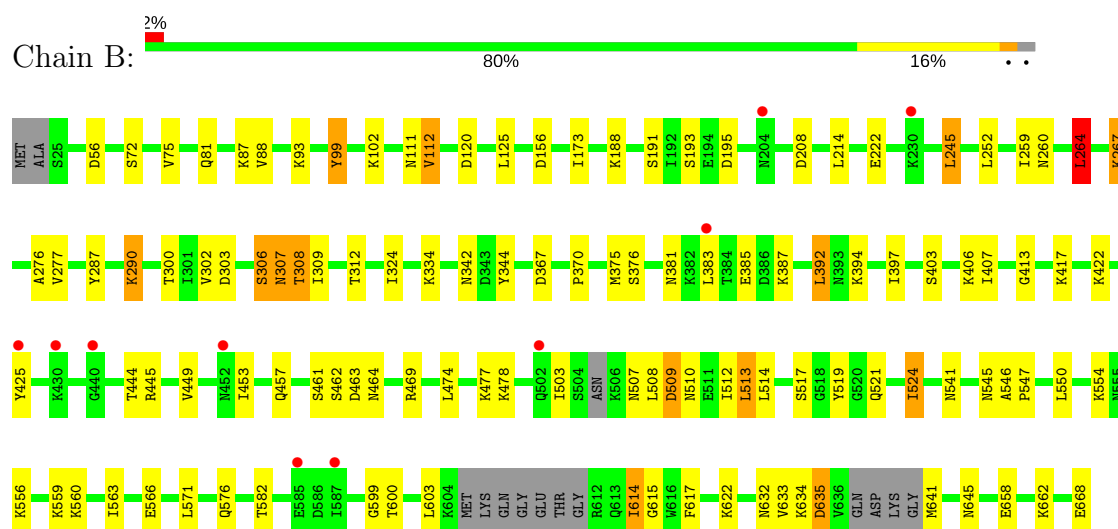
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Penicillin-binding protein 2'



#### • Molecule 1: Penicillin-binding protein 2'



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.85Å 103.47Å 186.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.29 – 2.90 53.29 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.8 (53.29-2.90) 91.8 (53.29-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.93 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, $R_{free}$	0.173 , 0.236 0.184 , 0.247	Depositor DCC
$R_{free}$ test set	1640 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.4	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 61.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10357	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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: BCT, RB6, CL, CD

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	0.51	0/5235	0.77	1/7035 (0.0%)
1	B	0.51	0/5141	0.76	0/6916
All	All	0.51	0/10376	0.77	1/13951 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	LYS	C-N-CA	5.47	135.37	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	5152	0	5141	44	0
1	B	5058	0	5027	38	0
2	A	45	0	6	2	0
2	B	36	0	22	6	0
3	A	12	0	0	0	0
3	B	4	0	0	0	0
4	A	3	0	0	0	0
4	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	18	0	0	0	0
6	B	21	0	0	3	0
All	All	10357	0	10196	88	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 4.

All (88) 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:99:TYR:HB2	1:B:112:VAL:HG22	1.72	0.71
1:A:166:GLY:HA3	1:A:242:ASN:HB2	1.72	0.71
2:B:701:RB6:CAR	2:B:701:RB6:H14	2.21	0.70
2:B:701:RB6:H14	2:B:701:RB6:H9	1.76	0.68
1:A:26:LYS:HG2	1:A:28:LYS:HG3	1.76	0.68
1:A:89:SER:HB3	1:A:92:LYS:HB2	1.76	0.67
1:A:112:VAL:HG13	1:A:134:PRO:HB3	1.77	0.67
1:A:414:LEU:HD13	1:A:567:ASN:HB3	1.77	0.66
2:B:701:RB6:H9	2:B:701:RB6:CAQ	2.27	0.64
2:B:701:RB6:CAR	2:B:701:RB6:CAQ	2.77	0.63
1:B:99:TYR:HB2	1:B:112:VAL:CG2	2.29	0.62
1:A:327:THR:HB	1:A:356:GLU:HB3	1.83	0.61
1:B:87:LYS:HG2	1:B:93:LYS:HE2	1.84	0.59
1:A:559:LYS:HB3	1:A:562:ILE:HD13	1.84	0.58
1:B:173:ILE:HD12	1:B:214:LEU:HD11	1.84	0.58
1:A:300:THR:HG22	1:A:312:THR:HA	1.86	0.57
1:B:306:SER:O	1:B:308:THR:N	2.33	0.57
1:B:245:LEU:HD13	1:B:334:LYS:HG3	1.86	0.56
1:B:478:LYS:HG3	6:B:820:HOH:O	2.05	0.56
1:B:300:THR:HG22	1:B:312:THR:HA	1.88	0.55
1:A:290:LYS:HB2	1:A:324:ILE:HD11	1.89	0.54
1:A:50:SER:O	1:A:54:LYS:HB2	2.08	0.54
1:A:164:ASN:OD1	1:A:242:ASN:HB3	2.08	0.53
1:B:392:LEU:O	6:B:819:HOH:O	2.19	0.52
1:A:477:LYS:O	1:A:481:LYS:HB2	2.09	0.52
1:B:445:ARG:HA	1:B:464:ASN:HD22	1.74	0.52
1:B:394:LYS:HA	1:B:397:ILE:HG12	1.91	0.52
1:B:510:ASN:HD21	1:B:512:ILE:HD12	1.74	0.52
1:B:633:VAL:HB	1:B:645:ASN:HD21	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:LEU:HD12	1:A:604:LYS:HG3	1.92	0.51
1:B:191:SER:HB3	1:B:376:SER:HB2	1.92	0.51
1:A:544:ILE:HB	1:A:559:LYS:HB2	1.91	0.51
1:A:175:PRO:HB2	1:A:208:ASP:HA	1.93	0.50
1:A:410:ALA:O	1:A:414:LEU:HG	2.11	0.50
1:B:403:SER:HB2	1:B:599:GLY:HA2	1.94	0.50
1:B:517:SER:HB3	1:B:524:ILE:HD11	1.95	0.49
1:B:615:GLY:N	1:B:633:VAL:O	2.45	0.49
1:A:255:TYR:CZ	1:A:371:PHE:HB3	2.47	0.49
1:A:601:ALA:O	1:A:613:GLN:HG3	2.12	0.49
1:B:287:TYR:CZ	1:B:550:LEU:HD11	2.48	0.48
1:A:408:LEU:HD22	1:A:534:ILE:HG21	1.96	0.48
1:A:386:ASP:HB3	1:A:390:PRO:HD3	1.95	0.48
1:A:143:HIS:HB3	1:A:145:GLU:OE1	2.13	0.48
1:B:302:VAL:HG22	1:B:309:ILE:HA	1.95	0.48
1:B:406:LYS:HE3	1:B:519:TYR:HB2	1.95	0.48
2:B:701:RB6:H14	2:B:701:RB6:H8	1.95	0.48
1:B:381:ASN:C	1:B:383:LEU:H	2.17	0.48
1:B:508:LEU:O	1:B:510:ASN:N	2.43	0.47
1:A:331:LYS:NZ	1:A:668:GLU:OXT	2.43	0.47
1:A:99:TYR:HD1	1:A:112:VAL:HG11	1.80	0.46
1:A:130:SER:HA	1:A:133:ILE:O	2.15	0.46
1:B:425:TYR:HD2	1:B:469:ARG:HH11	1.64	0.46
1:B:521:GLN:HB3	2:B:701:RB6:CB	2.47	0.45
1:B:614:ILE:HA	1:B:634:LYS:HA	1.98	0.45
1:A:602:GLU:HB3	1:A:603:LEU:H	1.65	0.45
1:A:173:ILE:HD12	1:A:214:LEU:HD11	1.98	0.45
1:A:344:TYR:CD1	1:A:634:LYS:HB3	2.51	0.45
1:A:153:LYS:HD3	1:A:161:GLU:HG2	1.99	0.44
1:A:364:PRO:HG2	1:A:388:LYS:HB3	1.98	0.44
1:B:508:LEU:HD23	1:B:513:LEU:HD12	2.00	0.44
1:B:259:ILE:HG12	1:B:264:LEU:HG	2.00	0.43
1:A:228:ALA:HA	1:A:233:LEU:HB2	2.00	0.43
1:A:42:PHE:HB3	1:A:63:THR:HA	2.01	0.43
1:B:413:GLY:HA2	1:B:474:LEU:HD21	2.01	0.43
1:B:277:VAL:O	6:B:821:HOH:O	2.21	0.43
1:B:344:TYR:O	1:B:633:VAL:HA	2.18	0.43
1:A:327:THR:OG1	1:A:549:LEU:HA	2.19	0.43
1:A:66:PRO:HG3	1:A:132:ILE:HG12	2.01	0.42
1:B:290:LYS:HB2	1:B:324:ILE:HD11	2.00	0.42
1:A:176:LYS:HG3	1:A:208:ASP:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:LYS:HG2	1:A:635:ASP:N	2.35	0.42
1:A:256:VAL:O	1:A:372:MET:HG2	2.19	0.42
1:B:367:ASP:O	1:B:370:PRO:HD2	2.19	0.42
1:B:658:GLU:HB2	1:B:662:LYS:HG2	2.01	0.42
1:A:424:SER:HA	1:A:453:ILE:O	2.20	0.41
1:B:453:ILE:HG23	1:B:457:GLN:HB3	2.02	0.41
1:A:521:GLN:HG3	2:A:701[A]:RB6:CBD	2.50	0.41
1:A:580:ASN:O	1:A:584:LYS:HB3	2.21	0.41
1:B:546:ALA:HA	1:B:547:PRO:HD3	1.96	0.41
1:B:267:LYS:HG2	1:B:267:LYS:H	1.68	0.41
1:A:252:LEU:O	1:A:283:LEU:HG	2.21	0.40
1:A:532:LEU:HA	1:A:532:LEU:HD23	1.97	0.40
1:B:615:GLY:HA3	1:B:641:MET:O	2.21	0.40
1:B:407:ILE:HG23	1:B:571:LEU:HD13	2.03	0.40
1:A:259:ILE:HD11	1:A:269:TYR:HB3	2.02	0.40
1:A:480:GLU:HG3	1:A:508:LEU:HD12	2.03	0.40
1:A:601:ALA:HB3	1:A:614:ILE:H	1.86	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	635/646 (98%)	589 (93%)	40 (6%)	6 (1%)	20	54
1	B	624/646 (97%)	571 (92%)	43 (7%)	10 (2%)	11	37
All	All	1259/1292 (97%)	1160 (92%)	83 (7%)	16 (1%)	14	43

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	ASP

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Mol	Chain	Res	Type
1	A	605	MET
1	A	637	GLN
1	B	276	ALA
1	B	306	SER
1	B	307	ASN
1	B	635	ASP
1	A	602	GLU
1	B	582	THR
1	B	509	ASP
1	B	617	PHE
1	B	264	LEU
1	B	417	LYS
1	A	176	LYS
1	A	518	GLY
1	B	88	VAL

### 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	573/576 (100%)	527 (92%)	46 (8%)	14	38
1	B	560/576 (97%)	501 (90%)	59 (10%)	8	24
All	All	1133/1152 (98%)	1028 (91%)	105 (9%)	10	31

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LYS
1	A	56	ASP
1	A	75	VAL
1	A	76	LYS
1	A	88	VAL
1	A	89	SER
1	A	96	ASP
1	A	99	TYR

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Mol	Chain	Res	Type
1	A	112	VAL
1	A	122	MET
1	A	125	LEU
1	A	128	ASP
1	A	156	ASP
1	A	194	GLU
1	A	195	ASP
1	A	199	GLN
1	A	208	ASP
1	A	223	TYR
1	A	229	LYS
1	A	245	LEU
1	A	252	LEU
1	A	262	GLU
1	A	267	LYS
1	A	277	VAL
1	A	318	LYS
1	A	320	ASP
1	A	365	SER
1	A	391	LEU
1	A	419	LEU
1	A	421	ASP
1	A	473	GLU
1	A	478	LYS
1	A	502	GLN
1	A	510	ASN
1	A	513	LEU
1	A	514	LEU
1	A	524	ILE
1	A	545	ASN
1	A	556	LYS
1	A	562	ILE
1	A	587	ILE
1	A	603	LEU
1	A	605	MET
1	A	607	GLN
1	A	614	ILE
1	A	622	LYS
1	B	56	ASP
1	B	72	SER
1	B	75	VAL
1	B	81	GLN

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Mol	Chain	Res	Type
1	B	99	TYR
1	B	102	LYS
1	B	111	ASN
1	B	112	VAL
1	B	120	ASP
1	B	125	LEU
1	B	156	ASP
1	B	188	LYS
1	B	193	SER
1	B	195	ASP
1	B	208	ASP
1	B	222	GLU
1	B	245	LEU
1	B	252	LEU
1	B	260	ASN
1	B	264	LEU
1	B	267	LYS
1	B	290	LYS
1	B	303	ASP
1	B	307	ASN
1	B	308	THR
1	B	342	ASN
1	B	375	MET
1	B	385	GLU
1	B	387	LYS
1	B	392	LEU
1	B	422	LYS
1	B	444	THR
1	B	449	VAL
1	B	461	SER
1	B	462	SER
1	B	463	ASP
1	B	477	LYS
1	B	503	ILE
1	B	507	ASN
1	B	509	ASP
1	B	513	LEU
1	B	514	LEU
1	B	524	ILE
1	B	541	ASN
1	B	545	ASN
1	B	554	LYS

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Mol	Chain	Res	Type
1	B	556	LYS
1	B	559	LYS
1	B	560	LYS
1	B	563	ILE
1	B	566	GLU
1	B	576	GLN
1	B	600	THR
1	B	603	LEU
1	B	614	ILE
1	B	622	LYS
1	B	632	ASN
1	B	635	ASP
1	B	668	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	91	ASN
1	A	113	GLN
1	A	510	ASN
1	A	593	ASN
1	A	607	GLN
1	B	502	GLN
1	B	545	ASN
1	B	576	GLN
1	B	645	ASN

### 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

Of 18 ligands modelled in this entry, 11 are monoatomic - leaving 7 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	RB6	A	701[A]	-	26,39,39	2.92	8 (30%)	25,55,55	4.23	8 (32%)
2	RB6	A	701[B]	-	26,39,39	2.90	8 (30%)	25,55,55	3.90	6 (24%)
3	BCT	A	702	-	0,3,3	0.00	-	0,3,3	0.00	-
3	BCT	A	703	-	0,3,3	0.00	-	0,3,3	0.00	-
3	BCT	A	704	-	0,3,3	0.00	-	0,3,3	0.00	-
2	RB6	B	701	1	26,39,39	2.84	9 (34%)	25,55,55	3.83	10 (40%)
3	BCT	B	702	-	0,3,3	0.00	-	0,3,3	0.00	-

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
2	RB6	A	701[A]	-	-	0/16/65/65	0/2/4/4
2	RB6	A	701[B]	-	-	0/16/65/65	0/2/4/4
3	BCT	A	702	-	-	0/0/0/0	0/0/0/0
3	BCT	A	703	-	-	0/0/0/0	0/0/0/0
3	BCT	A	704	-	-	0/0/0/0	0/0/0/0
2	RB6	B	701	1	-	0/16/65/65	0/2/4/4
3	BCT	B	702	-	-	0/0/0/0	0/0/0/0

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701[A]	RB6	CAF-CAG	-9.08	1.33	1.50
2	A	701[B]	RB6	CAF-CAG	-9.08	1.33	1.50
2	B	701	RB6	CAF-CAG	-8.06	1.35	1.50
2	B	701	RB6	CAR-SAS	-4.49	1.71	1.82
2	B	701	RB6	CBH-CAD	-4.35	1.45	1.52
2	A	701[A]	RB6	CAH-NAJ	-4.30	1.29	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701[B]	RB6	CAH-NAJ	-4.30	1.29	1.35
2	A	701[A]	RB6	CAF-CAE	-3.81	1.46	1.50
2	A	701[B]	RB6	CAF-CAE	-3.81	1.46	1.50
2	A	701[A]	RB6	CBH-CAD	-3.65	1.46	1.52
2	A	701[B]	RB6	CBH-CAD	-3.65	1.46	1.52
2	A	701[A]	RB6	CAR-SAS	-3.59	1.73	1.82
2	A	701[B]	RB6	CAR-SAS	-3.59	1.73	1.82
2	B	701	RB6	CAH-NAJ	-3.43	1.30	1.35
2	B	701	RB6	CAY-CAW	-3.17	1.44	1.50
2	A	701[A]	RB6	CAH-CAG	-3.12	1.44	1.49
2	A	701[B]	RB6	CAH-CAG	-3.12	1.44	1.49
2	B	701	RB6	CAH-CAG	-2.85	1.44	1.49
2	A	701[A]	RB6	CAY-CAW	-2.84	1.45	1.50
2	B	701	RB6	CAF-CAE	-2.55	1.47	1.50
2	A	701[B]	RB6	CAY-CAW	-2.33	1.46	1.50
2	B	701	RB6	OAX-CAW	-2.32	1.19	1.23
2	A	701[A]	RB6	CAQ-CAG	6.64	1.49	1.33
2	A	701[B]	RB6	CAQ-CAG	6.64	1.49	1.33
2	B	701	RB6	CAQ-CAG	6.95	1.49	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701[A]	RB6	CAP-CAQ-CAG	-12.07	103.52	112.26
2	A	701[B]	RB6	CAP-CAQ-CAG	-12.07	103.52	112.26
2	B	701	RB6	CAP-CAQ-CAG	-10.12	104.93	112.26
2	A	701[A]	RB6	OAX-CAW-CAY	-6.28	113.10	120.34
2	B	701	RB6	NBG-CBD-NBC	-3.40	118.54	123.06
2	B	701	RB6	OAX-CAW-CAY	-3.38	116.45	120.34
2	A	701[A]	RB6	NBG-CBD-NBC	-3.18	118.84	123.06
2	A	701[B]	RB6	NBG-CBD-NBC	-2.63	119.57	123.06
2	B	701	RB6	CAE-CAR-SAS	-2.40	110.53	115.01
2	B	701	RB6	OAI-CAH-NAJ	2.10	128.63	125.49
2	B	701	RB6	CB-NAC-CAD	3.86	127.41	118.32
2	B	701	RB6	CAY-CAW-N	4.24	121.58	114.41
2	A	701[A]	RB6	CB-NAC-CAD	4.67	129.30	118.32
2	A	701[B]	RB6	CB-NAC-CAD	4.67	129.30	118.32
2	B	701	RB6	CAR-SAS-CB	5.43	105.30	94.48
2	A	701[A]	RB6	CAR-SAS-CB	5.45	105.35	94.48
2	A	701[B]	RB6	CAR-SAS-CB	5.45	105.35	94.48
2	A	701[A]	RB6	OBA-NAZ-CAY	6.20	129.27	113.82
2	B	701	RB6	OBA-NAZ-CAY	6.28	129.46	113.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701[A]	RB6	CAY-CAW-N	6.56	125.52	114.41
2	A	701[B]	RB6	OBA-NAZ-CAY	7.34	132.09	113.82
2	A	701[A]	RB6	CAP-NAJ-CAH	9.73	119.39	112.79
2	A	701[B]	RB6	CAP-NAJ-CAH	9.73	119.39	112.79
2	B	701	RB6	CAP-NAJ-CAH	10.36	119.81	112.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701[A]	RB6	1	0
2	A	701[B]	RB6	1	0
2	B	701	RB6	6	0

## 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	641/646 (99%)	-0.11	16 (2%) 58 53	26, 59, 106, 165	0
1	B	632/646 (97%)	-0.09	10 (1%) 72 70	29, 69, 109, 143	0
All	All	1273/1292 (98%)	-0.10	26 (2%) 65 62	26, 63, 107, 165	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	610	THR	8.6
1	A	606	LYS	7.2
1	A	605	MET	6.2
1	A	607	GLN	5.8
1	A	612	ARG	4.2
1	A	609	GLU	4.2
1	A	611	GLY	4.0
1	B	440	GLY	3.2
1	A	186	ILE	3.2
1	B	502	GLN	3.2
1	B	204	ASN	3.0
1	B	430	LYS	2.8
1	A	508	LEU	2.7
1	B	585	GLU	2.6
1	B	425	TYR	2.6
1	A	641	MET	2.5
1	B	383	LEU	2.4
1	B	452	ASN	2.3
1	A	224	LEU	2.3
1	A	637	GLN	2.3
1	B	230	LYS	2.3
1	A	441	TYR	2.3
1	B	587	ILE	2.2
1	A	181	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	173	ILE	2.2
1	A	604	LYS	2.1

## 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 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(Å <sup>2</sup> )	Q<0.9
3	BCT	A	702	4/4	0.85	0.22	2.15	69,76,77,79	0
2	RB6	B	701	36/36	0.86	0.20	0.44	96,112,123,125	0
4	CD	B	704	1/1	1.00	0.17	0.41	46,46,46,46	0
4	CD	A	705	1/1	0.99	0.18	0.24	43,43,43,43	0
4	CD	B	703	1/1	0.99	0.17	0.24	41,41,41,41	0
5	CL	B	707	1/1	0.99	0.16	0.15	52,52,52,52	0
4	CD	A	707	1/1	0.99	0.17	0.09	60,60,60,60	0
5	CL	B	708	1/1	1.00	0.16	-0.00	44,44,44,44	0
2	RB6	A	701[B]	36/36	0.94	0.15	-0.43	55,78,91,93	9
2	RB6	A	701[A]	36/36	0.94	0.15	-0.57	55,68,91,93	9
5	CL	A	709	1/1	0.98	0.13	-1.61	47,47,47,47	0
5	CL	A	708	1/1	1.00	0.12	-1.98	41,41,41,41	0
4	CD	B	706	1/1	0.97	0.18	-	121,121,121,121	0
3	BCT	A	703	4/4	0.90	0.30	-	68,69,70,72	0
4	CD	B	705	1/1	0.89	0.08	-	142,142,142,142	0
3	BCT	A	704	4/4	0.94	0.10	-	70,73,73,75	0
3	BCT	B	702	4/4	0.80	0.26	-	102,103,104,104	0
4	CD	A	706	1/1	0.85	0.06	-	154,154,154,154	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.