



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:31 am BST

PDB ID : 4ETZ
Title : Crystal Structure of PelD 158-CT from Pseudomonas aeruginosa PAO1
Authors : Li, Z.; Chen, J.; Nair, S.K.
Deposited on : 2012-04-24
Resolution : 2.05 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 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 : 2.11
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) : 2.11

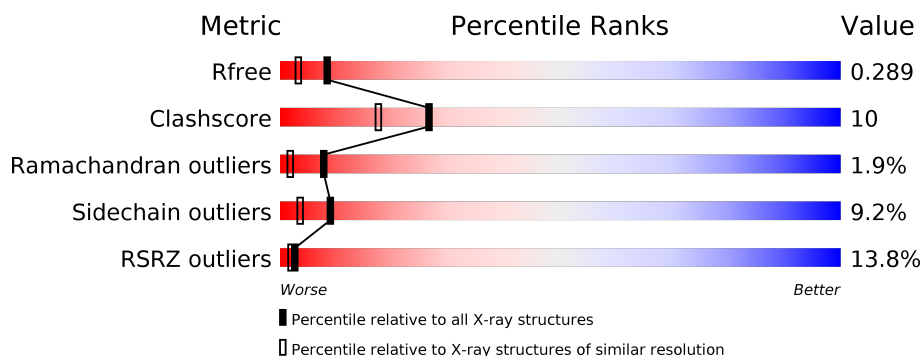
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 ≥ 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	297	<div> <div>10%</div> <div>68%</div> <div>25%</div> <div>...</div> </div>
1	B	297	<div> <div>16%</div> <div>73%</div> <div>22%</div> <div>..</div> </div>

2 Entry composition i

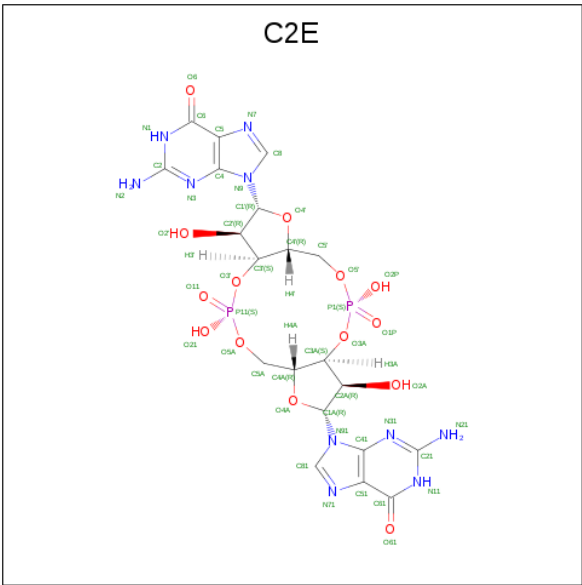
There are 3 unique types of molecules in this entry. The entry contains 4768 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PelD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2251	1414	411	420	6			
1	B	289	Total	C	N	O	S	0	0	0
			2285	1436	415	428	6			

- 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
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		

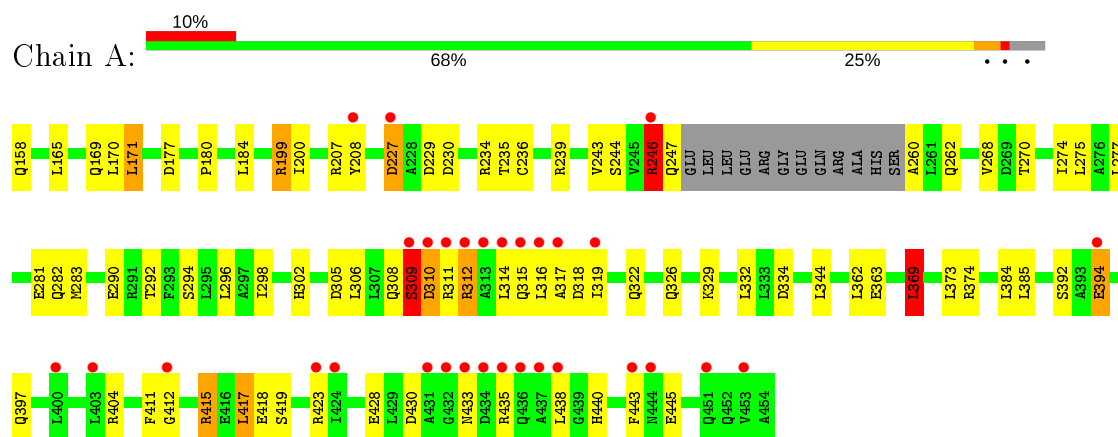
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	98	Total 98	O 98	0	0
3	B	42	Total 42	O 42	0	0

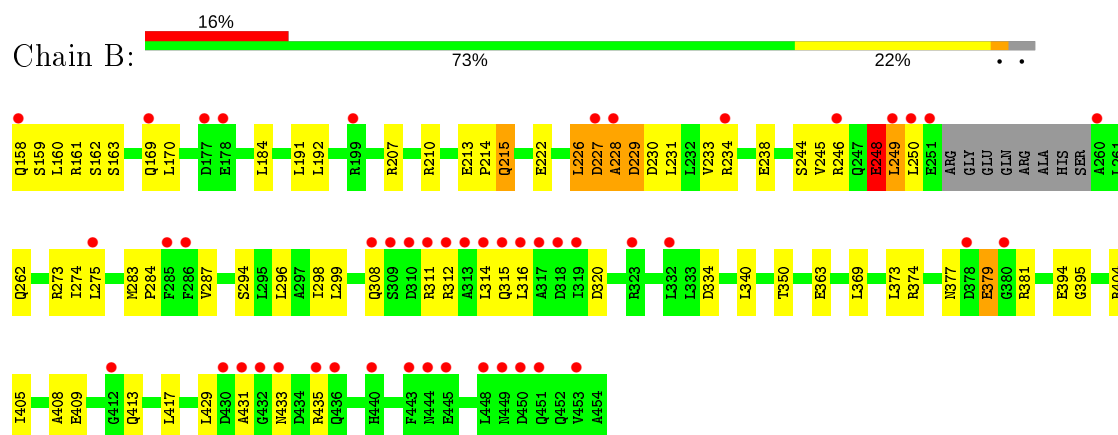
3 Residue-property plots [i](#)

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: PelD



• Molecule 1: PelD



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.32Å 41.31Å 110.85Å 90.00° 95.45° 90.00°	Depositor
Resolution (Å)	25.00 – 2.05 38.69 – 2.05	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-2.05) 99.7 (38.69-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.231 , 0.277 0.240 , 0.289	Depositor DCC
R_{free} test set	2016 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	39.9	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4768	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% 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	0.71	0/2280	0.80	2/3082 (0.1%)
1	B	0.55	0/2314	0.71	0/3128
All	All	0.63	0/4594	0.76	2/6210 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	GLU	C-N-CA	-6.19	109.30	122.30
1	A	369	LEU	CB-CG-CD1	6.15	121.45	111.00

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	2251	0	2283	56	0
1	B	2285	0	2317	41	0
2	A	46	0	22	0	0
2	B	46	0	22	1	0
3	A	98	0	0	10	0
3	B	42	0	0	4	0
All	All	4768	0	4644	95	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 10.

All (95) 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:296:LEU:HG	3:A:696:HOH:O	1.48	1.11
1:A:363:GLU:OE2	1:A:374:ARG:HD3	1.49	1.11
1:A:317:ALA:HB2	1:B:315:GLN:HA	1.48	0.95
1:B:229:ASP:HA	3:B:626:HOH:O	1.72	0.88
1:B:215:GLN:HB2	3:B:604:HOH:O	1.76	0.83
1:A:169:GLN:HB3	3:A:623:HOH:O	1.79	0.82
1:B:275:LEU:HD21	1:B:308:GLN:HG2	1.65	0.79
1:B:248:GLU:HA	1:B:249:LEU:HB3	1.68	0.76
1:A:246:ARG:NH1	1:A:290:GLU:OE2	2.18	0.76
1:A:244:SER:OG	1:A:246:ARG:HG3	1.86	0.75
1:A:165:LEU:O	1:A:169:GLN:HG2	1.88	0.74
1:A:322:GLN:O	1:A:326:GLN:HG2	1.89	0.72
1:B:229:ASP:HB2	1:B:234:ARG:HD2	1.74	0.70
1:A:208:TYR:HB2	3:A:603:HOH:O	1.91	0.70
1:B:227:ASP:HB2	1:B:230:ASP:HB2	1.73	0.70
1:B:163:SER:HB3	1:B:191:LEU:HD21	1.76	0.67
1:A:292:THR:O	1:A:296:LEU:HD13	1.95	0.66
1:A:306:LEU:HA	1:A:309:SER:HB2	1.78	0.65
1:A:270:THR:O	1:A:329:LYS:HE2	1.97	0.64
1:A:199:ARG:HG2	1:A:282:GLN:NE2	2.15	0.62
1:A:199:ARG:HG2	1:A:282:GLN:HE21	1.66	0.60
1:B:350:THR:HA	1:B:381:ARG:HD2	1.85	0.59
1:B:207:ARG:NH1	1:B:213:GLU:OE2	2.36	0.58
1:B:228:ALA:O	3:B:626:HOH:O	2.17	0.58
1:A:318:ASP:H	1:B:316:LEU:HD12	1.70	0.57
1:A:332:LEU:HD21	1:A:438:LEU:HD22	1.86	0.57
1:B:248:GLU:HA	1:B:249:LEU:CB	2.31	0.57
1:A:158:GLN:N	3:A:613:HOH:O	2.38	0.56
1:A:415:ARG:NH1	1:A:419:SER:OG	2.38	0.56
1:B:227:ASP:O	1:B:228:ALA:C	2.45	0.55
1:B:248:GLU:HG2	1:B:250:LEU:HD23	1.87	0.55
1:A:199:ARG:HB3	1:A:282:GLN:HG2	1.89	0.55
1:A:404:ARG:HG2	1:A:417:LEU:HD13	1.88	0.54
1:A:415:ARG:HH11	1:A:415:ARG:CG	2.20	0.54
1:B:229:ASP:CB	1:B:234:ARG:HD2	2.38	0.54
1:B:245:VAL:O	1:B:245:VAL:HG13	2.08	0.53
1:B:246:ARG:N	3:B:624:HOH:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:ASP:HB2	1:B:234:ARG:CD	2.39	0.52
1:B:210:ARG:NH1	1:B:274:ILE:HD11	2.25	0.51
1:B:405:ILE:O	1:B:409:GLU:HG3	2.11	0.51
1:A:315:GLN:HB3	1:A:322:GLN:HE22	1.75	0.51
1:B:363:GLU:OE2	1:B:374:ARG:HD3	2.11	0.51
1:A:260:ALA:N	3:A:609:HOH:O	2.44	0.50
1:A:305:ASP:O	1:A:309:SER:HB2	2.12	0.50
1:A:392:SER:OG	1:A:394:GLU:HG2	2.13	0.49
1:A:294:SER:O	1:A:298:ILE:HD12	2.13	0.49
1:A:236:CYS:HB2	1:A:243:VAL:HG22	1.95	0.48
1:A:207:ARG:HB3	1:A:208:TYR:HD2	1.78	0.48
1:A:309:SER:O	1:A:312:ARG:HB2	2.14	0.48
1:A:415:ARG:NH1	1:A:415:ARG:HG2	2.29	0.48
1:A:415:ARG:HH11	1:A:415:ARG:HG2	1.79	0.47
1:B:229:ASP:N	1:B:229:ASP:OD1	2.47	0.47
1:A:310:ASP:HA	3:A:655:HOH:O	2.14	0.47
1:A:312:ARG:HH12	1:A:314:LEU:HB2	1.79	0.47
1:A:262:GLN:HE22	1:A:283:MET:H	1.63	0.47
1:B:244:SER:OG	1:B:246:ARG:HG3	2.15	0.46
1:A:235:THR:HG22	1:A:243:VAL:HG11	1.97	0.46
1:B:248:GLU:HA	1:B:249:LEU:C	2.35	0.46
1:B:404:ARG:HG2	1:B:417:LEU:HD13	1.97	0.46
1:A:246:ARG:HE	1:A:247:GLN:HE21	1.64	0.46
1:B:262:GLN:HE22	1:B:283:MET:H	1.64	0.46
1:A:200:ILE:HB	1:A:281:GLU:HB3	1.98	0.46
1:A:430:ASP:HB3	1:A:433:ASN:H	1.82	0.44
1:A:227:ASP:CB	3:A:653:HOH:O	2.64	0.44
1:A:302:HIS:HE1	1:A:334:ASP:OD2	2.00	0.44
1:A:268:VAL:HG22	1:A:274:ILE:HG12	1.98	0.44
1:A:246:ARG:O	1:A:247:GLN:HB2	2.18	0.44
1:B:226:LEU:HD21	1:B:233:VAL:HG21	2.00	0.44
1:B:334:ASP:HB3	1:B:340:LEU:HB2	1.99	0.44
1:B:298:ILE:HD13	1:B:340:LEU:HD11	2.00	0.44
1:A:415:ARG:HB3	1:A:415:ARG:HH11	1.83	0.43
1:A:302:HIS:CE1	1:A:334:ASP:OD2	2.71	0.43
1:A:362:LEU:HB3	1:A:384:LEU:CD2	2.49	0.43
1:B:377:ASN:OD1	1:B:379:GLU:HG2	2.18	0.43
1:A:397:GLN:NE2	3:A:605:HOH:O	2.47	0.43
1:A:171:LEU:HD11	1:A:180:PRO:HB3	2.00	0.43
1:A:428:GLU:O	1:A:433:ASN:ND2	2.52	0.43
1:B:192:LEU:HD23	1:B:299:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:ALA:HB1	1:B:413:GLN:OE1	2.19	0.42
1:A:227:ASP:HB2	1:A:230:ASP:HB2	2.01	0.42
1:A:418:GLU:HG3	3:A:697:HOH:O	2.20	0.42
1:B:294:SER:O	1:B:298:ILE:HG13	2.19	0.42
1:B:158:GLN:HG3	1:B:161:ARG:NE	2.35	0.41
1:A:165:LEU:CD2	1:A:369:LEU:HD13	2.50	0.41
1:B:234:ARG:O	1:B:238:GLU:HB2	2.20	0.41
1:A:440:HIS:O	1:A:443:PHE:O	2.38	0.41
1:A:229:ASP:HB2	1:A:234:ARG:HD2	2.02	0.41
1:A:411:PHE:O	1:A:412:GLY:C	2.57	0.41
1:A:440:HIS:O	1:A:445:GLU:HB2	2.21	0.41
1:B:227:ASP:N	1:B:227:ASP:OD1	2.49	0.41
1:B:213:GLU:HA	1:B:214:PRO:HD3	1.87	0.41
1:B:395:GLY:O	2:B:501:C2E:H1'	2.21	0.41
1:B:429:LEU:HA	1:B:433:ASN:OD1	2.21	0.41
1:B:284:PRO:O	1:B:287:VAL:HG22	2.22	0.40
1:A:158:GLN:CA	3:A:613:HOH:O	2.69	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	281/297 (95%)	262 (93%)	14 (5%)	5 (2%)	8	2
1	B	285/297 (96%)	260 (91%)	19 (7%)	6 (2%)	7	1
All	All	566/594 (95%)	522 (92%)	33 (6%)	11 (2%)	8	2

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	435	ARG

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Mol	Chain	Res	Type
1	B	312	ARG
1	B	431	ALA
1	A	310	ASP
1	B	228	ALA
1	B	311	ARG
1	A	309	SER
1	B	248	GLU
1	A	246	ARG
1	A	316	LEU
1	B	435	ARG

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	237/247 (96%)	215 (91%)	22 (9%)	9	3
1	B	241/247 (98%)	219 (91%)	22 (9%)	9	3
All	All	478/494 (97%)	434 (91%)	44 (9%)	9	3

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	LEU
1	A	171	LEU
1	A	177	ASP
1	A	184	LEU
1	A	199	ARG
1	A	227	ASP
1	A	239	ARG
1	A	246	ARG
1	A	275	LEU
1	A	277	LEU
1	A	308	GLN
1	A	309	SER
1	A	311	ARG

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Mol	Chain	Res	Type
1	A	312	ARG
1	A	319	ILE
1	A	344	LEU
1	A	369	LEU
1	A	373	LEU
1	A	385	LEU
1	A	415	ARG
1	A	417	LEU
1	A	423	ARG
1	B	159	SER
1	B	160	LEU
1	B	162	SER
1	B	169	GLN
1	B	170	LEU
1	B	184	LEU
1	B	215	GLN
1	B	222	GLU
1	B	226	LEU
1	B	227	ASP
1	B	229	ASP
1	B	231	LEU
1	B	248	GLU
1	B	249	LEU
1	B	273	ARG
1	B	296	LEU
1	B	314	LEU
1	B	320	ASP
1	B	369	LEU
1	B	373	LEU
1	B	379	GLU
1	B	394	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	247	GLN
1	A	262	GLN
1	A	282	GLN
1	A	302	HIS
1	A	322	GLN
1	A	397	GLN
1	A	433	ASN

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Mol	Chain	Res	Type
1	A	440	HIS
1	A	451	GLN
1	B	169	GLN
1	B	262	GLN
1	B	322	GLN
1	B	326	GLN
1	B	433	ASN
1	B	440	HIS

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 carbohydrates 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	B	501	-	44,52,52	1.74	9 (20%)	54,82,82	2.15	12 (22%)
2	C2E	A	501	-	44,52,52	1.65	7 (15%)	54,82,82	1.92	11 (20%)

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	B	501	-	-	0/22/62/62	0/6/7/7
2	C2E	A	501	-	-	0/22/62/62	0/6/7/7

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	C2E	O6-C6	4.98	1.37	1.24
2	A	501	C2E	O6-C6	4.93	1.36	1.24
2	B	501	C2E	C6-C5	4.55	1.49	1.41
2	B	501	C2E	O61-C61	4.52	1.35	1.24
2	B	501	C2E	C61-C51	4.33	1.48	1.41
2	A	501	C2E	O61-C61	4.09	1.34	1.24
2	A	501	C2E	C6-C5	4.08	1.48	1.41
2	A	501	C2E	C61-C51	3.45	1.47	1.41
2	A	501	C2E	O4'-C1'	3.11	1.45	1.41
2	A	501	C2E	C5-C4	2.97	1.48	1.40
2	B	501	C2E	C5-C4	2.83	1.48	1.40
2	A	501	C2E	O4A-C1A	2.24	1.44	1.41
2	B	501	C2E	C51-C41	2.19	1.46	1.40
2	B	501	C2E	O4A-C1A	2.11	1.44	1.41
2	B	501	C2E	O4'-C1'	2.05	1.43	1.41
2	B	501	C2E	C2'-C1'	-2.01	1.50	1.53

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	C2E	C21-N31-C41	5.82	122.00	115.36
2	B	501	C2E	C21-N31-C41	5.64	121.80	115.36
2	B	501	C2E	C6-N1-C2	5.02	123.90	115.93
2	A	501	C2E	C6-N1-C2	4.87	123.67	115.93
2	B	501	C2E	C6-C5-C4	-4.83	116.19	120.80
2	A	501	C2E	C6-C5-C4	-4.72	116.29	120.80
2	B	501	C2E	C2-N3-C4	4.71	120.74	115.36
2	B	501	C2E	C61-C51-C41	-4.62	116.39	120.80
2	B	501	C2E	C5-C6-N1	-4.53	117.23	123.43
2	A	501	C2E	C5-C6-N1	-4.23	117.64	123.43
2	B	501	C2E	N3-C2-N1	-4.21	121.60	127.22
2	A	501	C2E	C2-N3-C4	4.15	120.10	115.36
2	A	501	C2E	N3-C2-N1	-4.06	121.81	127.22
2	A	501	C2E	N31-C21-N11	-3.68	122.31	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	C2E	N31-C21-N11	-3.65	122.35	127.22
2	A	501	C2E	C61-C51-C41	-3.61	117.35	120.80
2	B	501	C2E	C51-C61-N11	-3.36	118.83	123.43
2	B	501	C2E	C61-N11-C21	3.33	121.22	115.93
2	B	501	C2E	C41-C51-N71	-3.07	106.20	109.40
2	B	501	C2E	C4-C5-N7	-2.78	106.50	109.40
2	A	501	C2E	C61-N11-C21	2.70	120.21	115.93
2	A	501	C2E	C51-C61-N11	-2.54	119.96	123.43
2	A	501	C2E	C4-C5-N7	-2.13	107.18	109.40

There are no chirality outliers.

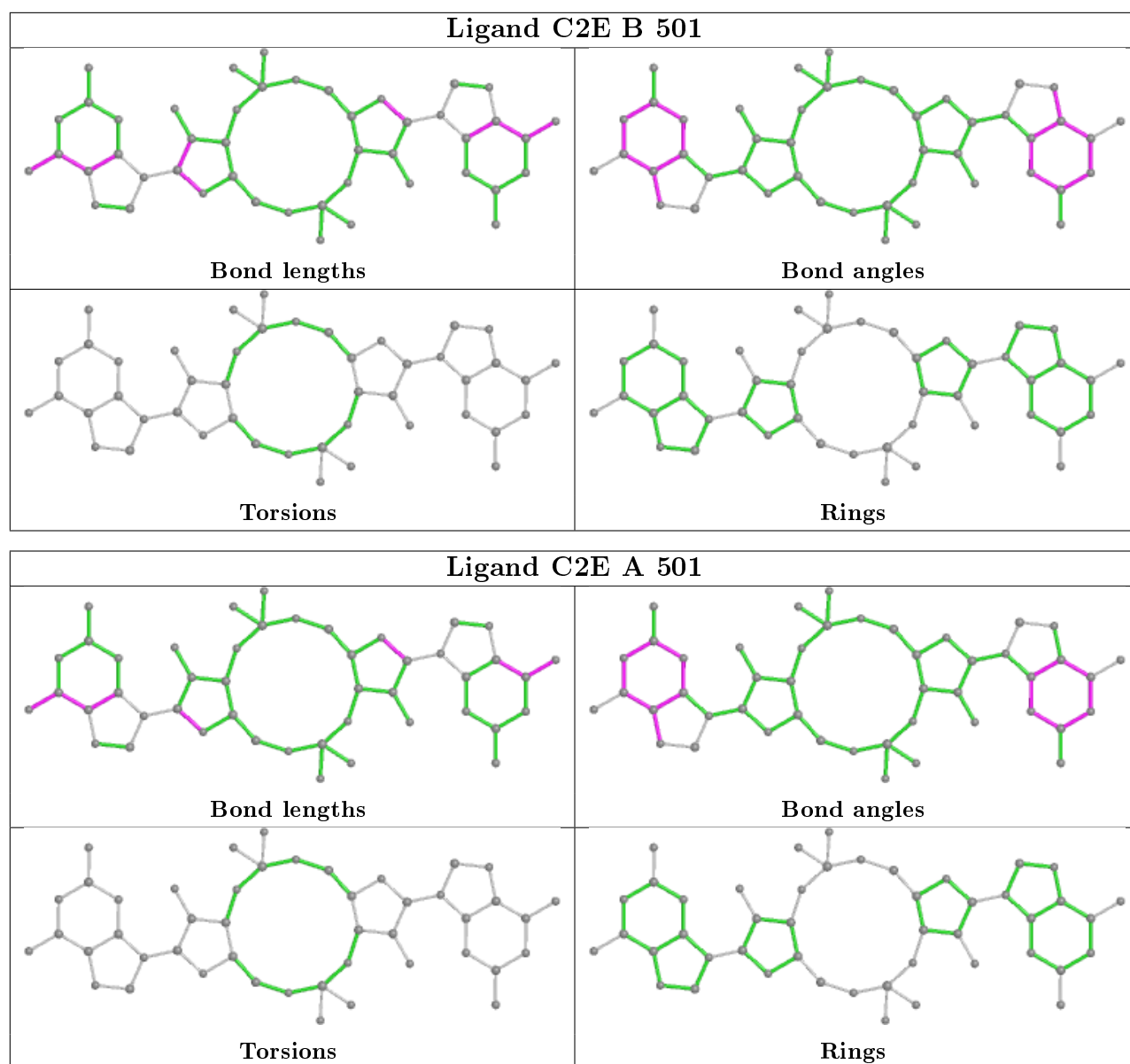
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	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 ⓘ

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, 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	285/297 (95%)	0.81	31 (10%) 5 5	29, 43, 80, 102	0
1	B	289/297 (97%)	1.08	48 (16%) 1 1	34, 55, 95, 130	0
All	All	574/594 (96%)	0.95	79 (13%) 2 2	29, 50, 90, 130	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	316	LEU	17.8
1	B	317	ALA	10.7
1	A	315	GLN	9.3
1	B	250	LEU	8.7
1	A	316	LEU	8.6
1	B	314	LEU	8.1
1	A	314	LEU	8.0
1	A	317	ALA	8.0
1	B	313	ALA	7.4
1	B	312	ARG	6.8
1	A	309	SER	6.6
1	B	319	ILE	6.5
1	B	311	ARG	6.2
1	B	436	GLN	6.2
1	A	313	ALA	6.2
1	B	318	ASP	6.1
1	B	431	ALA	5.6
1	A	311	ARG	5.1
1	B	444	ASN	5.0
1	B	451	GLN	4.9
1	A	208	TYR	4.9
1	B	315	GLN	4.9
1	A	433	ASN	4.8
1	A	312	ARG	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	433	ASN	4.6
1	B	309	SER	4.4
1	A	443	PHE	4.4
1	B	251	GLU	4.3
1	A	227	ASP	4.2
1	B	227	ASP	4.2
1	B	310	ASP	4.1
1	B	228	ALA	4.0
1	A	432	GLY	4.0
1	B	378	ASP	3.9
1	A	436	GLN	3.8
1	A	310	ASP	3.8
1	A	319	ILE	3.7
1	B	260	ALA	3.5
1	B	246	ARG	3.4
1	B	158	GLN	3.3
1	A	434	ASP	3.2
1	B	435	ARG	3.1
1	B	448	LEU	3.1
1	B	249	LEU	3.1
1	B	308	GLN	3.0
1	A	435	ARG	2.9
1	A	431	ALA	2.9
1	B	449	ASN	2.8
1	A	451	GLN	2.8
1	B	443	PHE	2.8
1	B	450	ASP	2.8
1	B	453	VAL	2.7
1	B	177	ASP	2.6
1	B	440	HIS	2.6
1	A	444	ASN	2.5
1	A	412	GLY	2.5
1	A	424	ILE	2.5
1	B	323	ARG	2.4
1	A	438	LEU	2.3
1	B	380	GLY	2.3
1	B	430	ASP	2.3
1	A	423	ARG	2.3
1	B	432	GLY	2.3
1	B	234	ARG	2.3
1	B	445	GLU	2.3
1	B	178	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	332	LEU	2.2
1	B	199	ARG	2.2
1	A	453	VAL	2.2
1	B	285	PHE	2.2
1	B	412	GLY	2.2
1	B	286	PHE	2.1
1	A	394	GLU	2.1
1	B	169	GLN	2.1
1	A	403	LEU	2.1
1	B	275	LEU	2.1
1	A	400	LEU	2.0
1	A	437	ALA	2.0
1	A	246	ARG	2.0

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 ⓘ

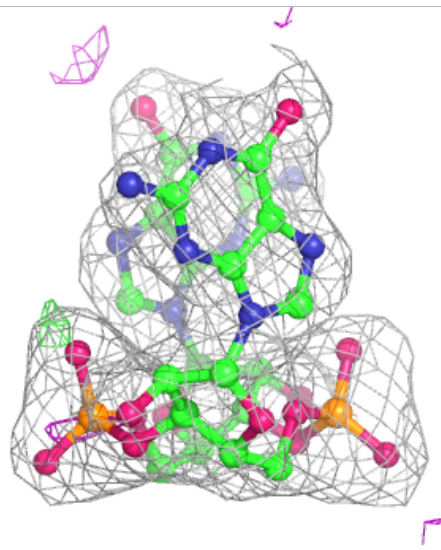
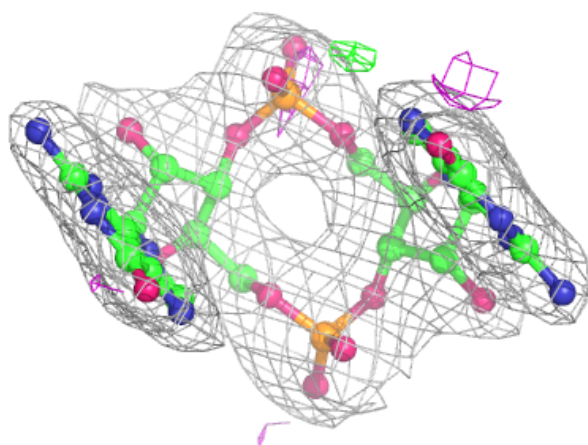
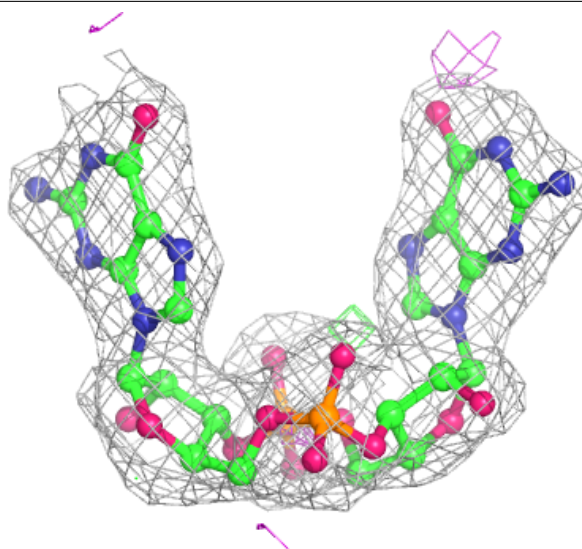
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	501	46/46	0.94	0.10	41,52,58,60	0
2	C2E	A	501	46/46	0.94	0.12	32,41,45,46	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.

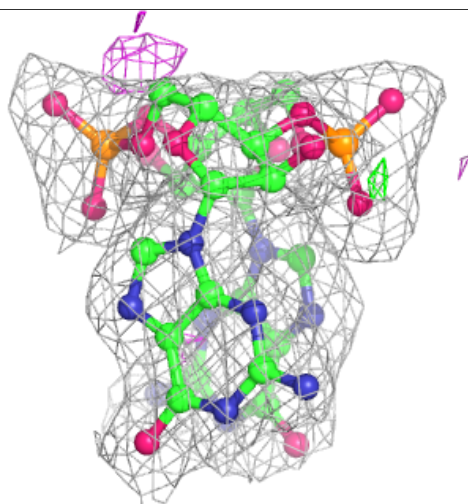
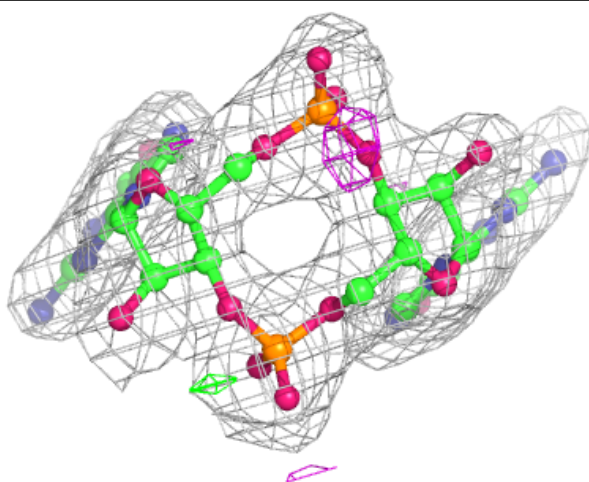
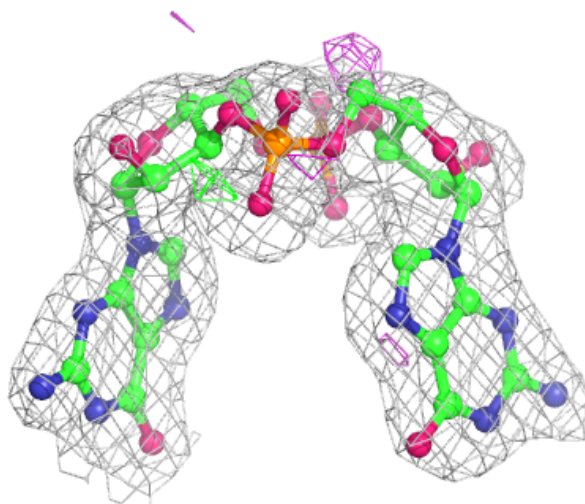
Electron density around C2E B 501:

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 C2E A 501:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.