Full wwPDB X-ray Structure Validation Report ⓘ

Sep 29, 2024 – 02:25 PM EDT

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

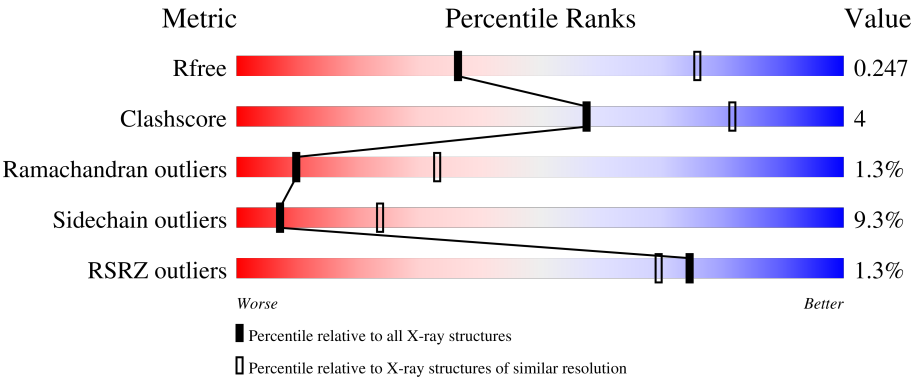
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

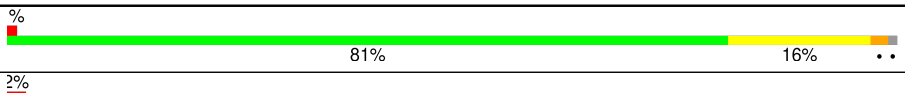
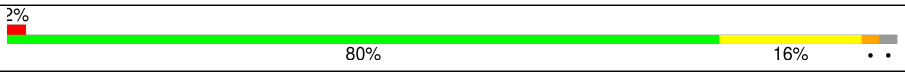
The reported resolution of this entry is 2.90 Å.

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}	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	
1	B	646	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10357 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.

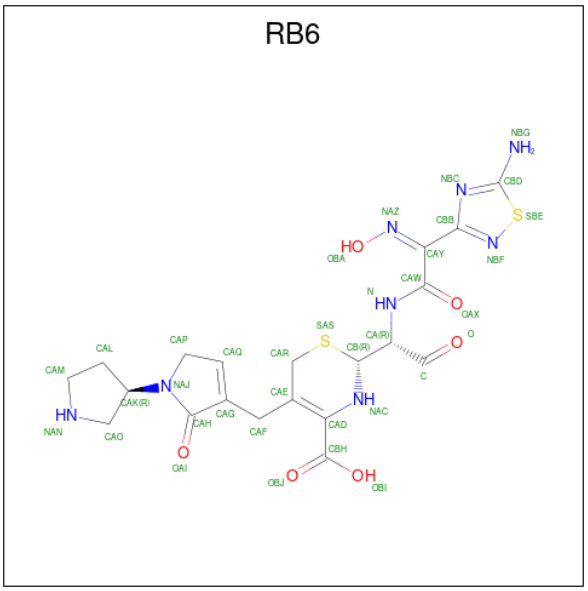
- Molecule 1 is a protein called Penicillin-binding protein 2'.

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

There are 2 discrepancies between the modelled and reference sequences:

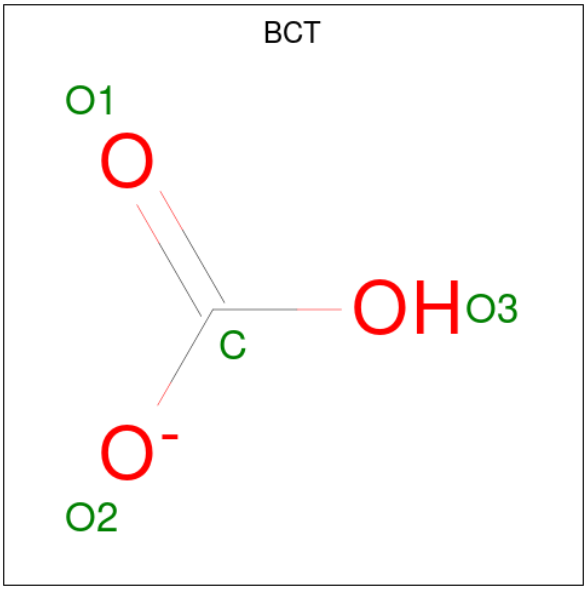
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	expression tag	UNP Q5HJW3
B	23	MET	-	expression tag	UNP Q5HJW3

- 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: $C_{20}H_{24}N_8O_6S_2$).



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: 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	A	3	Total	Cd	0	0
			3	3		
4	B	4	Total	Cd	0	0
			4	4		

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

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

- Molecule 6 is water.

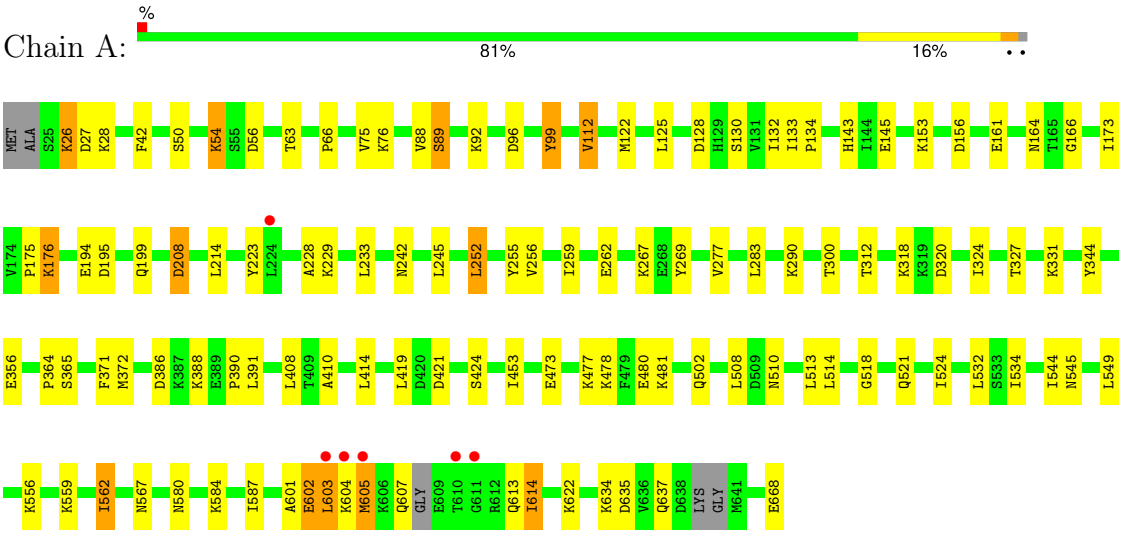
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	18	Total O 18 18	0	0
6	B	21	Total O 21 21	0	0

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.

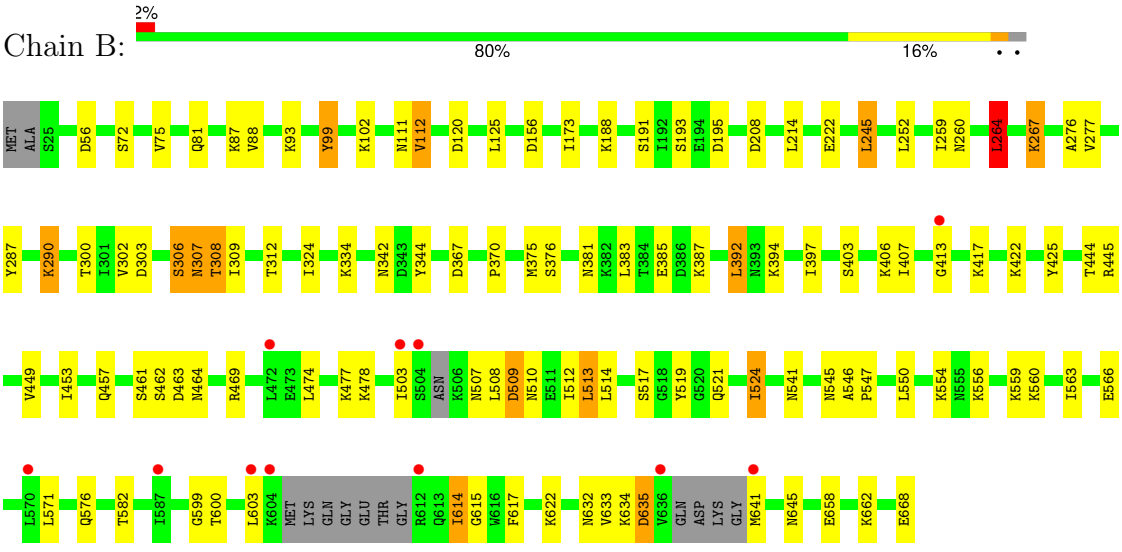
• Molecule 1: Penicillin-binding protein 2'

Chain A:



• Molecule 1: Penicillin-binding protein 2'

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	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 (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	60.4	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 63.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCT, CD, RB6, CL

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(^{o})	Ideal(^{o})
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

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:H14	2:B:701:RB6:CAR	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:CBD	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:42:PHE:HB3	1:A:63:THR:HA	2.01	0.43
1:A:228:ALA:HA	1:A:233:LEU:HB2	2.00	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:H	1:B:267:LYS:HG2	1.68	0.41
1:A:252:LEU:O	1:A:283:LEU:HG	2.21	0.40
1:A:532:LEU:HD23	1:A:532:LEU:HA	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 (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	635/646 (98%)	589 (93%)	40 (6%)	6 (1%)	14 43
1	B	624/646 (97%)	571 (92%)	43 (7%)	10 (2%)	8 28
All	All	1259/1292 (97%)	1160 (92%)	83 (7%)	16 (1%)	10 33

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 (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	573/576 (100%)	527 (92%)	46 (8%)	10 30
1	B	560/576 (97%)	501 (90%)	59 (10%)	5 18
All	All	1133/1152 (98%)	1028 (91%)	105 (9%)	7 23

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

Sometimes 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 (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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

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[B]	-	29,39,39	3.07	8 (27%)	27,55,55	4.17	9 (33%)
2	RB6	A	701[A]	-	29,39,39	3.09	8 (27%)	27,55,55	4.47	11 (40%)
3	BCT	A	702	-	3,3,3	0.52	0	2,3,3	0.23	0
2	RB6	B	701	1	29,39,39	3.01	9 (31%)	27,55,55	4.09	15 (55%)
3	BCT	B	702	-	3,3,3	0.51	0	2,3,3	0.68	0
3	BCT	A	703	-	3,3,3	0.53	0	2,3,3	0.67	0
3	BCT	A	704	-	3,3,3	0.52	0	2,3,3	0.78	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
2	RB6	A	701[A]	-	-	10/22/65/65	0/3/4/4
2	RB6	A	701[B]	-	-	11/22/65/65	0/3/4/4
2	RB6	B	701	1	-	6/22/65/65	0/3/4/4

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	-10.81	1.33	1.51
2	A	701[B]	RB6	CAF-CAG	-10.81	1.33	1.51
2	B	701	RB6	CAF-CAG	-9.60	1.35	1.51
2	B	701	RB6	CAQ-CAG	7.81	1.49	1.33
2	A	701[A]	RB6	CAQ-CAG	7.47	1.49	1.33
2	A	701[B]	RB6	CAQ-CAG	7.47	1.49	1.33
2	B	701	RB6	CAR-SAS	-5.13	1.71	1.82
2	A	701[A]	RB6	CAH-NAJ	-4.50	1.29	1.35
2	A	701[B]	RB6	CAH-NAJ	-4.50	1.29	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701[A]	RB6	CAR-SAS	-4.09	1.73	1.82
2	A	701[B]	RB6	CAR-SAS	-4.09	1.73	1.82
2	B	701	RB6	CB-SAS	-3.79	1.73	1.82
2	A	701[A]	RB6	CB-SAS	-3.76	1.73	1.82
2	A	701[B]	RB6	CB-SAS	-3.76	1.73	1.82
2	A	701[A]	RB6	CAH-CAG	-3.61	1.44	1.49
2	A	701[B]	RB6	CAH-CAG	-3.61	1.44	1.49
2	B	701	RB6	CAH-NAJ	-3.56	1.30	1.35
2	B	701	RB6	CAY-CAW	-3.50	1.44	1.50
2	B	701	RB6	CAH-CAG	-3.30	1.44	1.49
2	A	701[A]	RB6	CAY-CAW	-3.14	1.45	1.50
2	A	701[B]	RB6	CAY-CAW	-2.59	1.46	1.50
2	B	701	RB6	OAX-CAW	-2.28	1.19	1.23
2	A	701[A]	RB6	CAD-NAC	-2.10	1.33	1.37
2	A	701[B]	RB6	CAD-NAC	-2.10	1.33	1.37
2	B	701	RB6	CAD-CBH	-2.09	1.45	1.48

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701[A]	RB6	CAP-CAQ-CAG	-11.94	103.52	112.33
2	A	701[B]	RB6	CAP-CAQ-CAG	-11.94	103.52	112.33
2	B	701	RB6	CAP-NAJ-CAH	10.05	119.81	112.95
2	B	701	RB6	CAP-CAQ-CAG	-10.02	104.93	112.33
2	A	701[A]	RB6	CAP-NAJ-CAH	9.42	119.39	112.95
2	A	701[B]	RB6	CAP-NAJ-CAH	9.42	119.39	112.95
2	A	701[B]	RB6	OBA-NAZ-CAY	7.69	132.09	113.62
2	A	701[A]	RB6	CAE-CAF-CAG	6.84	129.33	114.47
2	A	701[B]	RB6	CAE-CAF-CAG	6.84	129.33	114.47
2	A	701[A]	RB6	CAY-CAW-N	6.75	125.52	114.40
2	B	701	RB6	OBA-NAZ-CAY	6.60	129.46	113.62
2	A	701[A]	RB6	OBA-NAZ-CAY	6.52	129.27	113.62
2	A	701[A]	RB6	OAX-CAW-CAY	-6.48	113.10	120.45
2	A	701[A]	RB6	CAR-SAS-CB	6.00	105.35	94.36
2	A	701[B]	RB6	CAR-SAS-CB	6.00	105.35	94.36
2	B	701	RB6	CAR-SAS-CB	5.97	105.30	94.36
2	A	701[A]	RB6	OBI-CBH-CAD	5.85	126.00	116.73
2	A	701[B]	RB6	OBI-CBH-CAD	5.85	126.00	116.73
2	B	701	RB6	OBI-CBH-CAD	5.31	125.15	116.73
2	B	701	RB6	C-CA-N	5.20	118.00	109.80
2	B	701	RB6	CAE-CAF-CAG	5.19	125.75	114.47
2	B	701	RB6	CAY-CAW-N	4.36	121.58	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701[A]	RB6	OBI-CBH-OBJ	-4.18	113.94	123.90
2	A	701[B]	RB6	OBI-CBH-OBJ	-4.18	113.94	123.90
2	B	701	RB6	NBG-CBD-NBC	-3.67	118.54	123.19
2	B	701	RB6	OAX-CAW-CAY	-3.53	116.45	120.45
2	A	701[A]	RB6	NBG-CBD-NBC	-3.43	118.84	123.19
2	A	701[A]	RB6	C-CA-N	3.14	114.75	109.80
2	A	701[B]	RB6	C-CA-N	3.14	114.75	109.80
2	B	701	RB6	CAE-CAR-SAS	-3.08	110.53	115.36
2	A	701[B]	RB6	NBG-CBD-NBC	-2.85	119.57	123.19
2	B	701	RB6	OBI-CBH-OBJ	-2.79	117.26	123.90
2	B	701	RB6	CAE-CAD-CBH	-2.10	120.05	125.85
2	B	701	RB6	CB-CA-N	2.09	114.35	109.93
2	B	701	RB6	OAI-CAH-NAJ	2.06	128.63	125.79

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701[A]	RB6	NAC-CAD-CBH-OBI
2	A	701[A]	RB6	CAR-CAE-CAF-CAG
2	A	701[A]	RB6	CAD-CAE-CAF-CAG
2	A	701[A]	RB6	CAO-CAK-NAJ-CAH
2	A	701[A]	RB6	CAL-CAK-NAJ-CAP
2	A	701[A]	RB6	CAO-CAK-NAJ-CAP
2	A	701[B]	RB6	N-CAW-CAY-CBB
2	A	701[B]	RB6	NAC-CAD-CBH-OBI
2	A	701[B]	RB6	CAR-CAE-CAF-CAG
2	A	701[B]	RB6	CAD-CAE-CAF-CAG
2	A	701[B]	RB6	CAO-CAK-NAJ-CAH
2	A	701[B]	RB6	CAL-CAK-NAJ-CAP
2	A	701[B]	RB6	CAO-CAK-NAJ-CAP
2	B	701	RB6	NAC-CAD-CBH-OBI
2	B	701	RB6	CAR-CAE-CAF-CAG
2	B	701	RB6	CAD-CAE-CAF-CAG
2	B	701	RB6	CAL-CAK-NAJ-CAP
2	B	701	RB6	CAO-CAK-NAJ-CAP
2	A	701[B]	RB6	OAX-CAW-CAY-CBB
2	A	701[A]	RB6	NAC-CAD-CBH-OBJ
2	A	701[B]	RB6	NAC-CAD-CBH-OBJ
2	A	701[B]	RB6	OAX-CAW-CAY-NAZ
2	A	701[A]	RB6	N-CAW-CAY-NAZ
2	A	701[B]	RB6	N-CAW-CAY-NAZ

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Mol	Chain	Res	Type	Atoms
2	A	701[A]	RB6	OAX-CAW-CAY-NAZ
2	B	701	RB6	OAX-CAW-CAY-NAZ
2	A	701[A]	RB6	OAX-CAW-CAY-CBB

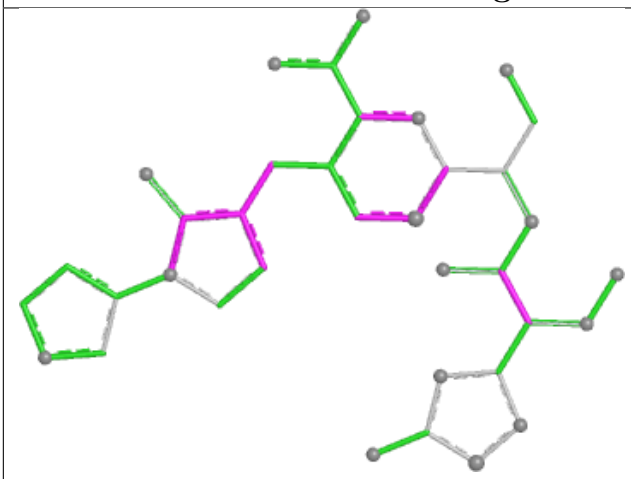
There are no ring outliers.

3 monomers are involved in 8 short contacts:

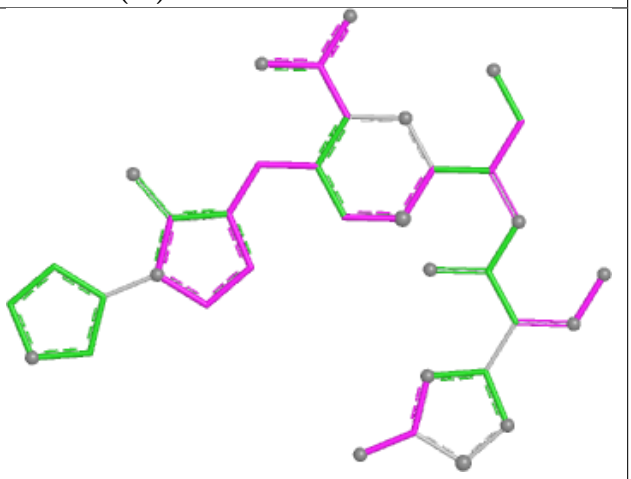
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701[B]	RB6	1	0
2	A	701[A]	RB6	1	0
2	B	701	RB6	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

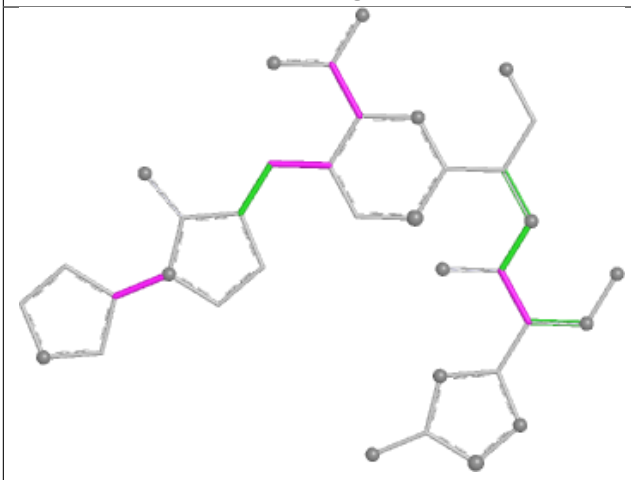
Ligand RB6 A 701 (B)



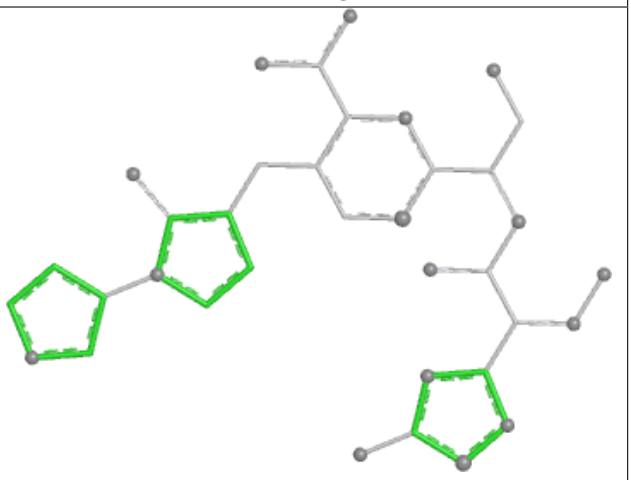
Bond lengths



Bond angles

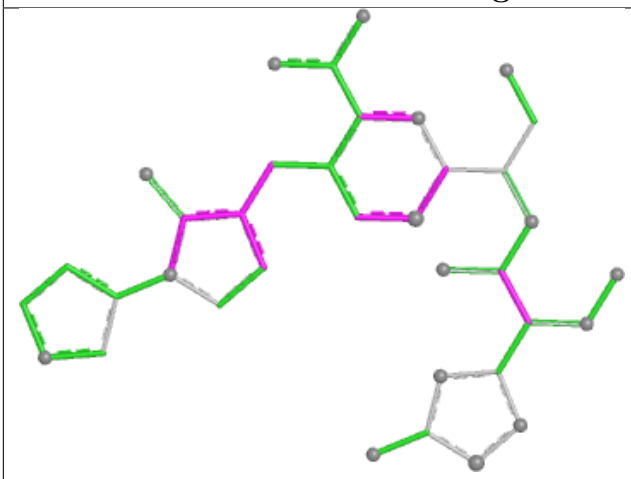


Torsions

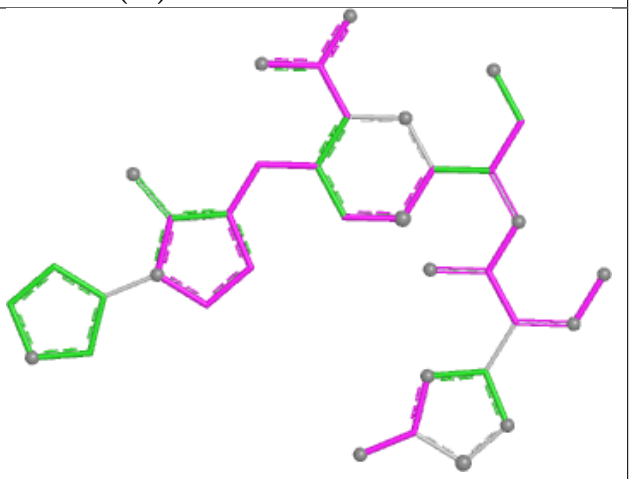


Rings

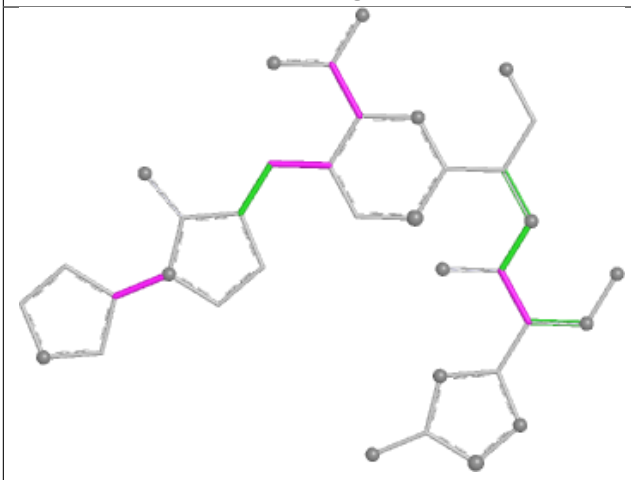
Ligand RB6 A 701 (A)



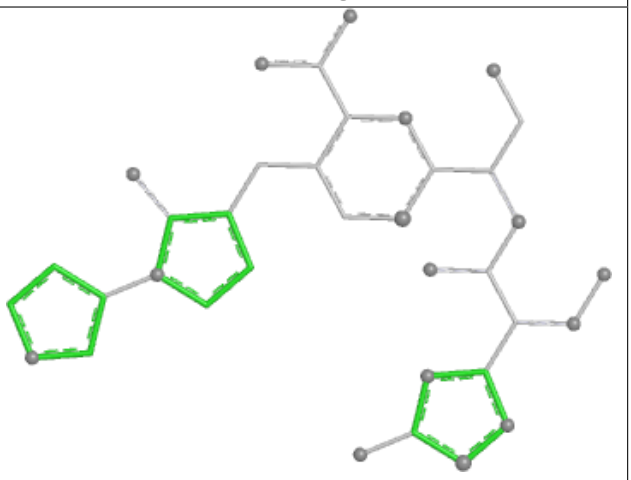
Bond lengths



Bond angles

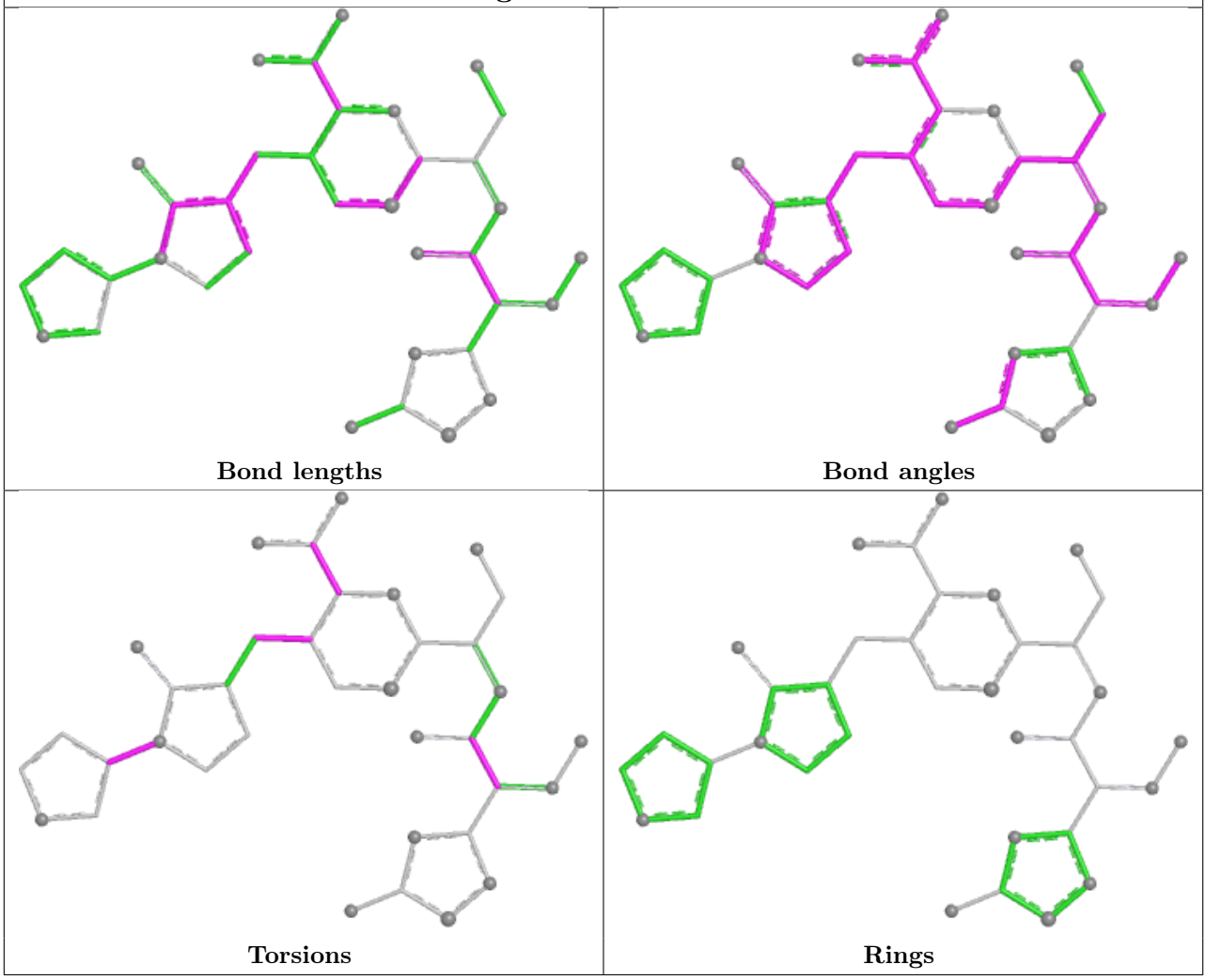


Torsions



Rings

Ligand RB6 B 701



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^{th} 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^2)	Q<0.9
1	A	641/646 (99%)	-0.45	6 (0%)	81	76	26, 59, 106, 165	0
1	B	632/646 (97%)	-0.26	11 (1%)	69	63	29, 69, 109, 143	0
All	All	1273/1292 (98%)	-0.36	17 (1%)	74	69	26, 63, 107, 165	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	636	VAL	4.9
1	B	612	ARG	3.6
1	B	503	ILE	3.4
1	B	413	GLY	3.0
1	A	604	LYS	2.9
1	B	504	SER	2.8
1	A	610	THR	2.6
1	B	641	MET	2.5
1	B	587	ILE	2.4
1	B	604	LYS	2.4
1	A	224	LEU	2.3
1	A	611	GLY	2.3
1	B	603	LEU	2.2
1	A	605	MET	2.2
1	A	603	LEU	2.1
1	B	570	LEU	2.1
1	B	472	LEU	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

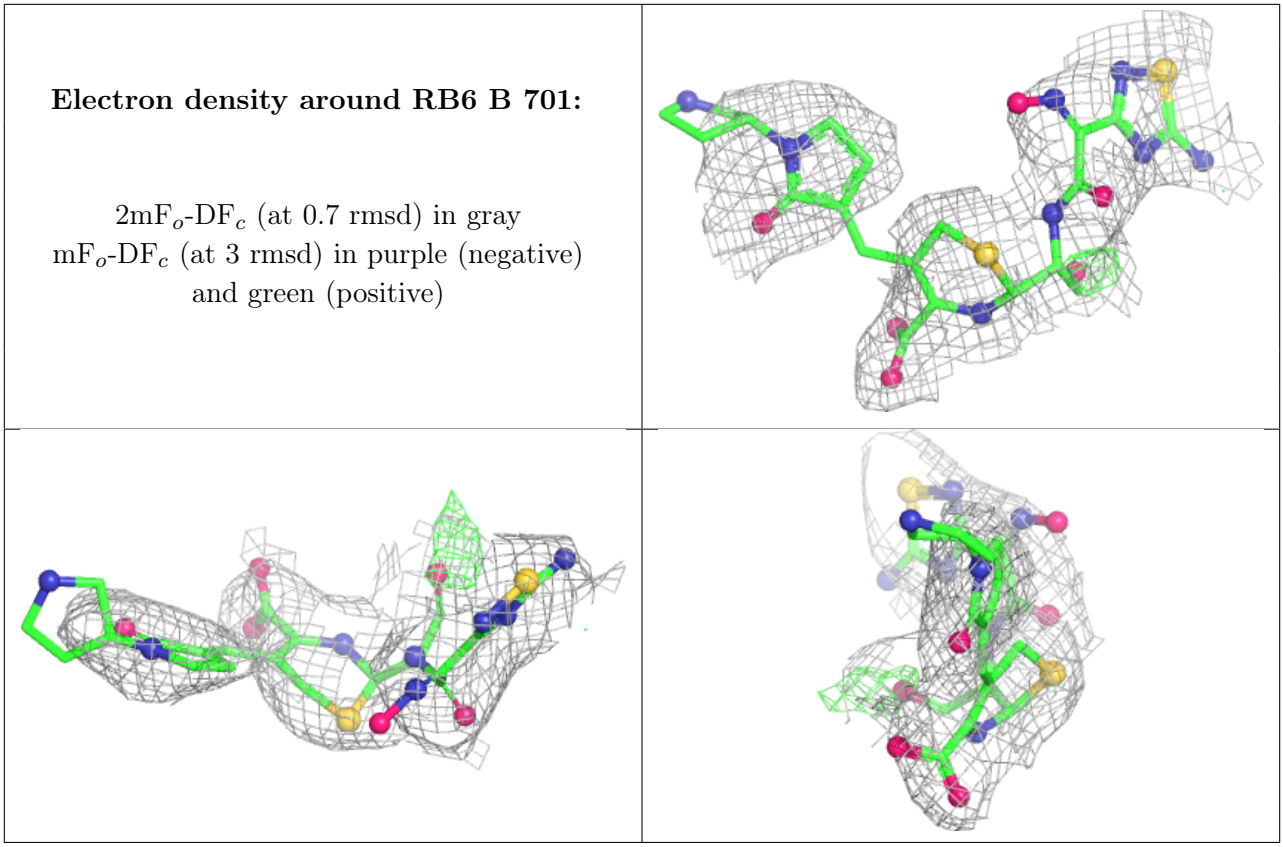
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BCT	B	702	4/4	0.78	0.08	102,103,104,104	0
2	RB6	B	701	36/36	0.81	0.12	96,112,123,125	0
3	BCT	A	702	4/4	0.83	0.20	69,76,77,79	0
3	BCT	A	703	4/4	0.84	0.13	68,69,70,72	0
3	BCT	A	704	4/4	0.86	0.11	70,73,73,75	0
4	CD	A	706	1/1	0.90	0.08	154,154,154,154	0
2	RB6	A	701[A]	36/36	0.93	0.08	55,68,91,93	9
2	RB6	A	701[B]	36/36	0.93	0.08	55,78,91,93	9
4	CD	B	705	1/1	0.94	0.07	142,142,142,142	0
4	CD	B	706	1/1	0.96	0.06	121,121,121,121	0
5	CL	A	708	1/1	0.99	0.05	41,41,41,41	0
5	CL	A	709	1/1	0.99	0.04	47,47,47,47	0
5	CL	B	707	1/1	0.99	0.04	52,52,52,52	0
4	CD	A	707	1/1	1.00	0.03	60,60,60,60	0
4	CD	B	703	1/1	1.00	0.03	41,41,41,41	0
4	CD	B	704	1/1	1.00	0.03	46,46,46,46	0
4	CD	A	705	1/1	1.00	0.04	43,43,43,43	0
5	CL	B	708	1/1	1.00	0.04	44,44,44,44	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

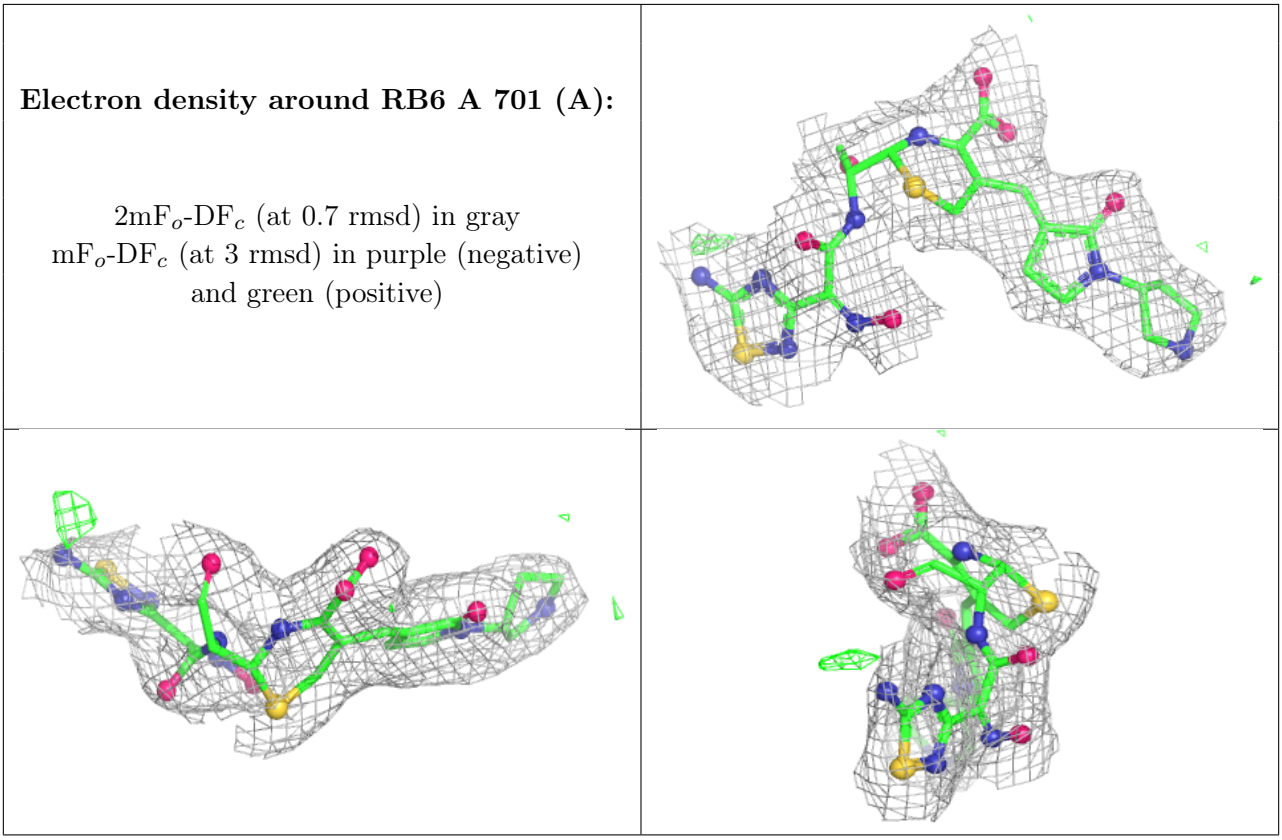
Electron density around RB6 B 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



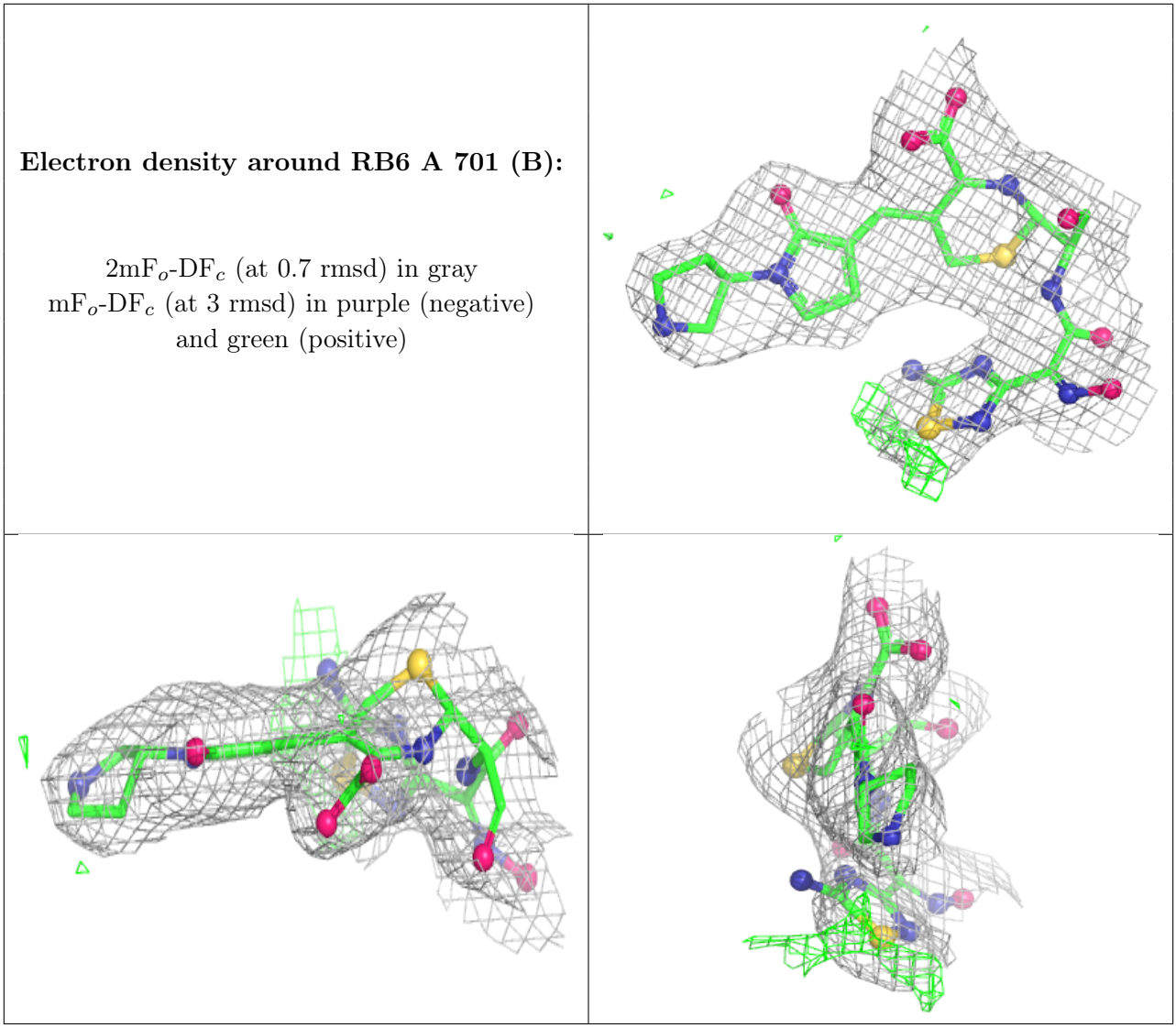
Electron density around RB6 A 701 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around RB6 A 701 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.