



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 11:36 PM GMT

PDB ID : 3PJT  
Title : Structure of Pseudomonas fluorescence LapD EAL domain complexed with c-di-GMP, C2221  
Authors : Sondermann, H.; Navarro, M.V.A.S.; Krasteva, P.  
Deposited on : 2010-11-10  
Resolution : 2.52 Å(reported)

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

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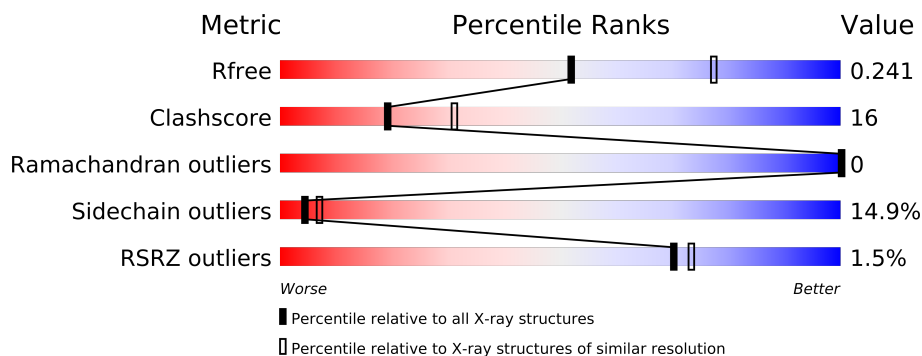
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.52 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))
$R_{free}$	66092	3240 (2.54-2.50)
Clashscore	79885	4080 (2.54-2.50)
Ramachandran outliers	78287	3990 (2.54-2.50)
Sidechain outliers	78261	3992 (2.54-2.50)
RSRZ outliers	66119	3241 (2.54-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	249	
1	B	249	

## 2 Entry composition i

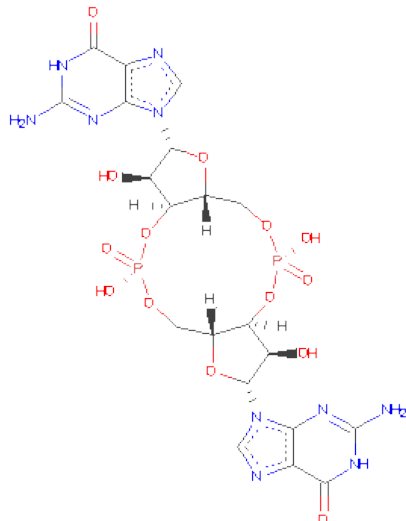
There are 3 unique types of molecules in this entry. The entry contains 4073 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cyclic dimeric GMP binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1933	1229	351	349	4			
1	B	240	Total	C	N	O	S	0	0	0
			1933	1229	351	349	4			

- Molecule 2 is 9,9'-[(2R,3R,3AS,5S,7AR,9R,10R,10AS,12S,14AR)-3,5,10,12-TETRAHYDROXY-5,12-DIOXIDOOCTAHYDRO-2H,7H-DIFURO[3,2-D:3',2'-J][1,3,7,9,2,8]TETRAOXADIPHOSPHACYCLODODECINE-2,9-DIYL]BIS(2-AMINO-1,9-DIHYDRO-6H-PURIN-6-ONE) (three-letter code: C2E) (formula: C<sub>20</sub>H<sub>24</sub>N<sub>10</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
2	B	1	Total	C	N	O	P	0	0
			46	20	10	14	2		

- Molecule 3 is water.

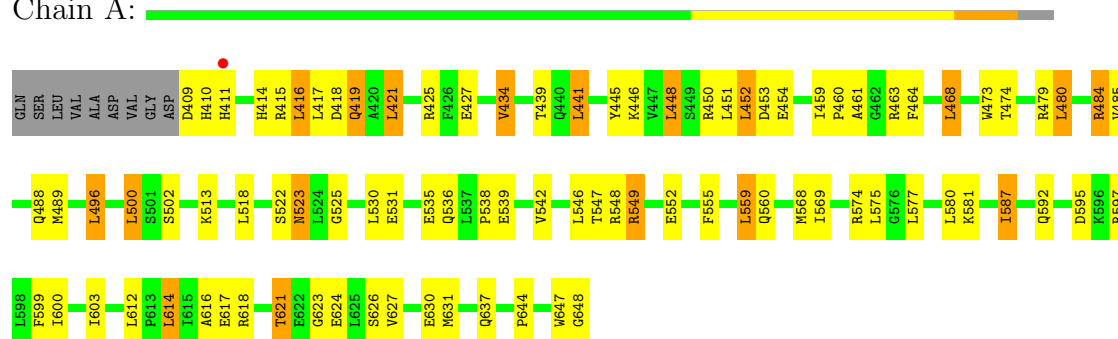
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	72	Total 72	O 72	0	0
3	B	43	Total 43	O 43	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

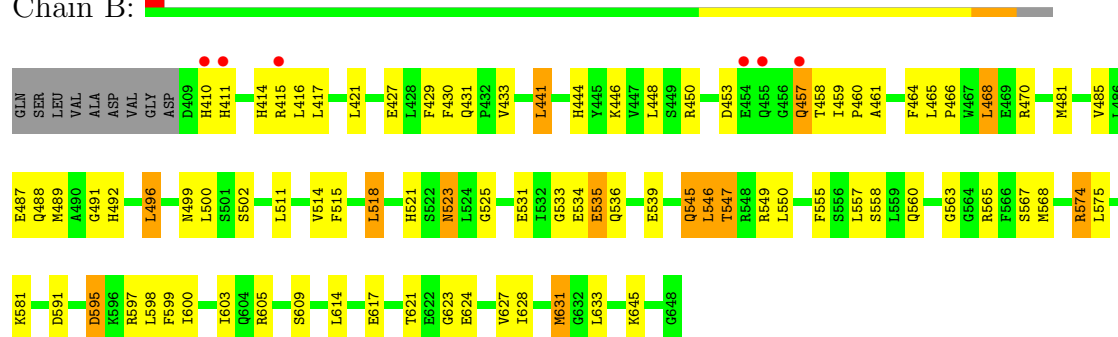
#### • Molecule 1: Cyclic dimeric GMP binding protein

Chain A:



#### • Molecule 1: Cyclic dimeric GMP binding protein

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	41.45Å 204.83Å 142.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.14 – 2.52 48.19 – 2.52	Depositor EDS
% Data completeness (in resolution range)	94.8 (34.14-2.52) 94.8 (48.19-2.52)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.55 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.289)	Depositor
R, $R_{free}$	0.181 , 0.245 0.177 , 0.241	Depositor DCC
$R_{free}$ test set	1922 reflections (9.55%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.3	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 33.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 20916 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4073	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: C2E

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	0/1970	0.66	1/2660 (0.0%)
1	B	0.45	0/1970	0.60	0/2660
All	All	0.48	0/3940	0.63	1/5320 (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	480	LEU	CA-CB-CG	7.31	132.10	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1933	0	1945	69	0
1	B	1933	0	1945	65	0
2	A	46	0	21	2	0
2	B	46	0	21	1	0
3	A	72	0	0	2	0
3	B	43	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4073	0	3932	129	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (129) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:484:ARG:HG3	1:A:484:ARG:HH11	0.92	1.07
1:B:523:ASN:HD22	1:B:523:ASN:H	1.06	1.02
1:A:621:THR:HG22	1:A:624:GLU:H	1.30	0.96
1:A:484:ARG:HG3	1:A:484:ARG:NH1	1.70	0.91
1:B:446:LYS:HE2	1:B:531:GLU:OE1	1.70	0.90
1:B:523:ASN:H	1:B:523:ASN:ND2	1.76	0.83
1:B:621:THR:HG22	1:B:624:GLU:H	1.45	0.78
1:B:599:PHE:CE2	1:B:603:ILE:HD11	2.19	0.77
1:A:417:LEU:O	1:A:421:LEU:HB2	1.87	0.75
1:A:523:ASN:HD22	1:A:523:ASN:H	1.31	0.74
1:B:410:HIS:O	1:B:414:HIS:HB2	1.88	0.73
1:A:484:ARG:HH11	1:A:484:ARG:CG	1.86	0.71
1:A:414:HIS:HB3	1:A:415:ARG:HD3	1.72	0.70
1:B:534:GLU:OE1	1:B:563:GLY:HA2	1.92	0.69
1:A:523:ASN:ND2	1:A:523:ASN:H	1.92	0.67
1:B:525:GLY:HA2	1:B:555:PHE:CE1	2.32	0.65
1:A:627:VAL:HG12	1:A:631:MET:HE2	1.78	0.65
1:A:618:ARG:H	1:A:637:GLN:NE2	1.95	0.65
1:B:446:LYS:NZ	1:B:499:ASN:OD1	2.31	0.64
1:B:600:ILE:HB	1:B:631:MET:HE1	1.80	0.62
2:B:2256:C2E:H512	2:B:2256:C2E:H81	1.80	0.62
1:A:434:VAL:HG13	1:A:439:THR:HA	1.80	0.62
1:B:464:PHE:HD1	1:B:468:LEU:HD22	1.64	0.62
1:A:489:MET:HG2	1:A:496:LEU:HD22	1.81	0.61
1:A:479:ARG:HD2	1:A:513:LYS:NZ	2.15	0.61
1:A:417:LEU:HD13	1:A:468:LEU:HD13	1.84	0.60
1:B:457:GLN:NE2	1:B:457:GLN:H	1.99	0.60
1:B:523:ASN:N	1:B:523:ASN:ND2	2.47	0.60
1:A:479:ARG:HD2	1:A:513:LYS:HZ1	1.67	0.59
1:A:461:ALA:HA	1:A:464:PHE:CE2	2.37	0.59
1:A:559:LEU:HD22	1:A:577:LEU:HD11	1.84	0.59
1:B:546:LEU:O	1:B:550:LEU:HG	2.01	0.59
2:A:2256:C2E:H81	2:A:2256:C2E:H512	1.85	0.59
1:A:538:PRO:HB2	1:A:542:VAL:HB	1.84	0.58
1:B:525:GLY:HA2	1:B:555:PHE:CD1	2.39	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:429:PHE:CD2	1:B:450:ARG:HG3	2.39	0.58
1:A:548:ARG:O	1:A:552:GLU:HG3	2.05	0.56
1:A:418:ASP:HB2	1:A:473:TRP:CH2	2.40	0.56
1:A:502:SER:HB3	1:A:536:GLN:HB2	1.88	0.55
1:B:481:MET:O	1:B:485:VAL:HG23	2.07	0.55
1:A:574:ARG:NH1	1:B:595:ASP:OD1	2.39	0.55
1:B:600:ILE:CG2	1:B:631:MET:HE2	2.37	0.54
1:A:574:ARG:HH12	1:B:595:ASP:CG	2.11	0.54
1:A:525:GLY:HA2	1:A:555:PHE:CD1	2.43	0.53
1:B:533:GLY:HA3	1:B:535:GLU:OE2	2.08	0.53
1:A:627:VAL:HG12	1:A:631:MET:CE	2.39	0.53
1:B:502:SER:HB3	1:B:536:GLN:HB2	1.92	0.52
1:A:603:ILE:HG22	1:A:614:LEU:HD21	1.92	0.52
1:A:621:THR:HG21	3:A:30:HOH:O	2.10	0.52
1:B:628:ILE:HG23	1:B:633:LEU:HD22	1.92	0.52
1:A:523:ASN:N	1:A:523:ASN:ND2	2.57	0.51
1:A:531:GLU:OE2	1:A:581:LYS:HE3	2.11	0.51
1:B:453:ASP:HB3	1:B:459:ILE:HD11	1.93	0.51
1:A:500:LEU:CD2	1:A:530:LEU:HD22	2.40	0.51
1:A:618:ARG:H	1:A:637:GLN:HE21	1.59	0.51
1:A:569:ILE:HG13	1:B:598:LEU:CD2	2.41	0.51
1:A:600:ILE:HG21	1:A:631:MET:HE3	1.92	0.51
1:A:525:GLY:HA2	1:A:555:PHE:CE1	2.46	0.50
1:A:580:LEU:HG	1:A:612:LEU:HD21	1.93	0.50
1:A:409:ASP:OD2	1:A:411:HIS:HD2	1.94	0.50
1:A:568:MET:HG3	1:A:568:MET:O	2.13	0.49
1:B:621:THR:HG22	1:B:623:GLY:N	2.27	0.48
1:B:417:LEU:HD13	1:B:468:LEU:HD13	1.94	0.48
1:B:464:PHE:CD1	1:B:468:LEU:HD22	2.48	0.48
1:B:489:MET:HG2	1:B:496:LEU:HD22	1.96	0.48
1:A:569:ILE:HG23	1:B:598:LEU:HD23	1.96	0.47
1:B:546:LEU:HD22	1:B:550:LEU:HD11	1.97	0.47
1:B:485:VAL:O	1:B:489:MET:HG3	2.15	0.47
1:A:416:LEU:HD13	1:A:451:LEU:HD21	1.96	0.47
1:A:647:TRP:O	1:A:648:GLY:C	2.51	0.47
1:A:621:THR:HG23	1:A:623:GLY:H	1.80	0.47
1:B:444:HIS:HE1	1:B:581:LYS:HZ1	1.63	0.47
1:B:411:HIS:O	1:B:415:ARG:HG2	2.14	0.47
1:A:445:TYR:HB2	1:A:496:LEU:HD12	1.97	0.47
1:A:453:ASP:HB2	3:A:49:HOH:O	2.15	0.47
1:B:450:ARG:HD3	1:B:460:PRO:HA	1.97	0.46
1:B:547:THR:HG21	1:B:575:LEU:O	2.14	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:448:LEU:HD23	1:A:644:PRO:HB3	1.97	0.46
1:A:425:ARG:NH1	1:A:452:LEU:O	2.47	0.46
1:A:560:GLN:HB2	1:A:617:GLU:OE2	2.15	0.46
1:A:415:ARG:CD	1:A:415:ARG:N	2.75	0.46
1:A:549:ARG:HA	1:A:549:ARG:HD3	1.54	0.46
1:A:411:HIS:HB3	1:A:415:ARG:HH12	1.81	0.46
1:B:491:GLY:HA3	3:B:650:HOH:O	2.15	0.45
1:A:569:ILE:HG13	1:B:598:LEU:HD23	1.97	0.45
1:B:465:LEU:N	1:B:466:PRO:CD	2.80	0.45
1:B:591:ASP:HA	1:B:627:VAL:HG21	2.00	0.44
1:A:415:ARG:O	1:A:419:GLN:HB2	2.18	0.44
1:B:565:ARG:O	1:B:568:MET:HG2	2.18	0.44
1:B:599:PHE:CZ	1:B:603:ILE:HD11	2.52	0.43
1:B:599:PHE:O	1:B:603:ILE:HG13	2.18	0.43
1:A:434:VAL:CG1	1:A:439:THR:HA	2.47	0.43
1:A:559:LEU:HD22	1:A:577:LEU:CD1	2.47	0.43
1:A:451:LEU:HB3	1:A:459:ILE:HB	1.99	0.43
1:A:416:LEU:HD23	1:A:416:LEU:HA	1.79	0.43
1:A:451:LEU:HD23	1:A:459:ILE:HD12	2.01	0.43
1:B:514:VAL:O	1:B:518:LEU:HD22	2.18	0.43
1:B:600:ILE:HB	1:B:631:MET:CE	2.48	0.43
1:A:500:LEU:HD21	1:A:530:LEU:HD13	2.01	0.42
1:A:484:ARG:CG	1:A:484:ARG:NH1	2.56	0.42
1:B:545:GLN:H	1:B:545:GLN:HG2	1.50	0.42
1:A:485:VAL:O	1:A:489:MET:HG3	2.19	0.42
1:A:626:SER:O	1:A:630:GLU:HG3	2.20	0.42
1:A:599:PHE:CD1	1:B:567:SER:HA	2.53	0.42
1:B:444:HIS:HE1	1:B:581:LYS:NZ	2.18	0.42
1:B:546:LEU:HD22	1:B:550:LEU:CD1	2.50	0.42
1:B:511:LEU:HG	1:B:515:PHE:HE2	1.84	0.42
1:B:431:GLN:HG2	3:B:55:HOH:O	2.19	0.42
1:A:595:ASP:OD2	1:B:574:ARG:NH2	2.53	0.42
1:B:492:HIS:HB2	3:B:29:HOH:O	2.20	0.42
1:B:557:LEU:HG	1:B:558:SER:N	2.35	0.42
1:B:521:HIS:HA	1:B:523:ASN:HD21	1.85	0.41
1:A:547:THR:HG21	1:A:575:LEU:O	2.21	0.41
1:B:457:GLN:CD	1:B:457:GLN:H	2.23	0.41
1:B:597:ARG:NH1	3:B:12:HOH:O	2.53	0.41
1:B:441:LEU:HA	1:B:441:LEU:HD22	1.77	0.41
1:A:468:LEU:HD12	1:A:468:LEU:HA	1.95	0.41
1:A:446:LYS:NZ	2:A:2256:C2E:O2P	2.48	0.41
1:A:587:ILE:HG12	1:A:616:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:434:VAL:HG22	1:A:441:LEU:O	2.21	0.41
1:B:430:PHE:CD2	1:B:430:PHE:N	2.88	0.41
1:B:461:ALA:HA	1:B:464:PHE:CE2	2.57	0.40
1:B:453:ASP:O	1:B:453:ASP:OD1	2.38	0.40
1:B:581:LYS:HB3	1:B:617:GLU:OE2	2.21	0.40
1:B:453:ASP:C	1:B:453:ASP:OD1	2.59	0.40
1:A:500:LEU:HD21	1:A:530:LEU:HD22	2.03	0.40
1:B:633:LEU:HD12	1:B:633:LEU:N	2.37	0.40
1:B:433:VAL:HG21	1:B:581:LYS:HZ1	1.87	0.40
1:A:450:ARG:NE	1:A:460:PRO:HA	2.37	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	238/249 (96%)	233 (98%)	5 (2%)	0	100	100
1	B	238/249 (96%)	225 (94%)	13 (6%)	0	100	100
All	All	476/498 (96%)	458 (96%)	18 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	201/208 (97%)	170 (85%)	31 (15%)	4	6
1	B	201/208 (97%)	172 (86%)	29 (14%)	5	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	402/416 (97%)	342 (85%)	60 (15%)	<b>4</b> <b>7</b>

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	410	HIS
1	A	416	LEU
1	A	419	GLN
1	A	421	LEU
1	A	427	GLU
1	A	434	VAL
1	A	441	LEU
1	A	448	LEU
1	A	452	LEU
1	A	454	GLU
1	A	463	ARG
1	A	468	LEU
1	A	474	THR
1	A	480	LEU
1	A	484	ARG
1	A	488	GLN
1	A	496	LEU
1	A	500	LEU
1	A	518	LEU
1	A	522	SER
1	A	523	ASN
1	A	535	GLU
1	A	539	GLU
1	A	546	LEU
1	A	549	ARG
1	A	559	LEU
1	A	587	ILE
1	A	592	GLN
1	A	597	ARG
1	A	614	LEU
1	A	621	THR
1	B	416	LEU
1	B	421	LEU
1	B	427	GLU
1	B	441	LEU
1	B	448	LEU
1	B	457	GLN

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Mol	Chain	Res	Type
1	B	458	THR
1	B	468	LEU
1	B	470	ARG
1	B	487	GLU
1	B	488	GLN
1	B	496	LEU
1	B	500	LEU
1	B	518	LEU
1	B	523	ASN
1	B	535	GLU
1	B	539	GLU
1	B	545	GLN
1	B	546	LEU
1	B	547	THR
1	B	549	ARG
1	B	560	GLN
1	B	574	ARG
1	B	595	ASP
1	B	605	ARG
1	B	609	SER
1	B	614	LEU
1	B	631	MET
1	B	645	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	411	HIS
1	A	523	ASN
1	A	592	GLN
1	A	637	GLN
1	B	419	GLN
1	B	440	GLN
1	B	444	HIS
1	B	457	GLN
1	B	523	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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	C2E	A	2256	-	52,52,52	2.63	13 (25%)	76,82,82	2.79	22 (28%)
2	C2E	B	2256	-	52,52,52	2.68	12 (23%)	76,82,82	2.58	24 (31%)

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	C2E	A	2256	-	-	0/30/62/62	0/0/7/7
2	C2E	B	2256	-	-	0/30/62/62	0/0/7/7

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2256	C2E	C21-N21	7.58	1.44	1.32
2	B	2256	C2E	C21-N21	7.54	1.44	1.32
2	B	2256	C2E	C2-N2	7.24	1.43	1.32
2	B	2256	C2E	O61-C61	7.19	1.38	1.24
2	A	2256	C2E	O61-C61	7.06	1.38	1.24
2	B	2256	C2E	O6-C6	7.06	1.38	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2256	C2E	O6-C6	6.86	1.38	1.24
2	A	2256	C2E	C2-N2	6.44	1.42	1.32
2	A	2256	C2E	C2'-C1'	-6.38	1.44	1.53
2	B	2256	C2E	C2'-C3'	-5.48	1.40	1.53
2	B	2256	C2E	C2'-C1'	-5.12	1.46	1.53
2	A	2256	C2E	C2'-C3'	-4.99	1.41	1.53
2	B	2256	C2E	C1A-N91	3.49	1.59	1.48
2	A	2256	C2E	C1'-N9	3.40	1.59	1.48
2	B	2256	C2E	C1'-N9	3.30	1.59	1.48
2	B	2256	C2E	C4-N9	-3.15	1.33	1.37
2	A	2256	C2E	C1A-N91	3.12	1.58	1.48
2	B	2256	C2E	O2A-C2A	-2.98	1.35	1.43
2	A	2256	C2E	O2A-C2A	-2.69	1.36	1.43
2	B	2256	C2E	C2A-C3A	-2.62	1.46	1.53
2	A	2256	C2E	C4-N9	-2.35	1.34	1.37
2	B	2256	C2E	O5A-C5A	-2.30	1.35	1.44
2	A	2256	C2E	O4'-C4'	-2.25	1.39	1.45
2	A	2256	C2E	C2A-C3A	-2.20	1.47	1.53
2	A	2256	C2E	O5A-C5A	-2.16	1.35	1.44

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2256	C2E	C6-C5-N7	-13.29	132.35	134.14
2	A	2256	C2E	O4A-C1A-N91	10.83	118.51	108.44
2	B	2256	C2E	O4A-C1A-N91	10.38	118.09	108.44
2	B	2256	C2E	C6-C5-N7	-8.52	132.99	134.14
2	A	2256	C2E	N3-C4-N9	5.83	135.46	126.91
2	B	2256	C2E	N3-C4-N9	5.27	134.63	126.91
2	A	2256	C2E	C5-C4-N3	-5.21	118.39	125.94
2	B	2256	C2E	N31-C41-N91	4.95	134.18	126.91
2	A	2256	C2E	C21-N31-C41	4.85	121.91	115.09
2	A	2256	C2E	N31-C41-N91	4.82	133.98	126.91
2	B	2256	C2E	C51-C41-N31	-4.76	119.05	125.94
2	A	2256	C2E	C51-C41-N31	-4.63	119.23	125.94
2	B	2256	C2E	C21-N31-C41	4.52	121.45	115.09
2	B	2256	C2E	C5-C4-N3	-4.50	119.42	125.94
2	B	2256	C2E	C8-N9-C4	4.21	110.11	106.90
2	B	2256	C2E	C5A-C4A-C3A	-4.07	100.02	114.19
2	B	2256	C2E	C4'-O4'-C1'	-3.93	105.48	109.75
2	A	2256	C2E	C8-N9-C4	3.89	109.87	106.90
2	A	2256	C2E	C5A-C4A-C3A	-3.86	100.73	114.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2256	C2E	C2-N3-C4	3.76	120.38	115.09
2	A	2256	C2E	O5'-P1-O3A	3.58	114.87	104.68
2	A	2256	C2E	C2-N3-C4	3.57	120.10	115.09
2	B	2256	C2E	C41-C51-N71	-3.46	106.56	109.52
2	B	2256	C2E	C4A-O4A-C1A	-3.38	106.08	109.75
2	B	2256	C2E	C81-N91-C41	3.26	109.39	106.90
2	B	2256	C2E	O5'-P1-O3A	3.24	113.91	104.68
2	B	2256	C2E	C3'-C2'-C1'	2.71	106.42	99.98
2	A	2256	C2E	C81-N91-C41	2.58	108.87	106.90
2	A	2256	C2E	C4-C5-N7	-2.51	107.37	109.52
2	A	2256	C2E	O5A-P11-O3'	2.49	111.79	104.68
2	A	2256	C2E	C2'-C1'-N9	2.44	119.53	113.27
2	A	2256	C2E	C41-C51-N71	-2.43	107.44	109.52
2	B	2256	C2E	C2'-C1'-N9	2.39	119.41	113.27
2	B	2256	C2E	O4'-C1'-N9	2.28	110.56	108.44
2	A	2256	C2E	N21-C21-N11	2.27	120.35	117.86
2	B	2256	C2E	O5A-P11-O3'	2.26	111.11	104.68
2	A	2256	C2E	N7-C8-N9	-2.24	108.03	114.36
2	A	2256	C2E	C2A-C3A-C4A	2.22	107.49	103.16
2	B	2256	C2E	C61-C51-N71	2.18	134.43	134.14
2	B	2256	C2E	O5A-P11-O11	-2.13	101.03	109.37
2	B	2256	C2E	N7-C8-N9	-2.13	108.34	114.36
2	B	2256	C2E	N71-C81-N91	-2.12	108.35	114.36
2	A	2256	C2E	C4A-O4A-C1A	-2.09	107.47	109.75
2	A	2256	C2E	N71-C81-N91	-2.07	108.50	114.36
2	B	2256	C2E	C4-C5-N7	-2.05	107.76	109.52
2	A	2256	C2E	C3'-C2'-C1'	2.05	104.86	99.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	240/249 (96%)	-0.28	1 (0%) 90 92	18, 30, 51, 82	0
1	B	240/249 (96%)	-0.11	6 (2%) 54 58	24, 40, 61, 94	0
All	All	480/498 (96%)	-0.20	7 (1%) 70 73	18, 35, 58, 94	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	455	GLN	3.8
1	B	457	GLN	3.2
1	B	411	HIS	3.2
1	B	410	HIS	2.9
1	A	411	HIS	2.9
1	B	415	ARG	2.5
1	B	454	GLU	2.2

### 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 ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	C2E	A	2256	46/46	0.12	-0.23	17,26,29,31	0
2	C2E	B	2256	46/46	0.12	-0.74	24,30,33,36	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.