



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:09 AM UTC

PDB ID : 1EZ2 / pdb_00001ez2
Title : THREE-DIMENSIONAL STRUCTURE OF THE ZINC-CONTAINING PHOSPHOTRIESTERASE WITH BOUND SUBSTRATE ANALOG DIISOPROPYLMETHYL PHOSPHONATE.
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Deposited on : 2000-05-09
Resolution : 1.90 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

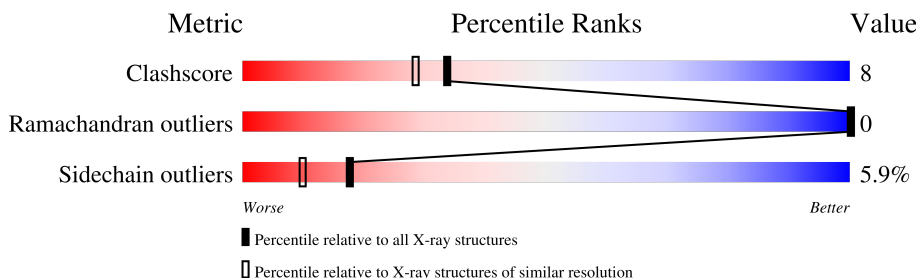
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	331	 76% 20% ..
1	B	331	 77% 20% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5344 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 PHOSPHOTRIESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2511	1590	446	468	7			
1	B	329	Total	C	N	O	S	0	2	0
			2521	1599	446	469	7			

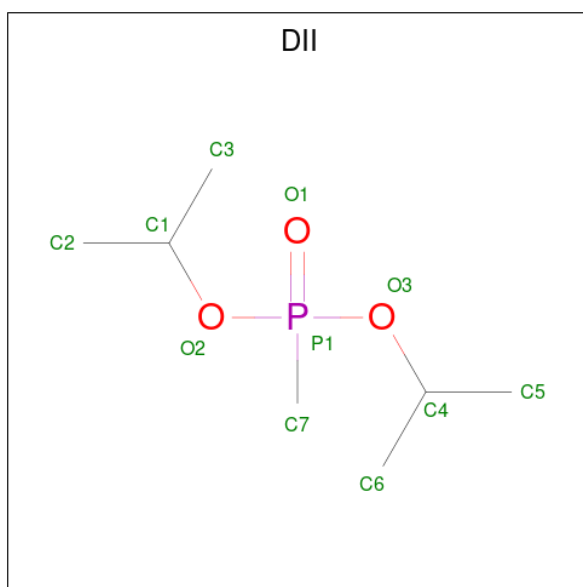
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	KCX	LYS	modified residue	UNP P0A434
B	169	KCX	LYS	modified residue	UNP P0A434

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is METHYLPHOSPHONIC ACID DIISOPROPYL ESTER (CCD ID: DII) (formula: C₇H₁₇O₃P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			11	7	3	1		
3	B	1	Total	C	O	P	0	0
			11	7	3	1		

- Molecule 4 is water.

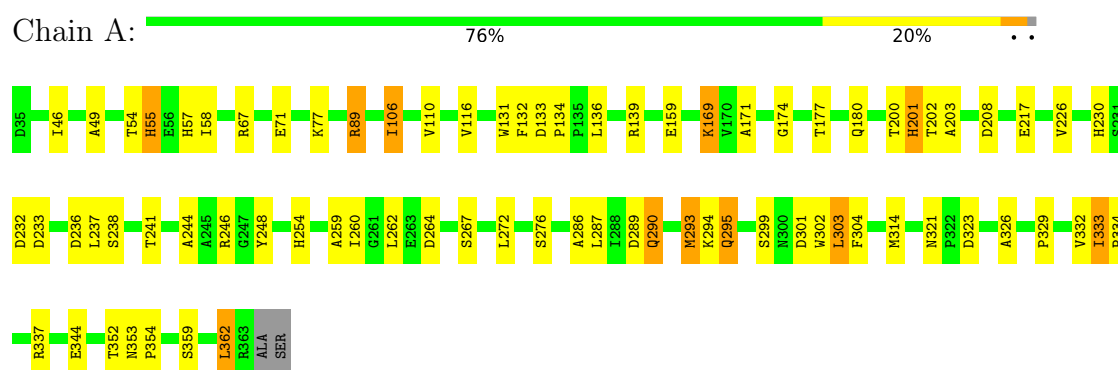
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	140	Total	O	0	0
			140	140		
4	B	146	Total	O	0	0
			146	146		

3 Residue-property plots

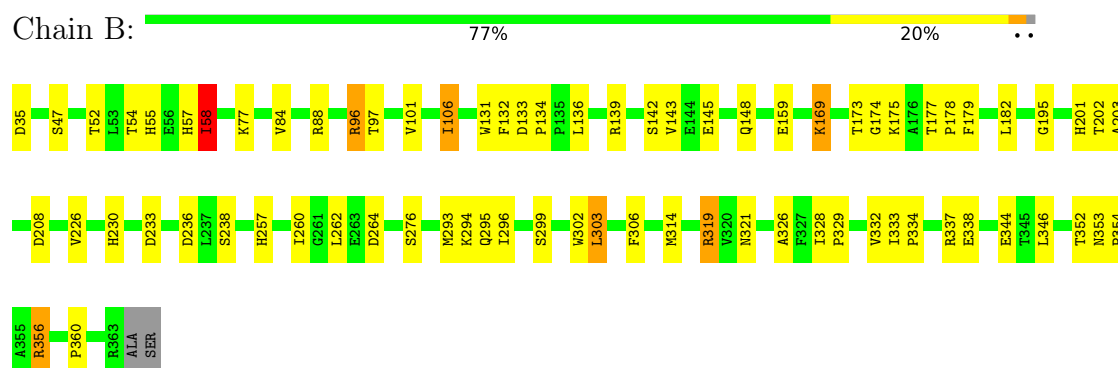
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: PHOSPHOTRIESTERASE



• Molecule 1: PHOSPHOTRIESTERASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	129.40 Å 91.00 Å 69.20 Å 90.00° 91.60° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90	Depositor
% Data completeness (in resolution range)	92.0 (20.00-1.90)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.183 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5344	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KCX, DII, ZN

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	1.16	1/2546 (0.0%)	1.43	18/3458 (0.5%)
1	B	1.11	0/2566	1.42	12/3486 (0.3%)
All	All	1.13	1/5112 (0.0%)	1.43	30/6944 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	HIS	CA-CB	5.20	1.59	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	179	PHE	CA-CB-CG	-9.17	104.63	113.80
1	A	54	THR	N-CA-C	8.42	123.12	113.01
1	B	58	ILE	N-CA-C	-7.18	103.17	111.00
1	A	272	LEU	N-CA-C	7.02	121.08	112.23
1	A	106	ILE	N-CA-C	-6.90	104.87	112.80
1	A	226	VAL	N-CA-C	6.77	117.86	108.12
1	B	352	THR	N-CA-C	6.76	118.31	111.07
1	B	54	THR	N-CA-C	6.71	121.32	113.20
1	A	203	ALA	N-CA-C	-6.68	95.02	107.71
1	A	200	THR	N-CA-C	6.46	119.54	109.52
1	A	58	ILE	N-CA-C	-6.46	103.96	111.00
1	B	203	ALA	N-CA-C	-6.38	94.52	107.41
1	B	332	VAL	N-CA-C	6.36	116.53	110.42
1	B	106	ILE	N-CA-C	-6.18	105.69	112.80
1	A	333	ILE	CA-C-O	6.16	122.82	118.69
1	A	159	GLU	CB-CA-C	-6.06	109.57	116.54
1	B	306	PHE	N-CA-CB	-6.01	101.61	110.86
1	B	174	GLY	N-CA-C	-5.84	103.61	112.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	THR	N-CA-C	5.71	117.18	111.07
1	B	226	VAL	N-CA-C	5.56	116.49	108.48
1	A	304	PHE	CA-CB-CG	-5.46	108.34	113.80
1	A	171	ALA	N-CA-C	5.40	117.47	108.99
1	A	362	LEU	N-CA-CB	5.36	118.91	110.56
1	A	232	ASP	N-CA-C	-5.30	106.78	113.20
1	A	254	HIS	CA-CB-CG	-5.28	108.52	113.80
1	B	257	HIS	CA-CB-CG	-5.27	108.53	113.80
1	A	174	GLY	N-CA-C	-5.13	104.74	112.84
1	A	332	VAL	N-CA-C	5.12	115.34	110.53
1	A	49	ALA	N-CA-C	5.02	116.76	111.28
1	B	159	GLU	CB-CA-C	-5.02	110.77	116.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	2511	0	2527	37	0
1	B	2521	0	2537	40	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	11	0	17	0	0
3	B	11	0	17	1	0
4	A	140	0	0	1	0
4	B	146	0	0	3	0
All	All	5344	0	5098	78	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 8.

All (78) 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:B:96:ARG:CG	1:B:96:ARG:HH11	2.02	0.71
1:A:248:TYR:O	1:A:295:GLN:HG2	1.90	0.71
1:B:333:ILE:HB	1:B:334:PRO:HD3	1.73	0.69
1:B:35:ASP:N	4:B:2588:HOH:O	2.26	0.68
1:B:96:ARG:HH11	1:B:96:ARG:HG2	1.58	0.67
1:A:333:ILE:HB	1:A:334:PRO:HD3	1.82	0.61
1:B:319:ARG:HG2	1:B:319:ARG:HH11	1.65	0.61
1:B:319:ARG:HG2	1:B:319:ARG:NH1	2.18	0.58
1:A:230:HIS:O	1:A:233:ASP:HB2	2.03	0.57
1:B:333:ILE:HG23	1:B:346:LEU:HD13	1.87	0.57
1:A:169:KCX:OQ1	1:A:201:HIS:HB2	2.05	0.56
1:B:173:THR:O	1:B:173:THR:HG23	2.04	0.55
1:A:259:ALA:O	1:A:262:LEU:HB2	2.07	0.55
1:A:236:ASP:OD2	1:A:238:SER:OG	2.24	0.53
1:A:133:ASP:N	1:A:134:PRO:CD	2.73	0.52
1:A:131:TRP:CG	1:A:132:PHE:H	2.29	0.51
1:B:57:HIS:O	1:B:303:LEU:HA	2.11	0.51
1:B:236:ASP:OD2	1:B:238:SER:OG	2.28	0.50
1:B:319:ARG:HH11	1:B:319:ARG:CG	2.24	0.50
1:A:177:THR:OG1	1:A:180:GLN:HG3	2.12	0.50
1:A:202:THR:HB	1:A:208:ASP:HB2	1.94	0.50
1:A:106:ILE:HG22	1:A:106:ILE:O	2.12	0.50
1:A:353:ASN:HB2	1:A:354:PRO:HD3	1.94	0.49
1:A:71:GLU:H	1:A:71:GLU:CD	2.18	0.49
1:B:353:ASN:HB2	1:B:354:PRO:HD3	1.93	0.49
1:B:142:SER:OG	1:B:145:GLU:HG3	2.13	0.49
1:A:55:HIS:CE1	1:A:169:KCX:CX	2.97	0.48
1:B:202:THR:HB	1:B:208:ASP:HB2	1.96	0.48
3:B:2403:DII:H1	4:B:2609:HOH:O	2.12	0.47
1:B:143:VAL:HB	1:B:182:LEU:HD22	1.95	0.47
1:A:57:HIS:O	1:A:303:LEU:HA	2.14	0.47
1:B:136:LEU:CD2	1:B:139:ARG:NH2	2.78	0.46
1:B:294:LYS:O	1:B:356:ARG:NH2	2.48	0.46
1:A:55:HIS:HE1	1:A:169:KCX:OQ1	1.99	0.46
1:B:169:KCX:OQ2	1:B:201:HIS:HB2	2.15	0.46
1:B:136:LEU:HG	1:B:139:ARG:NH2	2.31	0.45
1:A:293:MET:HB3	4:A:1521:HOH:O	2.16	0.45
1:A:286:ALA:O	1:A:290:GLN:HG2	2.16	0.45
1:B:96:ARG:NH1	4:B:2646:HOH:O	2.48	0.45
1:B:177:THR:HB	1:B:178:PRO:HD2	1.98	0.45
1:A:46:ILE:HD12	1:A:359:SER:OG	2.17	0.44
1:A:326:ALA:C	1:A:329:PRO:HD2	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:GLU:O	1:B:148:GLN:HB2	2.17	0.44
1:B:52:THR:HA	1:B:97:THR:O	2.18	0.44
1:B:131:TRP:CG	1:B:132:PHE:H	2.36	0.44
1:B:133:ASP:N	1:B:134:PRO:CD	2.81	0.43
1:B:333:ILE:N	1:B:334:PRO:CD	2.81	0.43
1:B:84:VAL:O	1:B:88:ARG:HG3	2.18	0.43
1:B:293:MET:HA	1:B:296:ILE:HD12	2.01	0.43
1:A:55:HIS:CD2	1:A:301:ASP:OD2	2.71	0.43
1:A:244:ALA:O	1:A:295:GLN:NE2	2.51	0.43
1:B:326:ALA:C	1:B:329:PRO:HD2	2.44	0.43
1:A:262:LEU:C	1:A:264:ASP:N	2.73	0.43
1:A:133:ASP:N	1:A:134:PRO:HD3	2.33	0.43
1:B:106:ILE:HG22	1:B:106:ILE:O	2.19	0.43
1:A:136:LEU:CD2	1:A:139:ARG:NH2	2.82	0.43
1:B:195:GLY:O	1:B:360:PRO:HA	2.18	0.42
1:B:96:ARG:HD3	1:B:96:ARG:HA	1.74	0.42
1:A:55:HIS:HE1	1:A:169:KCX:CX	2.33	0.42
1:A:237:LEU:HD21	1:A:286:ALA:HB1	2.02	0.42
1:B:58:ILE:HD13	1:B:58:ILE:HA	1.83	0.42
1:B:262:LEU:C	1:B:264:ASP:N	2.77	0.42
1:A:262:LEU:HD23	1:A:262:LEU:HA	1.76	0.41
1:A:302:TRP:CH2	1:A:321:ASN:HB3	2.55	0.41
1:A:260:ILE:HD12	1:A:276:SER:HA	2.02	0.41
1:A:262:LEU:C	1:A:264:ASP:H	2.27	0.41
1:A:89:ARG:HH22	1:A:323:ASP:HA	1.86	0.41
1:A:326:ALA:O	1:A:329:PRO:HD2	2.20	0.41
1:B:328:ILE:HB	1:B:329:PRO:HD3	2.02	0.41
1:A:286:ALA:O	1:A:289:ASP:HB2	2.20	0.41
1:A:293:MET:HG2	1:A:294:LYS:N	2.36	0.41
1:B:353:ASN:N	1:B:354:PRO:CD	2.84	0.41
1:A:287:LEU:HD23	1:A:287:LEU:HA	1.88	0.40
1:B:230:HIS:O	1:B:233:ASP:HB2	2.22	0.40
1:A:217:GLU:OE1	1:A:246:ARG:NH2	2.53	0.40
1:B:55:HIS:CE1	1:B:101:VAL:HG21	2.56	0.40
1:B:302:TRP:CH2	1:B:321:ASN:HB3	2.56	0.40
1:B:260:ILE:HD12	1:B:276:SER:HA	2.04	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	326/331 (98%)	313 (96%)	13 (4%)	0	100	100
1	B	328/331 (99%)	321 (98%)	7 (2%)	0	100	100
All	All	654/662 (99%)	634 (97%)	20 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	262/265 (99%)	245 (94%)	17 (6%)	15	8
1	B	264/265 (100%)	250 (95%)	14 (5%)	20	12
All	All	526/530 (99%)	495 (94%)	31 (6%)	18	10

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
1	A	77	LYS
1	A	89	ARG
1	A	110	VAL
1	A	116	VAL
1	A	201	HIS
1	A	241	THR
1	A	267	SER

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Mol	Chain	Res	Type
1	A	290	GLN
1	A	293	MET
1	A	295	GLN
1	A	299	SER
1	A	303	LEU
1	A	314	MET
1	A	337	ARG
1	A	344	GLU
1	A	362	LEU
1	B	47	SER
1	B	58	ILE
1	B	77	LYS
1	B	96	ARG
1	B	175	LYS
1	B	295	GLN
1	B	299	SER
1	B	303	LEU
1	B	314	MET
1	B	319	ARG
1	B	337	ARG
1	B	338	GLU
1	B	344	GLU
1	B	356	ARG

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

Mol	Chain	Res	Type
1	A	212	GLN
1	A	290	GLN
1	A	295	GLN
1	B	290	GLN

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	KCX	B	169	2,1	10,11,12	2.24	1 (10%)	6,12,14	1.93	1 (16%)
1	KCX	A	169	2,1	10,11,12	2.36	2 (20%)	6,12,14	0.71	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	KCX	B	169	2,1	-	3/9/10/12	-
1	KCX	A	169	2,1	-	0/9/10/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	169	KCX	CX-NZ	6.86	1.47	1.35
1	B	169	KCX	CX-NZ	6.60	1.47	1.35
1	A	169	KCX	OQ1-CX	2.33	1.26	1.21

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	169	KCX	CE-NZ-CX	-4.50	114.35	121.98

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	169	KCX	C-CA-CB-CG
1	B	169	KCX	OQ2-CX-NZ-CE
1	B	169	KCX	CG-CD-CE-NZ

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	169	KCX	1	0
1	A	169	KCX	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z > 2$
3	DII	A	1403	2	8,10,10	2.07	2 (25%)	9,14,14	0.91	0
3	DII	B	2403	2	8,10,10	1.92	1 (12%)	9,14,14	1.28	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
3	DII	A	1403	2	-	0/10/10/10	-
3	DII	B	2403	2	-	2/10/10/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1403	DII	P1-C7	-4.96	1.64	1.77
3	B	2403	DII	P1-C7	-4.82	1.64	1.77
3	A	1403	DII	P1-O1	2.65	1.51	1.47

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2403	DII	C4-O3-P1-O1
3	B	2403	DII	C4-O3-P1-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2403	DII	1	0

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.