



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:37 AM UTC

PDB ID : 8ZIJ / pdb_00008zij
Title : The holo structure of gamma-lyase CndF
Authors : Gao, Y.; Tang, Y.; Zhou, J.
Deposited on : 2024-05-14
Resolution : 2.59 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
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

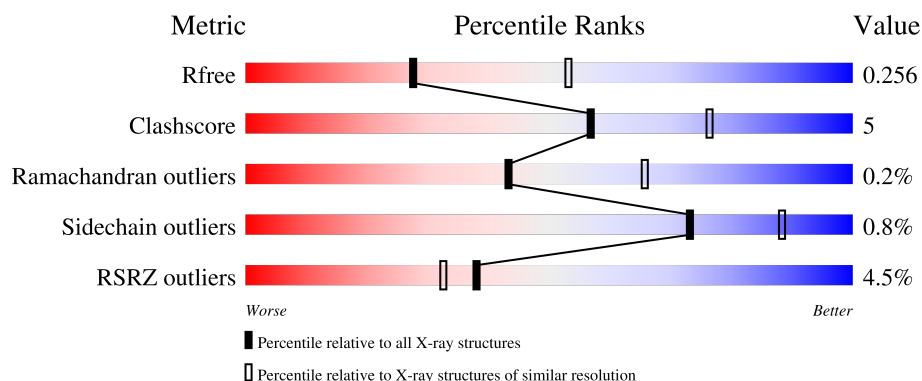
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

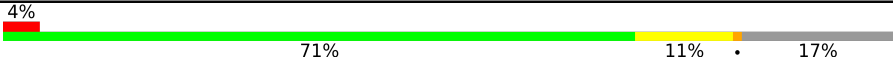
The reported resolution of this entry is 2.59 Å.

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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	568	
1	B	568	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7428 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 PLP dependent gamma-lyase CndF.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	476	Total	C	N	O	S		0	0	0
			3668	2338	621	693	16				
1	A	473	Total	C	N	O	P	S	0	0	0
			3656	2325	617	697	1	16			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

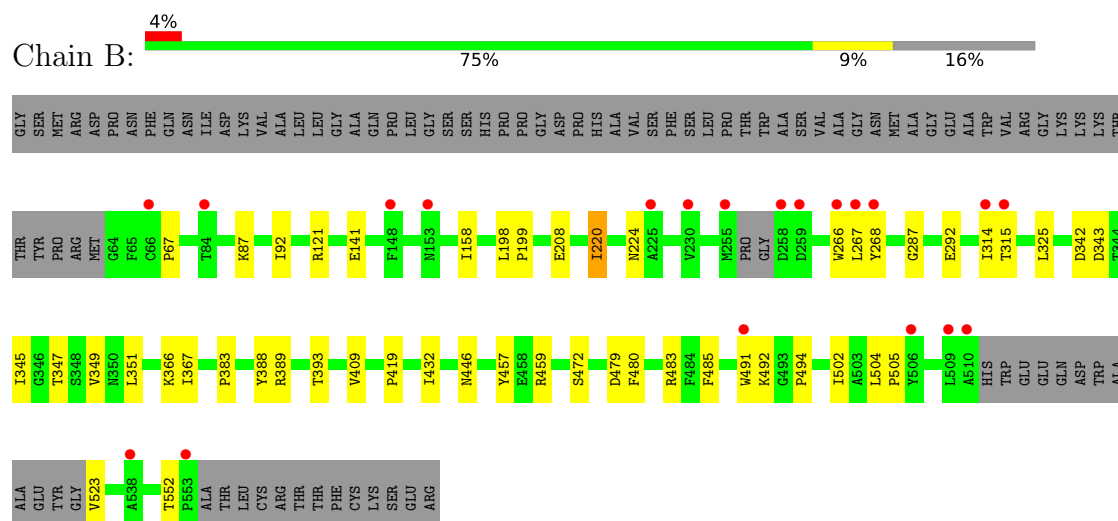
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	43	Total 43	O 43	0	0
4	A	55	Total 55	O 55	0	0

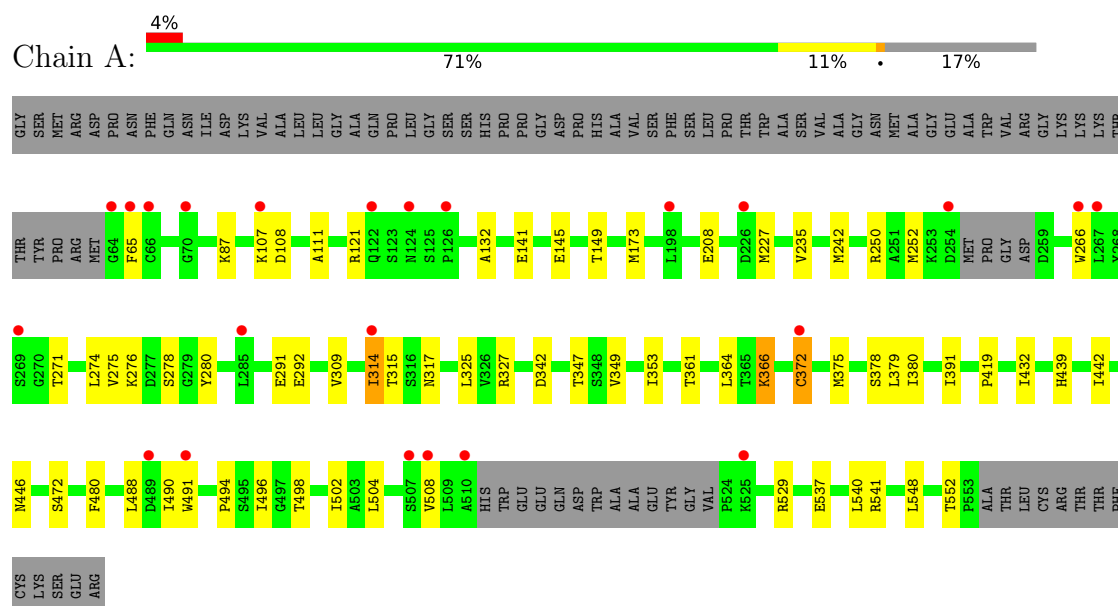
3 Residue-property plots [i](#)

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: PLP dependent gamma-lyase CndF



• Molecule 1: PLP dependent gamma-lyase CndF



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.43Å 102.53Å 128.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.60 – 2.59 47.60 – 2.59	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.60-2.59) 100.0 (47.60-2.59)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.214 , 0.255 0.218 , 0.256	Depositor DCC
R_{free} test set	1740 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7428	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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: CL, LLP, PO4

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	0.46	0/3715	0.55	4/5055 (0.1%)
1	B	0.32	0/3743	0.39	0/5094
All	All	0.40	0/7458	0.48	4/10149 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	ARG	N-CA-C	11.48	123.35	111.07
1	A	314	ILE	CA-C-N	5.53	132.10	121.54
1	A	314	ILE	C-N-CA	5.53	132.10	121.54
1	A	107	LYS	N-CA-C	-5.17	106.13	112.90

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	3656	0	3541	39	0
1	B	3668	0	3570	29	0
2	B	5	0	0	0	0
3	A	1	0	0	0	0
4	A	55	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	43	0	0	1	0
All	All	7428	0	7111	67	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 5.

All (67) 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:132:ALA:HB1	1:A:173:MET:HE2	1.69	0.75
1:A:314:ILE:HD12	1:A:325:LEU:HD11	1.70	0.72
1:B:198:LEU:HB3	1:B:199:PRO:HD2	1.75	0.67
1:A:291:GLU:HG3	1:A:327:ARG:NH1	2.11	0.65
1:A:494:PRO:HA	1:A:504:LEU:HD22	1.78	0.65
1:B:314:ILE:HD13	1:B:325:LEU:HD11	1.83	0.60
1:A:108:ASP:OD2	1:A:111:ALA:HB2	2.02	0.60
1:A:439:HIS:HB3	1:A:442:ILE:HD13	1.83	0.59
1:B:494:PRO:HA	1:B:504:LEU:HD22	1.84	0.58
1:A:315:THR:HG21	4:A:748:HOH:O	2.02	0.57
1:A:314:ILE:HD13	1:A:353:ILE:HG21	1.85	0.57
1:A:314:ILE:HD12	1:A:325:LEU:CD1	2.37	0.55
1:B:389:ARG:O	1:B:393:THR:HG23	2.06	0.55
1:A:361:THR:HG22	1:A:379:LEU:HD12	1.90	0.54
1:B:479:ASP:O	1:B:483:ARG:HG3	2.07	0.54
1:A:252:MET:HE1	1:A:391:ILE:HG12	1.89	0.53
1:A:291:GLU:HG3	1:A:327:ARG:HH11	1.72	0.53
1:A:488:LEU:HG	1:A:490:ILE:HG12	1.91	0.52
1:A:87:LYS:HD2	1:A:141:GLU:HA	1.92	0.52
1:A:252:MET:HG3	1:A:309:VAL:HB	1.92	0.51
1:A:480:PHE:HE2	1:A:552:THR:HG22	1.75	0.51
1:A:537:GLU:O	1:A:541:ARG:HB2	2.12	0.49
1:A:349:VAL:HG21	1:A:419:PRO:HA	1.95	0.49
1:A:432:ILE:HG13	1:A:540:LEU:HD23	1.95	0.49
1:B:67:PRO:HD3	1:A:375:MET:HG2	1.95	0.48
1:A:276:LYS:HA	1:A:280:TYR:O	2.13	0.47
1:A:266:TRP:CH2	1:A:342:ASP:HB2	2.50	0.47
1:B:314:ILE:HG22	1:B:343:ASP:HA	1.96	0.47
1:A:317:ASN:HD21	1:A:529:ARG:NH1	2.13	0.46
1:A:548:LEU:O	1:A:552:THR:HG23	2.16	0.46
1:B:87:LYS:HG3	1:B:141:GLU:HA	1.96	0.46
1:A:235:VAL:HG22	1:A:380:ILE:HG12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:PHE:CZ	1:B:492:LYS:HG2	2.52	0.45
1:A:271:THR:O	1:A:275:VAL:HG23	2.17	0.45
1:B:446:ASN:HB2	1:B:472:SER:OG	2.17	0.45
1:B:349:VAL:HG21	1:B:419:PRO:HA	1.97	0.45
1:A:366:LLP:O3	1:A:366:LLP:NZ	2.40	0.45
1:B:485:PHE:CZ	1:B:505:PRO:HD3	2.52	0.44
1:A:314:ILE:HD13	1:A:353:ILE:CG2	2.46	0.44
1:B:266:TRP:CH2	1:B:342:ASP:HB2	2.53	0.44
1:A:242:MET:HG3	1:A:274:LEU:CD1	2.47	0.43
1:A:242:MET:HG3	1:A:274:LEU:HD11	1.99	0.43
1:A:372:CYS:SG	1:A:498:THR:HG22	2.58	0.43
1:A:145:GLU:HB2	1:A:149:THR:OG1	2.19	0.43
1:B:121:ARG:HD2	4:B:702:HOH:O	2.18	0.43
1:A:508:VAL:H	1:A:508:VAL:HG23	1.49	0.42
1:B:366:LLP:HB2	1:B:367:ILE:H	1.56	0.42
1:B:491:TRP:O	1:B:502:ILE:HA	2.19	0.42
1:A:446:ASN:HB2	1:A:472:SER:OG	2.20	0.42
1:A:491:TRP:O	1:A:502:ILE:HA	2.20	0.42
1:B:220:ILE:HG13	1:B:220:ILE:O	2.20	0.42
1:B:292:GLU:H	1:B:292:GLU:CD	2.28	0.42
1:B:224:ASN:O	1:B:224:ASN:OD1	2.38	0.41
1:B:315:THR:O	1:B:345:ILE:HD12	2.21	0.41
1:A:208:GLU:OE1	1:A:208:GLU:N	2.49	0.41
1:B:351:LEU:HD21	1:B:457:TYR:CZ	2.55	0.41
1:B:480:PHE:HE2	1:B:552:THR:HG22	1.85	0.41
1:B:267:LEU:HD21	1:B:287:GLY:O	2.21	0.41
1:B:383:PRO:HA	1:B:388:TYR:CD1	2.56	0.41
1:B:267:LEU:HB2	1:B:268:TYR:CD2	2.56	0.41
1:A:364:LEU:HD21	1:A:378:SER:HB3	2.03	0.41
1:B:432:ILE:HD13	1:B:432:ILE:HA	1.88	0.40
1:B:208:GLU:HG2	1:B:409:VAL:HA	2.04	0.40
1:B:92:ILE:HD11	1:B:158:ILE:HG13	2.01	0.40
1:A:250:ARG:HG3	1:A:278:SER:OG	2.21	0.40
1:A:366:LLP:HG2	1:A:496:ILE:HG13	2.02	0.40
1:B:268:TYR:OH	1:B:523:VAL:HG11	2.21	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	466/568 (82%)	455 (98%)	10 (2%)	1 (0%)	43	66
1	B	469/568 (83%)	459 (98%)	9 (2%)	1 (0%)	43	66
All	All	935/1136 (82%)	914 (98%)	19 (2%)	2 (0%)	43	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	347	THR
1	B	347	THR

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	389/478 (81%)	385 (99%)	4 (1%)	68	86
1	B	392/478 (82%)	390 (100%)	2 (0%)	81	92
All	All	781/956 (82%)	775 (99%)	6 (1%)	73	88

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	220	ILE
1	B	459	ARG
1	A	65	PHE
1	A	227	MET

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Mol	Chain	Res	Type
1	A	292	GLU
1	A	372	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	168	ASN
1	A	168	ASN
1	A	387	HIS
1	A	434	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	LLP	A	366	1	23,24,25	1.48	2 (8%)	25,32,34	1.13	2 (8%)
1	LLP	B	366	1	7,8,25	0.51	0	3,8,34	0.23	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	A	366	1	-	5/16/17/19	0/1/1/1
1	LLP	B	366	1	-	4/6/7/19	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	366	LLP	C4'-NZ	4.87	1.43	1.27
1	A	366	LLP	C2-N1	2.66	1.38	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	366	LLP	C4-C4'-NZ	-3.46	108.08	124.04
1	A	366	LLP	C5-C6-N1	-2.28	120.12	123.83

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	366	LLP	C-CA-CB-CG
1	B	366	LLP	O-C-CA-CB
1	A	366	LLP	C-CA-CB-CG
1	A	366	LLP	O-C-CA-CB
1	B	366	LLP	CG-CD-CE-NZ
1	A	366	LLP	CA-CB-CG-CD
1	B	366	LLP	CA-CB-CG-CD
1	A	366	LLP	C3-C4-C4'-NZ
1	A	366	LLP	C4-C4'-NZ-CE

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	366	LLP	2	0
1	B	366	LLP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	B	601	-	4,4,4	0.94	0	6,6,6	0.56	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	472/568 (83%)	0.25	23 (4%) 35 29	34, 49, 75, 97	0
1	B	475/568 (83%)	0.31	20 (4%) 40 35	38, 52, 74, 87	0
All	All	947/1136 (83%)	0.28	43 (4%) 38 32	34, 50, 74, 97	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	255	MET	5.5
1	B	510	ALA	5.4
1	B	314	ILE	5.4
1	A	510	ALA	4.8
1	A	267	LEU	4.7
1	A	64	GLY	3.7
1	A	266	TRP	3.6
1	B	315	THR	3.4
1	B	258	ASP	3.4
1	A	508	VAL	3.2
1	B	553	PRO	3.1
1	A	507	SER	2.9
1	B	268	TYR	2.8
1	B	509	LEU	2.7
1	B	230	VAL	2.7
1	A	254	ASP	2.6
1	A	66	CYS	2.6
1	A	126	PRO	2.6
1	B	538	ALA	2.6
1	A	491	TRP	2.6
1	A	65	PHE	2.6
1	B	491	TRP	2.5
1	A	525	LYS	2.5
1	A	489	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	107	LYS	2.4
1	A	372	CYS	2.4
1	A	269	SER	2.4
1	A	122	GLN	2.4
1	B	267	LEU	2.4
1	A	198	LEU	2.4
1	A	226	ASP	2.4
1	B	66	CYS	2.3
1	A	285	LEU	2.3
1	A	124	ASN	2.3
1	A	70	GLY	2.3
1	B	153	ASN	2.2
1	B	84	THR	2.2
1	B	148	PHE	2.2
1	B	225	ALA	2.2
1	A	314	ILE	2.2
1	B	266	TRP	2.1
1	B	259	ASP	2.0
1	B	506	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	LLP	B	366	9/25	0.94	0.09	40,45,48,48	0
1	LLP	A	366	24/25	0.94	0.11	34,48,56,58	0

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
3	CL	A	601	1/1	0.95	0.10	73,73,73,73	0
2	PO4	B	601	5/5	0.96	0.07	45,49,53,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.