



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 08:49 AM EST

PDB ID : 3PJT
Title : Structure of Pseudomonas fluorescense 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 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
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) : 2.36

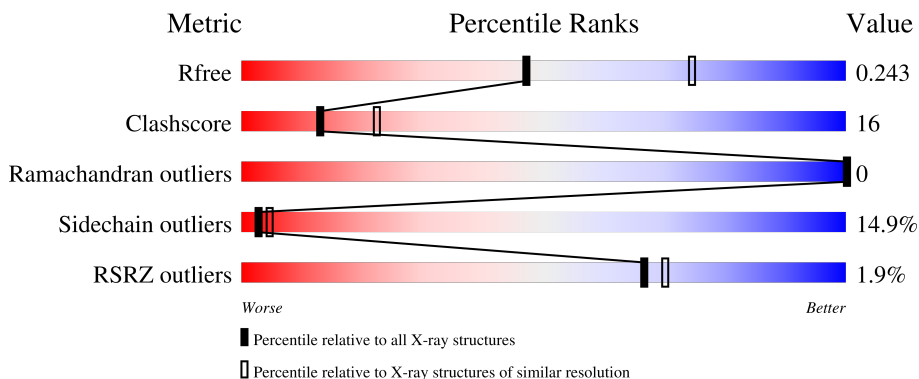
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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}	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (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 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 $\leq 5\%$. 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	249	
1	B	249	

2 Entry composition i

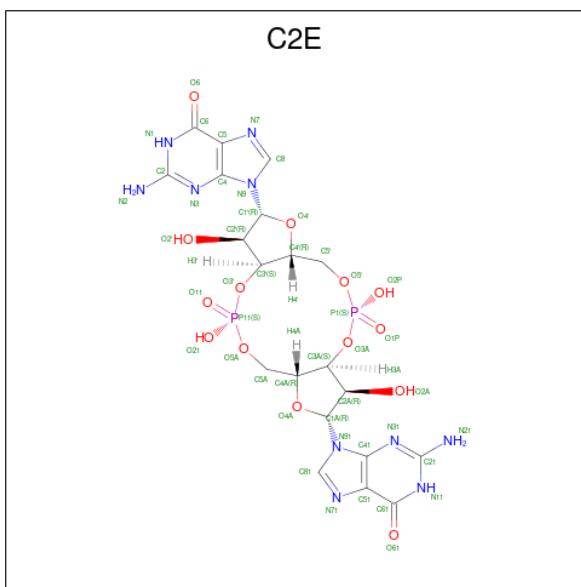
There are 3 unique types of molecules in this entry. The entry contains 4073 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cyclic dimeric GMP binding protein.

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

- Molecule 2 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydroxy-5,12-dioxidoctahydro-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: C₂₀H₂₄N₁₀O₁₄P₂).



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

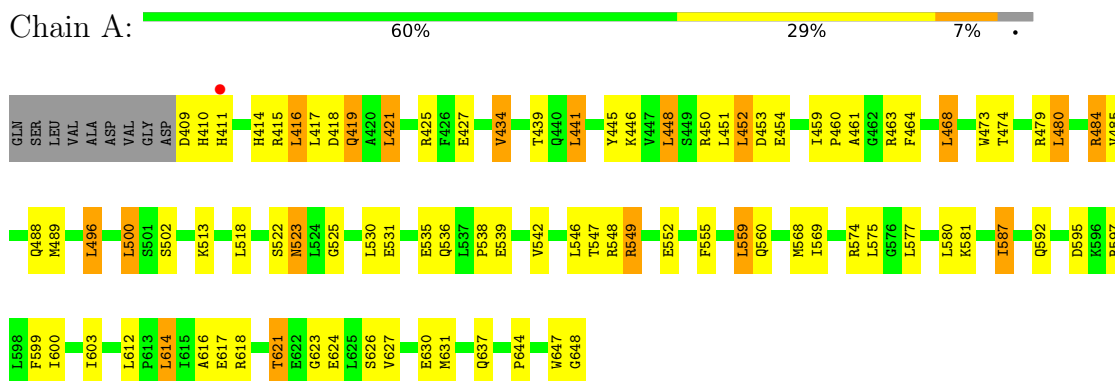
- Molecule 3 is water.

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

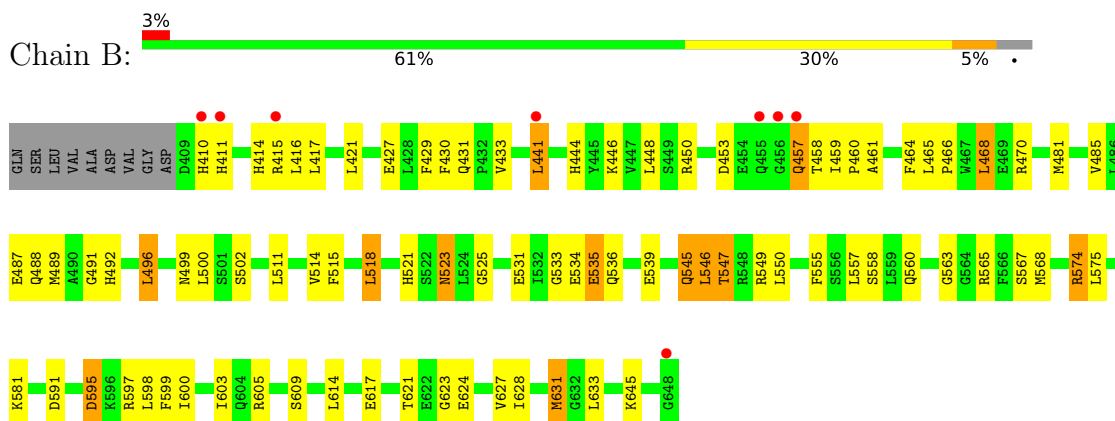
3 Residue-property plots [i](#)

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: Cyclic dimeric GMP binding protein



- Molecule 1: Cyclic dimeric GMP binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	4.55 (at 2.51Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, R_{free}	0.181 , 0.245 0.180 , 0.243	Depositor DCC
R_{free} test set	2000 reflections (9.56%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtrriage
Anisotropy	0.483	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4073	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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 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	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
All	All	4073	0	3932	129	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 16.

All (129) 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:484:ARG:HH11	1:A:484:ARG:HG3	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:H	1:A:523:ASN:HD22	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:H	1:A:523:ASN:ND2	1.92	0.67
1:B:525:GLY:HA2	1:B:555:PHE:CE1	2.32	0.65
1:A:618:ARG:H	1:A:637:GLN:NE2	1.95	0.65
1:A:627:VAL:HG12	1:A:631:MET:HE2	1.78	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:H81	2:B:2256:C2E:H512	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:ND2	1:B:523:ASN:N	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
2:A:2256:C2E:H81	2:A:2256:C2E:H512	1.85	0.59
1:B:546:LEU:O	1:B:550:LEU:HG	2.01	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:603:ILE:HG22	1:A:614:LEU:HD21	1.92	0.52
1:B:502:SER:HB3	1:B:536:GLN:HB2	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:ND2	1:A:523:ASN:N	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:569:ILE:HG13	1:B:598:LEU:CD2	2.41	0.51
1:A:618:ARG:H	1:A:637:GLN:HE21	1.59	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:O	1:A:568:MET:HG3	2.13	0.49
1:B:417:LEU:HD13	1:B:468:LEU:HD13	1.94	0.48
1:B:621:THR:HG22	1:B:623:GLY:N	2.27	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: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:B:485:VAL:O	1:B:489:MET:HG3	2.15	0.47
1:B:546:LEU:HD22	1:B:550:LEU:HD11	1.97	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
1:A:448:LEU:HD23	1:A:644:PRO:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:A:415:ARG:CD	2.75	0.46
1:A:549:ARG:HD3	1:A:549:ARG:HA	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: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:B:599:PHE:O	1:B:603:ILE:HG13	2.18	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:NH1	1:A:484:ARG:CG	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:599:PHE:CD1	1:B:567:SER:HA	2.53	0.42
1:A:626:SER:O	1:A:630:GLU:HG3	2.20	0.42
1:B:444:HIS:HE1	1:B:581:LYS:NZ	2.18	0.42
1:A:595:ASP:OD2	1:B:574:ARG:NH2	2.53	0.42
1:B:431:GLN:HG2	3:B:55:HOH:O	2.19	0.42
1:B:511:LEU:HG	1:B:515:PHE:HE2	1.84	0.42
1:B:546:LEU:HD22	1:B:550:LEU:CD1	2.50	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:A:547:THR:HG21	1:A:575:LEU:O	2.21	0.41
1:B:521:HIS:HA	1:B:523:ASN:HD21	1.85	0.41
1:B:441:LEU:HD22	1:B:441:LEU:HA	1.77	0.41
1:B:457:GLN:H	1:B:457:GLN:CD	2.23	0.41
1:B:597:ARG:NH1	3:B:12:HOH:O	2.53	0.41
1:A:446:LYS:NZ	2:A:2256:C2E:O2P	2.48	0.41
1:A:468:LEU:HD12	1:A:468:LEU:HA	1.95	0.41
1:A:587:ILE:HG12	1:A:616:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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:453:ASP:O	1:B:453:ASP:OD1	2.38	0.40
1:B:461:ALA:HA	1:B:464:PHE:CE2	2.57	0.40
1:B:581:LYS:HB3	1:B:617:GLU:OE2	2.21	0.40
1:B:453:ASP:OD1	1:B:453:ASP:C	2.59	0.40
1:A:500:LEU:HD21	1:A:530:LEU:HD22	2.03	0.40
1:A:450:ARG:NE	1:A:460:PRO:HA	2.37	0.40
1:B:433:VAL:HG21	1:B:581:LYS:HZ1	1.87	0.40
1:B:633:LEU:N	1:B:633:LEU:HD12	2.37	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	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 [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	201/208 (97%)	170 (85%)	31 (15%)	2	4
1	B	201/208 (97%)	172 (86%)	29 (14%)	3	5
All	All	402/416 (97%)	342 (85%)	60 (15%)	3	5

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

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Mol	Chain	Res	Type
1	B	448	LEU
1	B	457	GLN
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

Sometimes 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 [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](#)

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	-	44,52,52	2.59	14 (31%)	52,82,82	1.51	10 (19%)
2	C2E	B	2256	-	44,52,52	2.58	12 (27%)	52,82,82	1.53	8 (15%)

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	-	-	7/22/62/62	0/6/7/7
2	C2E	B	2256	-	-	5/22/62/62	0/6/7/7

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2256	C2E	O61-C61	7.53	1.38	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2256	C2E	O61-C61	7.40	1.38	1.23
2	B	2256	C2E	O6-C6	7.40	1.38	1.23
2	A	2256	C2E	O6-C6	7.21	1.38	1.23
2	A	2256	C2E	C2'-C1'	-6.18	1.44	1.53
2	B	2256	C2E	C2'-C3'	-5.71	1.40	1.52
2	A	2256	C2E	C2'-C3'	-5.20	1.41	1.52
2	B	2256	C2E	C2'-C1'	-5.00	1.46	1.53
2	A	2256	C2E	C21-N21	4.21	1.44	1.34
2	B	2256	C2E	C21-N21	4.18	1.44	1.34
2	B	2256	C2E	C2-N2	3.99	1.43	1.34
2	A	2256	C2E	C51-C61	-3.74	1.39	1.47
2	B	2256	C2E	C5-C6	-3.54	1.40	1.47
2	A	2256	C2E	C5-C6	-3.48	1.40	1.47
2	A	2256	C2E	C2-N2	3.46	1.42	1.34
2	B	2256	C2E	O2A-C2A	-3.06	1.35	1.43
2	B	2256	C2E	C51-C61	-2.95	1.41	1.47
2	A	2256	C2E	O2A-C2A	-2.76	1.36	1.43
2	B	2256	C2E	C2A-C3A	-2.70	1.46	1.52
2	A	2256	C2E	C6-N1	-2.46	1.34	1.37
2	B	2256	C2E	O5A-C5A	-2.46	1.35	1.44
2	A	2256	C2E	O4'-C4'	-2.34	1.39	1.45
2	A	2256	C2E	O5A-C5A	-2.31	1.35	1.44
2	A	2256	C2E	C2A-C3A	-2.26	1.47	1.52
2	A	2256	C2E	C3A-C4A	-2.05	1.47	1.52
2	B	2256	C2E	C61-N11	-2.02	1.34	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2256	C2E	C5A-C4A-C3A	-4.34	100.02	114.40
2	A	2256	C2E	C5A-C4A-C3A	-4.13	100.73	114.40
2	B	2256	C2E	C81-N71-C51	3.11	108.91	102.99
2	B	2256	C2E	C3'-C2'-C1'	2.95	106.42	99.89
2	A	2256	C2E	C8-N7-C5	2.94	108.59	102.99
2	B	2256	C2E	C5-C6-N1	2.91	119.09	113.95
2	A	2256	C2E	C51-C61-N11	2.86	119.00	113.95
2	A	2256	C2E	C81-N71-C51	2.84	108.40	102.99
2	B	2256	C2E	C2-N1-C6	-2.71	120.11	125.10
2	A	2256	C2E	C2-N1-C6	-2.70	120.13	125.10
2	B	2256	C2E	C51-C61-N11	2.64	118.61	113.95
2	B	2256	C2E	C8-N7-C5	2.54	107.83	102.99
2	A	2256	C2E	C5-C6-N1	2.53	118.42	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2256	C2E	O61-C61-C51	-2.50	119.48	124.37
2	A	2256	C2E	C2A-C3A-C4A	2.40	107.49	103.22
2	A	2256	C2E	C3'-C2'-C1'	2.24	104.86	99.89
2	B	2256	C2E	O5A-P11-O11	-2.06	101.03	109.07
2	A	2256	C2E	C21-N11-C61	-2.02	121.38	125.10

There are no chirality outliers.

All (12) torsion outliers are listed below:

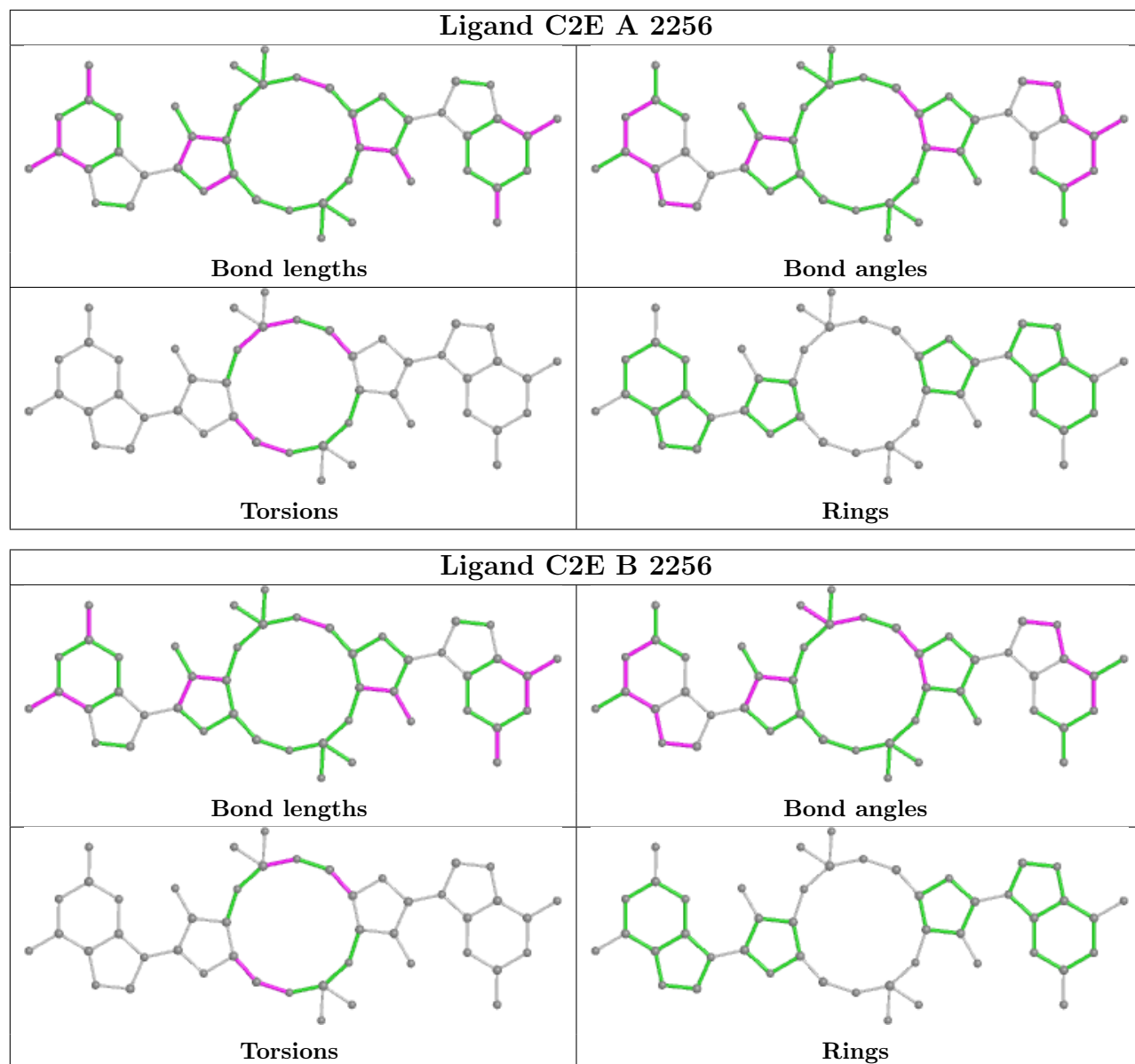
Mol	Chain	Res	Type	Atoms
2	B	2256	C2E	C3A-C4A-C5A-O5A
2	A	2256	C2E	O4A-C4A-C5A-O5A
2	A	2256	C2E	C3A-C4A-C5A-O5A
2	B	2256	C2E	O4A-C4A-C5A-O5A
2	A	2256	C2E	C4'-C5'-O5'-P1
2	B	2256	C2E	C4'-C5'-O5'-P1
2	A	2256	C2E	C3'-O3'-P11-O5A
2	A	2256	C2E	C3'-O3'-P11-O11
2	B	2256	C2E	O4'-C4'-C5'-O5'
2	A	2256	C2E	C5A-O5A-P11-O11
2	B	2256	C2E	C5A-O5A-P11-O11
2	A	2256	C2E	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2256	C2E	2	0
2	B	2256	C2E	1	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 than 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.



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 [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, 95th 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	240/249 (96%)	-0.21	1 (0%) 92 93	18, 30, 51, 82	0
1	B	240/249 (96%)	-0.05	8 (3%) 46 50	24, 40, 61, 94	0
All	All	480/498 (96%)	-0.13	9 (1%) 66 70	18, 35, 58, 94	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	411	HIS	3.8
1	B	455	GLN	3.6
1	B	457	GLN	3.5
1	B	410	HIS	3.2
1	A	411	HIS	3.0
1	B	415	ARG	2.6
1	B	456	GLY	2.3
1	B	648	GLY	2.1
1	B	441	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.

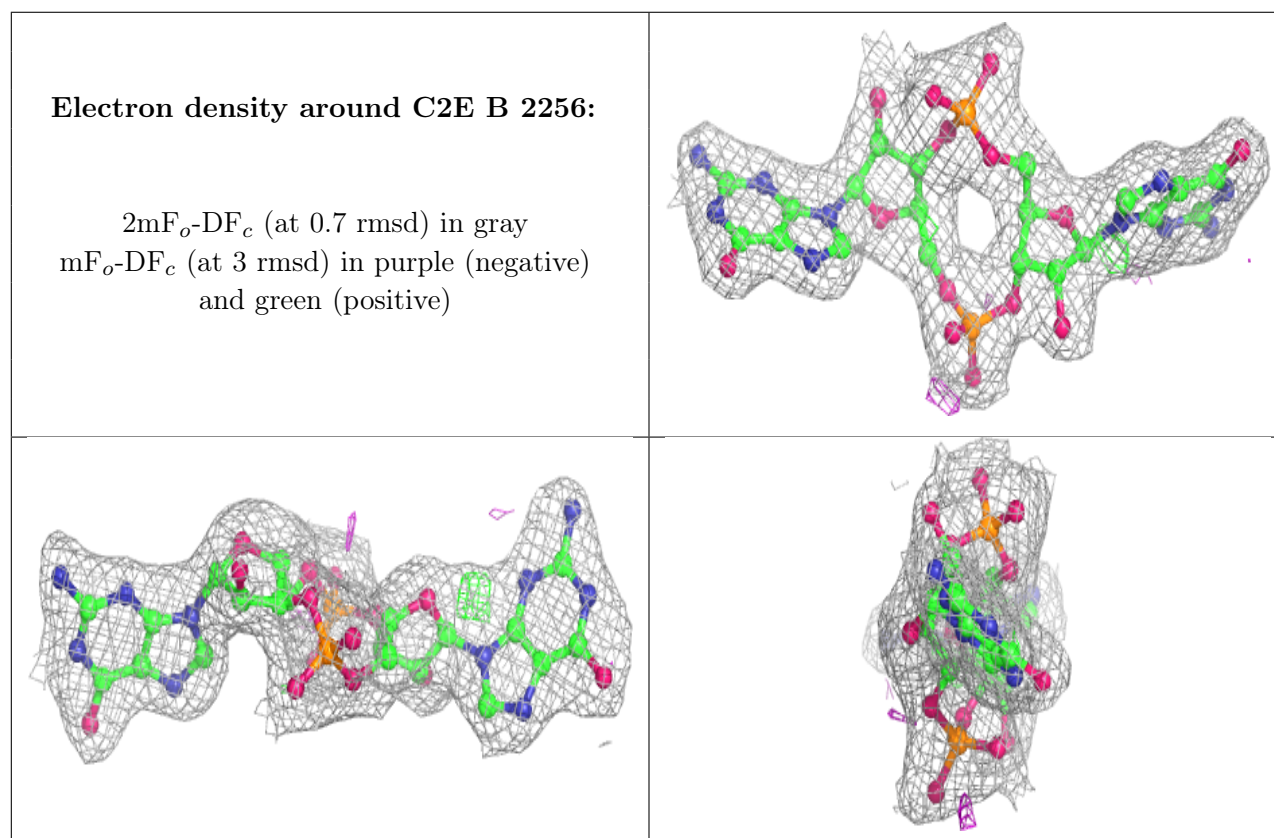
6.4 Ligands [i](#)

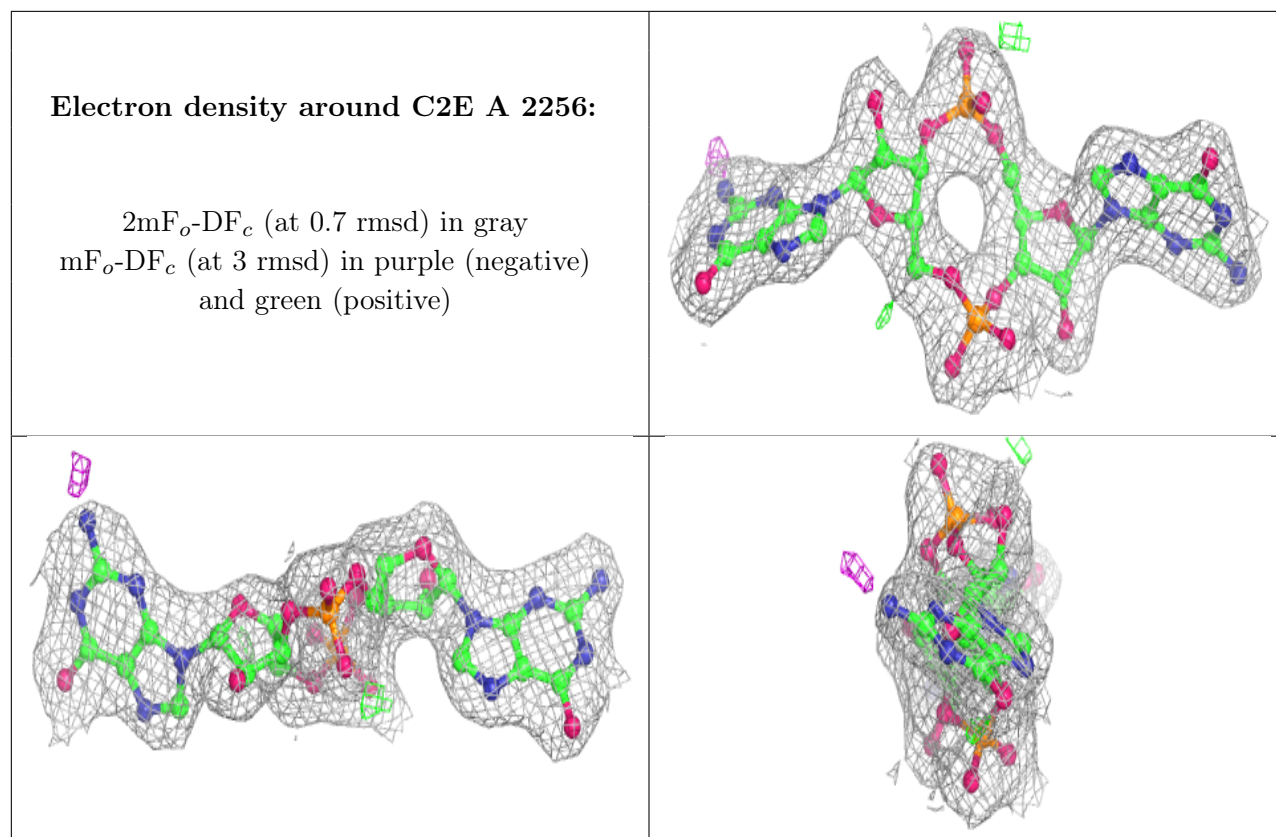
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th 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(\AA^2)	Q<0.9
2	C2E	B	2256	46/46	0.97	0.13	24,30,33,36	0
2	C2E	A	2256	46/46	0.98	0.13	17,26,29,31	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.