



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:01 PM UTC

PDB ID : 4ETZ / pdb_00004etz
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 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

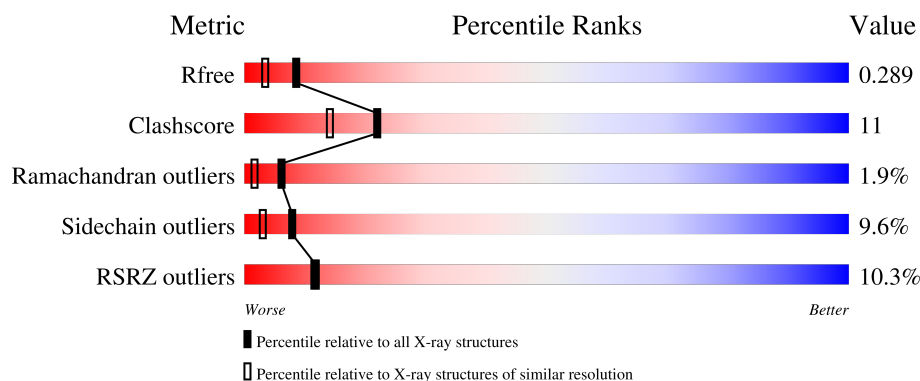
1 Overall quality at a glance

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}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (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 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	297	9% 66% 26% . . .
1	B	297	11% 72% 22% . .

2 Entry composition [i](#)

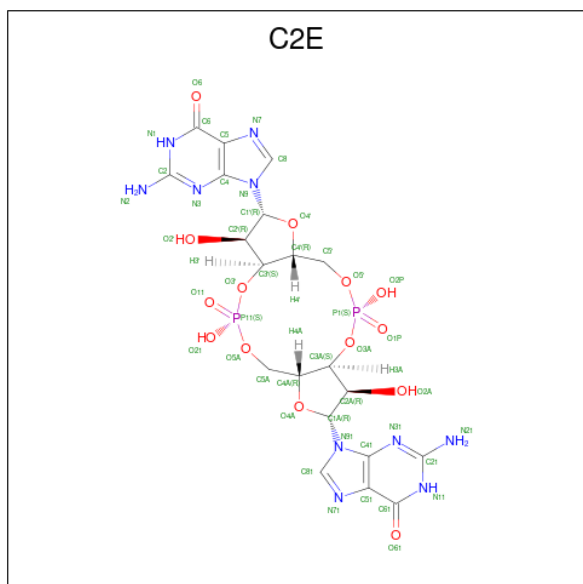
There are 3 unique types of molecules in this entry. The entry contains 4768 atoms, of which 0 are hydrogens and 0 are deuteriums.

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) (CCD ID: C2E) (formula: C₂₀H₂₄N₁₀O₁₄P₂).

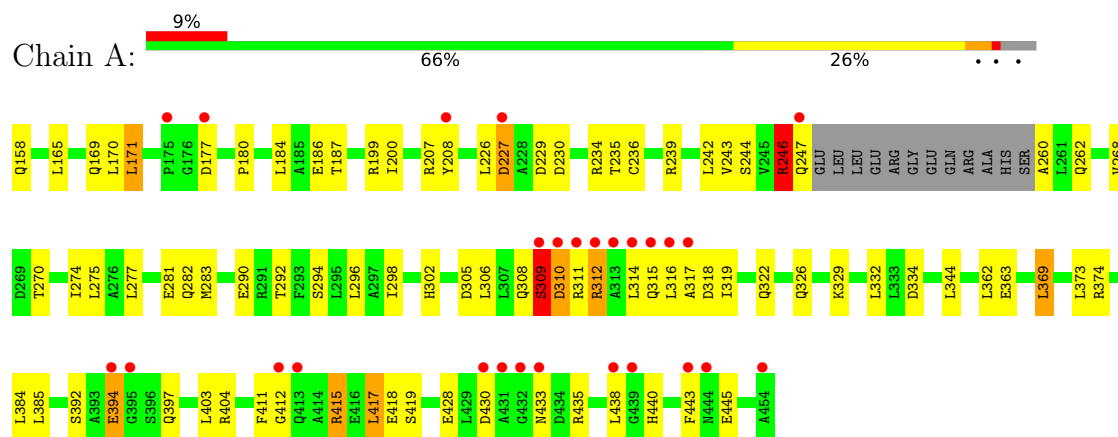


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	98	Total 98	O 98	0	0
3	B	42	Total 42	O 42	0	0

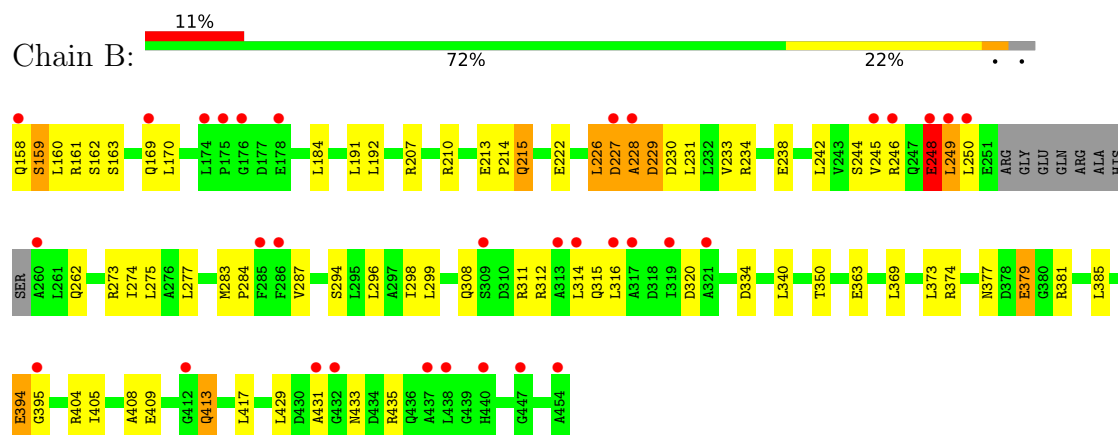
3 Residue-property plots

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: 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 25.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-2.05) 99.7 (25.00-2.05)	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 , 45.5	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	0.84	0/2280	0.99	3/3082 (0.1%)
1	B	0.67	0/2314	0.92	3/3128 (0.1%)
All	All	0.76	0/4594	0.95	6/6210 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	GLU	N-CA-C	-6.88	100.80	110.50
1	B	159	SER	N-CA-C	-6.27	104.36	111.07
1	A	394	GLU	CA-C-N	-6.18	109.30	121.41
1	A	394	GLU	C-N-CA	-6.18	109.30	121.41
1	B	394	GLU	N-CA-C	-5.63	101.95	110.28
1	B	413	GLN	N-CA-C	-5.19	106.20	112.54

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	59	0
1	B	2285	0	2317	42	0
2	A	46	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	99	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 11.

All (99) 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:227:ASP:O	1:B:228:ALA:C	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:229:ASP:HB2	1:B:234:ARG:CD	2.39	0.52
1:B:248:GLU:HA	1:B:249:LEU:C	2.35	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:OD1	1:B:229:ASP:N	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:A:186:GLU:OE2	1:A:187:THR:OG1	2.24	0.46
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: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:411:PHE:O	1:A:412:GLY:C	2.57	0.45
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:298:ILE:HD13	1:B:340:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:ASP:HB3	1:B:340:LEU:HB2	1.99	0.44
1:A:415:ARG:HH11	1:A:415:ARG:HB3	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:242:LEU:C	1:A:242:LEU:HD23	2.44	0.43
1:A:397:GLN:NE2	3:A:605:HOH:O	2.47	0.43
1:B:242:LEU:HD23	1:B:242:LEU:C	2.43	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
1:A:186:GLU:CD	1:A:187:THR:H	2.27	0.42
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:440:HIS:O	1:A:445:GLU:HB2	2.21	0.41
1:B:227:ASP:OD1	1:B:227:ASP:N	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 [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	281/297 (95%)	262 (93%)	14 (5%)	5 (2%)	6	2
1	B	285/297 (96%)	260 (91%)	19 (7%)	6 (2%)	5	1
All	All	566/594 (95%)	522 (92%)	33 (6%)	11 (2%)	6	2

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	435	ARG
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%)	8	3
1	B	241/247 (98%)	217 (90%)	24 (10%)	7	3
All	All	478/494 (97%)	432 (90%)	46 (10%)	8	3

All (46) 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	226	LEU

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Mol	Chain	Res	Type
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
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	403	LEU
1	A	415	ARG
1	A	417	LEU
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	277	LEU
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	385	LEU
1	B	394	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18)

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
1	A	440	HIS
1	A	451	GLN
1	B	169	GLN
1	B	215	GLN
1	B	262	GLN
1	B	322	GLN
1	B	326	GLN
1	B	338	HIS
1	B	433	ASN
1	B	440	HIS
1	B	449	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](#)

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	501	-	52,52,52	1.71	6 (11%)	78,82,82	1.85	13 (16%)
2	C2E	B	501	-	52,52,52	1.77	7 (13%)	78,82,82	1.84	14 (17%)

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	501	-	-	0/30/62/62	0/6/7/7
2	C2E	B	501	-	-	0/30/62/62	0/6/7/7

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	C2E	O6-C6	7.12	1.37	1.23
2	A	501	C2E	O6-C6	7.05	1.36	1.23
2	B	501	C2E	O61-C61	6.51	1.35	1.23
2	A	501	C2E	O61-C61	5.94	1.34	1.23
2	A	501	C2E	C5-C4	3.65	1.48	1.38
2	B	501	C2E	C5-C4	3.51	1.48	1.38
2	B	501	C2E	C51-C41	2.91	1.46	1.38
2	A	501	C2E	C61-N11	-2.66	1.33	1.38
2	A	501	C2E	C51-C41	2.39	1.45	1.38
2	B	501	C2E	C51-N71	-2.14	1.34	1.39
2	B	501	C2E	C4-N9	-2.06	1.32	1.38
2	B	501	C2E	C41-N91	-2.06	1.32	1.38
2	A	501	C2E	C51-N71	-2.06	1.34	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	C2E	C51-C41-N31	-6.44	118.14	128.39
2	B	501	C2E	C51-C41-N31	-5.64	119.41	128.39
2	A	501	C2E	C21-N31-C41	5.63	122.00	112.30
2	B	501	C2E	C21-N31-C41	5.51	121.80	112.30
2	A	501	C2E	N91-C41-N31	5.12	136.19	125.95
2	B	501	C2E	C5-C4-N3	-5.07	120.32	128.39
2	A	501	C2E	C5-C4-N3	-4.99	120.44	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	C2E	C2-N3-C4	4.90	120.74	112.30
2	A	501	C2E	C2-N3-C4	4.53	120.10	112.30
2	A	501	C2E	N9-C4-N3	4.48	134.90	125.95
2	B	501	C2E	C61-C51-N71	3.91	137.41	130.29
2	B	501	C2E	C6-C5-N7	3.85	137.30	130.29
2	B	501	C2E	N91-C41-N31	3.65	133.25	125.95
2	A	501	C2E	C6-C5-N7	3.43	136.52	130.29
2	B	501	C2E	N9-C4-N3	3.38	132.71	125.95
2	A	501	C2E	O61-C61-C51	-3.20	118.09	126.53
2	B	501	C2E	C41-C51-N71	-2.82	106.20	110.67
2	A	501	C2E	C21-N11-C61	-2.70	120.21	125.11
2	A	501	C2E	C51-C61-N11	2.64	119.96	113.25
2	B	501	C2E	C4-C5-N7	-2.63	106.50	110.67
2	B	501	C2E	C2A-C1A-N91	-2.41	106.56	113.25
2	A	501	C2E	C61-C51-N71	2.39	134.64	130.29
2	A	501	C2E	C4-C5-N7	-2.20	107.18	110.67
2	A	501	C2E	C2A-C1A-N91	-2.19	107.14	113.25
2	B	501	C2E	C51-C61-N11	2.19	118.83	113.25
2	B	501	C2E	C21-N11-C61	-2.15	121.22	125.11
2	B	501	C2E	O61-C61-C51	-2.08	121.04	126.53

There are no chirality outliers.

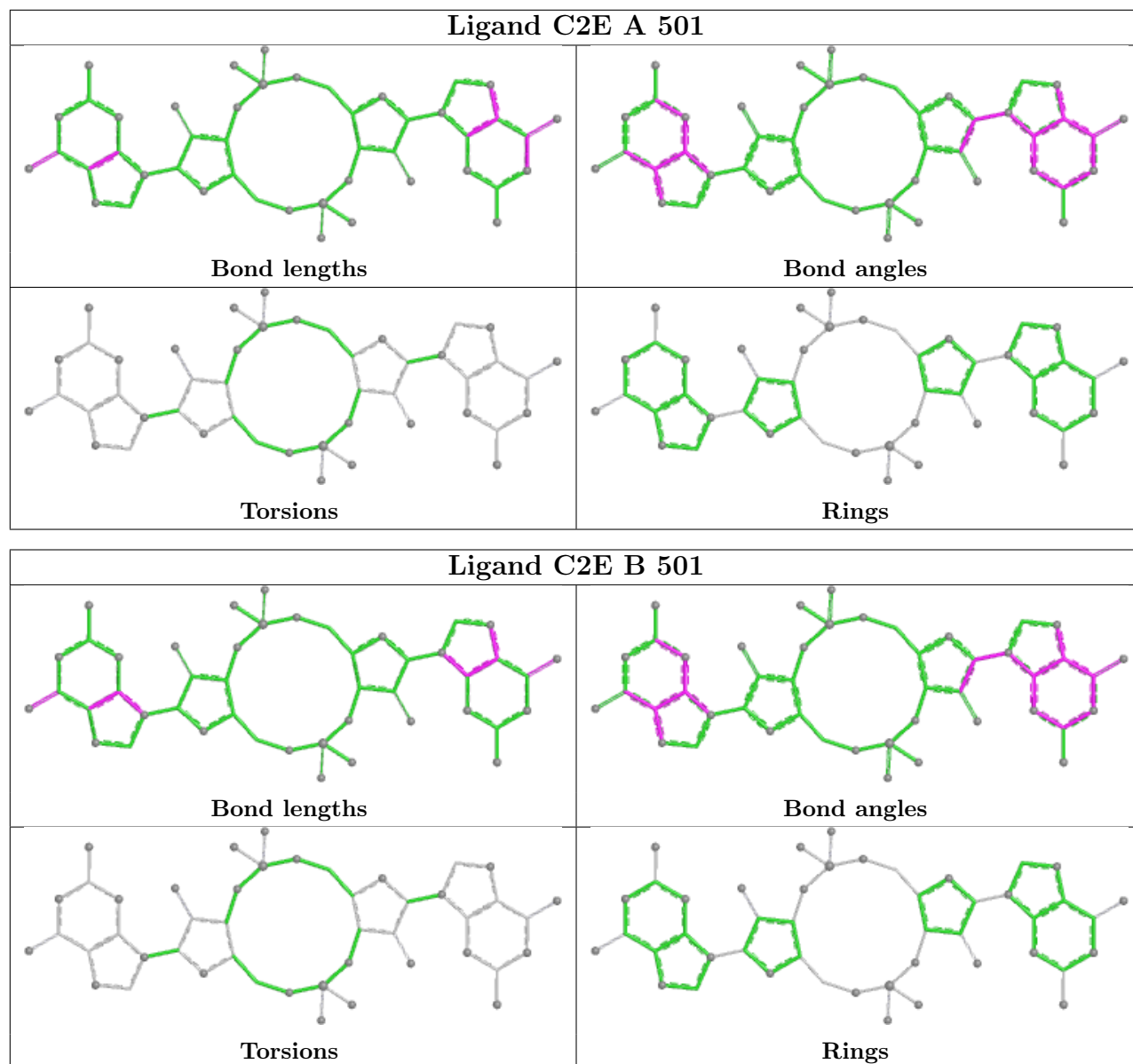
There are no torsion outliers.

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%)	0.50	27 (9%) 14 13	29, 43, 80, 102	0
1	B	289/297 (97%)	0.76	32 (11%) 10 10	34, 55, 95, 130	0
All	All	574/594 (96%)	0.64	59 (10%) 12 11	29, 50, 90, 130	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	316	LEU	6.5
1	B	314	LEU	6.3
1	A	316	LEU	6.2
1	A	309	SER	5.7
1	A	314	LEU	5.5
1	B	317	ALA	5.5
1	A	208	TYR	4.7
1	B	250	LEU	4.5
1	B	260	ALA	4.5
1	B	249	LEU	4.5
1	A	227	ASP	4.3
1	B	431	ALA	4.1
1	A	310	ASP	3.9
1	B	227	ASP	3.7
1	A	317	ALA	3.6
1	B	313	ALA	3.4
1	B	319	ILE	3.2
1	A	432	GLY	3.1
1	B	454	ALA	3.1
1	A	412	GLY	3.0
1	B	228	ALA	3.0
1	A	312	ARG	3.0
1	A	315	GLN	3.0
1	B	286	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	394	GLU	2.8
1	A	431	ALA	2.7
1	B	245	VAL	2.7
1	B	178	GLU	2.7
1	B	321	ALA	2.6
1	A	311	ARG	2.6
1	B	175	PRO	2.6
1	B	309	SER	2.4
1	B	246	ARG	2.4
1	A	443	PHE	2.4
1	A	444	ASN	2.4
1	B	158	GLN	2.3
1	A	177	ASP	2.3
1	B	169	GLN	2.3
1	A	430	ASP	2.3
1	B	176	GLY	2.3
1	B	412	GLY	2.3
1	A	313	ALA	2.2
1	A	395	GLY	2.2
1	B	174	LEU	2.2
1	B	438	LEU	2.2
1	B	285	PHE	2.1
1	A	439	GLY	2.1
1	B	395	GLY	2.1
1	A	438	LEU	2.1
1	B	248	GLU	2.1
1	A	433	ASN	2.1
1	A	413	GLN	2.1
1	A	175	PRO	2.1
1	B	432	GLY	2.1
1	A	454	ALA	2.1
1	B	440	HIS	2.0
1	B	437	ALA	2.0
1	A	247	GLN	2.0
1	B	447	GLY	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

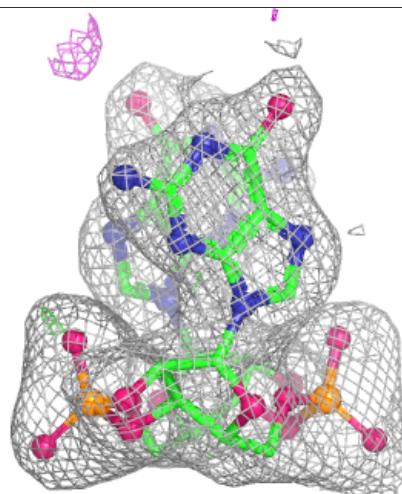
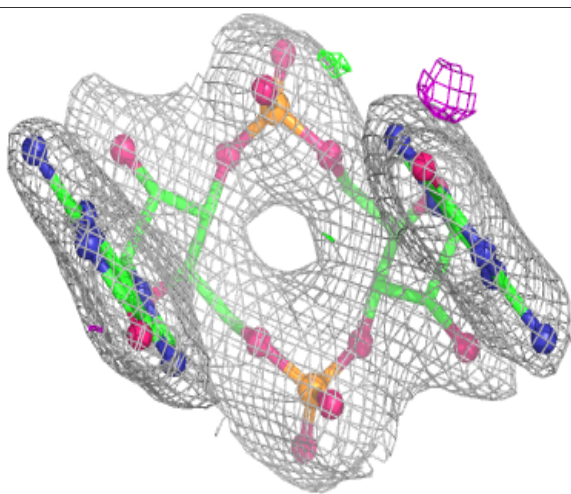
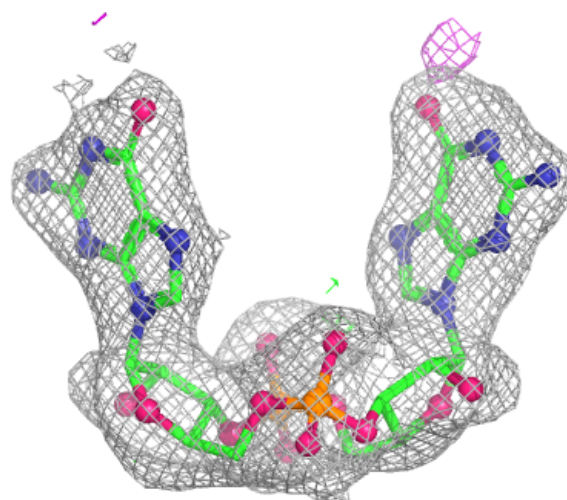
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	C2E	B	501	46/46	0.91	0.08	41,52,58,60	0
2	C2E	A	501	46/46	0.93	0.08	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.

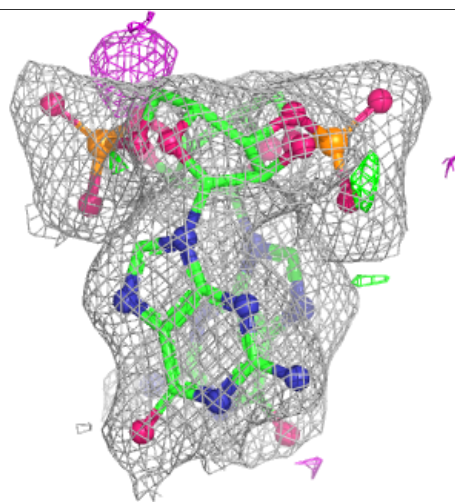
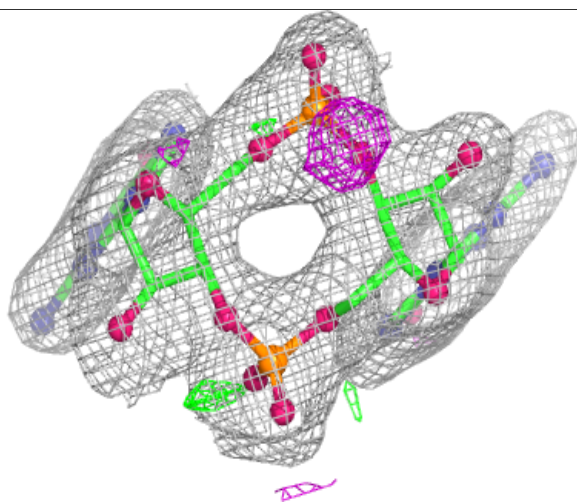
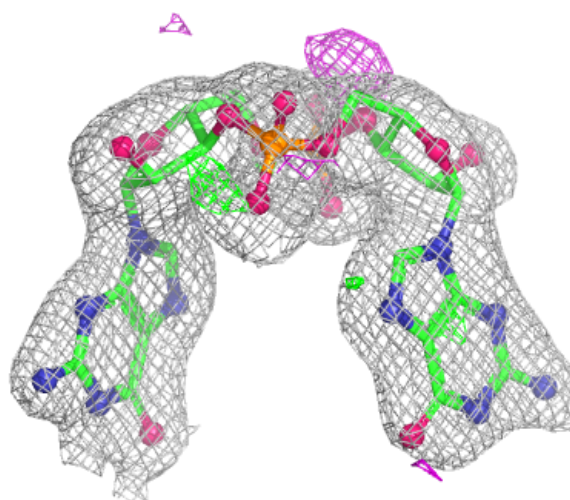
Electron density around C2E B 501:

$2mF_o-DF_c$ (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.