



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:38 AM UTC

PDB ID : 5LNV / pdb_00005lnv
Title : Crystal structure of Arabidopsis thaliana Pdx1-I320 complex from multiple crystals
Authors : Rodrigues, M.J.; Windeisen, V.; Zhang, Y.; Guedez, G.; Weber, S.; Strohmeier, M.; Hanes, J.W.; Royant, A.; Evans, G.; Sinning, I.; Ealick, S.E.; Begley, T.P.; Tews, I.
Deposited on : 2016-08-06
Resolution : 2.24 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

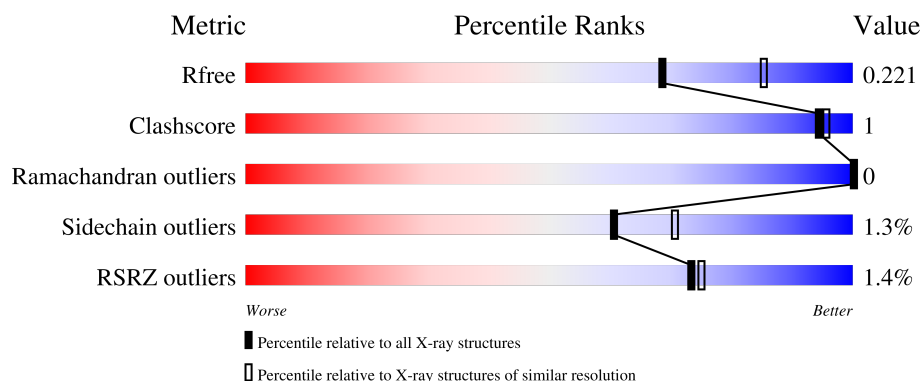
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	316	% 84% 12%
1	B	316	2% 81% 7% 12%
1	C	316	2% 82% 5% 13%
1	D	316	% 84% 13%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8941 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 Pyridoxal 5'-phosphate synthase subunit PDX1.3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2076	1296	378	384	18			
1	B	278	Total	C	N	O	S	0	1	0
			2092	1305	383	386	18			
1	C	276	Total	C	N	O	S	0	0	0
			2069	1291	377	383	18			
1	D	275	Total	C	N	O	S	0	0	0
			2063	1288	376	381	18			

There are 28 discrepancies between the modelled and reference sequences:

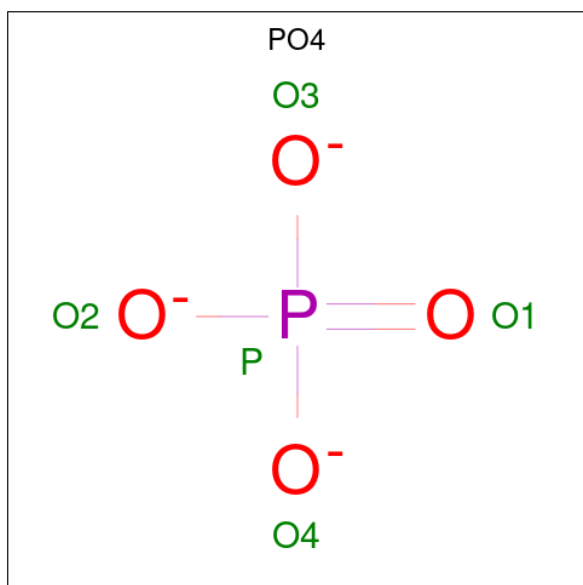
Chain	Residue	Modelled	Actual	Comment	Reference
A	311	GLU	-	expression tag	UNP Q8L940
A	312	HIS	-	expression tag	UNP Q8L940
A	313	HIS	-	expression tag	UNP Q8L940
A	314	HIS	-	expression tag	UNP Q8L940
A	315	HIS	-	expression tag	UNP Q8L940
A	316	HIS	-	expression tag	UNP Q8L940
A	317	HIS	-	expression tag	UNP Q8L940
B	311	GLU	-	expression tag	UNP Q8L940
B	312	HIS	-	expression tag	UNP Q8L940
B	313	HIS	-	expression tag	UNP Q8L940
B	314	HIS	-	expression tag	UNP Q8L940
B	315	HIS	-	expression tag	UNP Q8L940
B	316	HIS	-	expression tag	UNP Q8L940
B	317	HIS	-	expression tag	UNP Q8L940
C	311	GLU	-	expression tag	UNP Q8L940
C	312	HIS	-	expression tag	UNP Q8L940
C	313	HIS	-	expression tag	UNP Q8L940
C	314	HIS	-	expression tag	UNP Q8L940
C	315	HIS	-	expression tag	UNP Q8L940
C	316	HIS	-	expression tag	UNP Q8L940
C	317	HIS	-	expression tag	UNP Q8L940

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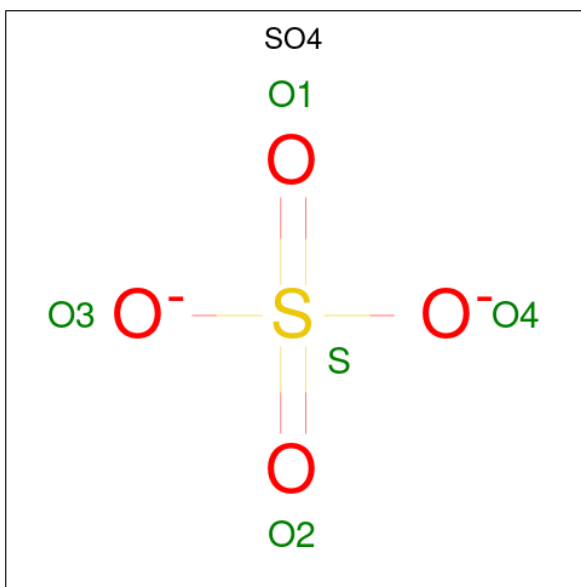
Chain	Residue	Modelled	Actual	Comment	Reference
D	311	GLU	-	expression tag	UNP Q8L940
D	312	HIS	-	expression tag	UNP Q8L940
D	313	HIS	-	expression tag	UNP Q8L940
D	314	HIS	-	expression tag	UNP Q8L940
D	315	HIS	-	expression tag	UNP Q8L940
D	316	HIS	-	expression tag	UNP Q8L940
D	317	HIS	-	expression tag	UNP Q8L940

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



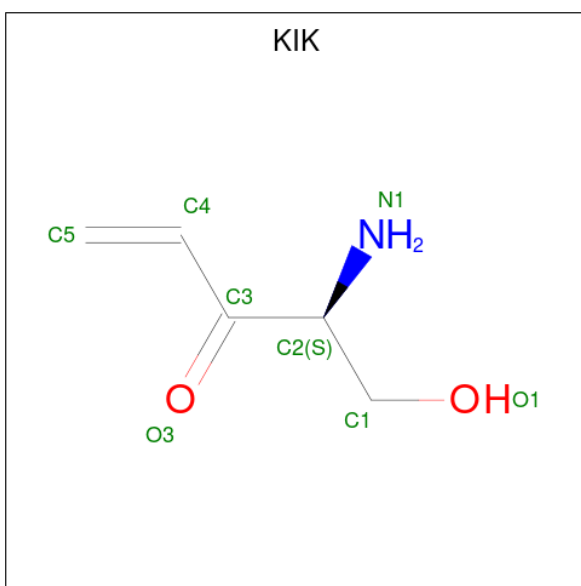
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is (4 {S})-4-azanyl-5-oxidanyl-pent-1-en-3-one (CCD ID: KIK) (formula: C₅H₉NO₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 7 5 1 1	0	0
4	B	1	Total C N O 7 5 1 1	0	0
4	C	1	Total C N O 7 5 1 1	0	0
4	D	1	Total C N O 7 5 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	154	Total O 154 154	0	0
5	B	153	Total O 153 153	0	0
5	C	138	Total O 138 138	0	0
5	D	128	Total O 128 128	0	0

HIS
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4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	178.58Å 178.58Å 117.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.75 – 2.24 46.75 – 2.24	Depositor EDS
% Data completeness (in resolution range)	97.0 (46.75-2.24) 97.0 (46.75-2.24)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.35 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.177 , 0.220 0.179 , 0.221	Depositor DCC
R_{free} test set	3294 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8941	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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: SO4, PO4, KIK

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	0.80	0/2103	0.91	0/2837
1	B	0.79	0/2119	0.92	1/2858 (0.0%)
1	C	0.78	0/2096	0.92	2/2827 (0.1%)
1	D	0.80	0/2090	0.94	1/2818 (0.0%)
All	All	0.79	0/8408	0.92	4/11340 (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	C	192	ARG	N-CA-C	6.19	117.70	111.07
1	C	175	ILE	N-CA-C	5.59	115.79	110.42
1	B	143	VAL	CB-CA-C	-5.27	103.55	110.98
1	D	175	ILE	N-CA-C	5.08	115.80	110.62

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	2076	0	2106	4	0
1	B	2092	0	2120	8	0
1	C	2069	0	2097	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2063	0	2093	3	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	7	0	0	0	0
4	B	7	0	0	0	0
4	C	7	0	0	0	0
4	D	7	0	0	0	0
5	A	154	0	0	1	0
5	B	153	0	0	0	0
5	C	138	0	0	0	0
5	D	128	0	0	0	0
All	All	8941	0	8416	21	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 1.

All (21) 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:C:101:ILE:HB	1:C:126:LEU:HD12	1.82	0.62
1:C:40:MET:HE3	1:C:56:ALA:HB2	1.87	0.55
1:A:101:ILE:HB	1:A:126:LEU:HD12	1.87	0.55
1:B:81:PRO:HB3	1:B:113:ILE:HD11	1.91	0.52
1:C:96:MET:HE2	1:C:117:TYR:CD1	2.45	0.52
1:B:101:ILE:HB	1:B:126:LEU:HD12	1.93	0.50
1:B:88:LYS:HA	1:B:95:VAL:HG21	1.93	0.50
1:B:41:ASP:HB2	1:B:252:GLY:HA2	1.95	0.49
1:D:202:PHE:CE2	1:D:206:LEU:HD11	2.48	0.48
1:B:98:LYS:HG2	1:B:119:ASP:HB3	1.96	0.48
1:C:174:ILE:CG1	1:C:241:MET:HE3	2.44	0.47
1:D:41:ASP:HB2	1:D:252:GLY:HA2	1.97	0.47
1:A:98:LYS:HG2	1:A:119:ASP:HB3	1.99	0.45
1:B:174:ILE:HD11	1:B:241:MET:HE3	1.98	0.44
1:D:116:ASP:O	1:D:141:PRO:HD2	2.17	0.43
1:C:177:ALA:O	1:C:181:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ARG:NH2	5:A:504:HOH:O	2.53	0.41
1:B:122:GLU:OE2	1:B:164:ARG:NH1	2.46	0.41
1:C:98:LYS:HG2	1:C:119:ASP:HB3	2.03	0.41
1:A:78:MET:HB2	1:A:106:GLU:CD	2.46	0.41
1:B:192[B]:ARG:HA	1:B:192[B]:ARG:HD2	1.90	0.41

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	275/316 (87%)	271 (98%)	4 (2%)	0	100	100
1	B	277/316 (88%)	269 (97%)	8 (3%)	0	100	100
1	C	274/316 (87%)	267 (97%)	7 (3%)	0	100	100
1	D	273/316 (86%)	266 (97%)	7 (3%)	0	100	100
All	All	1099/1264 (87%)	1073 (98%)	26 (2%)	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	214/246 (87%)	211 (99%)	3 (1%)	59	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	215/246 (87%)	210 (98%)	5 (2%)	44	53
1	C	213/246 (87%)	211 (99%)	2 (1%)	70	78
1	D	212/246 (86%)	211 (100%)	1 (0%)	81	86
All	All	854/984 (87%)	843 (99%)	11 (1%)	61	71

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	290	GLU
1	A	293	VAL
1	B	53	GLU
1	B	92	THR
1	B	147	ARG
1	B	249	VAL
1	B	295	ILE
1	C	249	VAL
1	C	279	GLU
1	D	88	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	82	GLN
1	A	185	ASN
1	A	243	GLN
1	A	296	ASN
1	B	108	GLN
1	C	82	GLN
1	C	108	GLN
1	C	148	ASN
1	D	215	GLN

5.3.3 RNA ⓘ

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](#)

12 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	$\# Z > 2$
4	KIK	B	403	1	5,6,7	0.91	0	5,7,8	1.30	0
4	KIK	C	403	1	5,6,7	0.92	0	5,7,8	1.28	0
3	SO4	D	402	-	4,4,4	0.45	0	6,6,6	0.33	0
3	SO4	C	402	-	4,4,4	0.42	0	6,6,6	0.49	0
4	KIK	A	403	1	5,6,7	0.99	1 (20%)	5,7,8	1.27	0
3	SO4	A	402	-	4,4,4	0.29	0	6,6,6	0.29	0
2	PO4	A	401	-	4,4,4	1.62	1 (25%)	6,6,6	0.98	0
2	PO4	D	401	-	4,4,4	1.23	0	6,6,6	0.52	0
2	PO4	B	401	-	4,4,4	1.23	0	6,6,6	1.06	0
4	KIK	D	403	1	5,6,7	0.95	1 (20%)	5,7,8	1.29	0
2	PO4	C	401	-	4,4,4	1.23	0	6,6,6	0.46	0
3	SO4	B	402	-	4,4,4	0.18	0	6,6,6	0.29	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
4	KIK	B	403	1	-	2/3/6/8	-
4	KIK	C	403	1	-	2/3/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	KIK	A	403	1	-	2/3/6/8	-
4	KIK	D	403	1	-	2/3/6/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	PO4	P-O2	-2.17	1.48	1.54
4	A	403	KIK	C2-C3	-2.15	1.50	1.53
4	D	403	KIK	C2-C3	-2.04	1.50	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	KIK	O3-C3-C4-C5
4	B	403	KIK	O3-C3-C4-C5
4	C	403	KIK	O3-C3-C4-C5
4	D	403	KIK	O3-C3-C4-C5
4	A	403	KIK	C1-C2-C3-C4
4	B	403	KIK	C1-C2-C3-C4
4	C	403	KIK	C1-C2-C3-C4
4	D	403	KIK	C1-C2-C3-C4

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 [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	277/316 (87%)	-0.49	3 (1%) 78 79	16, 24, 41, 54	0
1	B	278/316 (87%)	-0.31	5 (1%) 67 69	14, 27, 45, 63	1 (0%)
1	C	276/316 (87%)	-0.11	5 (1%) 67 69	19, 30, 53, 64	0
1	D	275/316 (87%)	-0.20	3 (1%) 78 79	16, 28, 51, 63	0
All	All	1106/1264 (87%)	-0.28	16 (1%) 73 75	14, 27, 49, 64	1 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	298	ASN	5.0
1	C	293	VAL	3.8
1	C	297	LEU	3.8
1	B	293	VAL	3.7
1	D	295	ILE	3.7
1	D	297	LEU	3.6
1	D	293	VAL	3.3
1	A	293	VAL	2.9
1	C	294	GLY	2.8
1	C	295	ILE	2.7
1	B	295	ILE	2.6
1	B	21	LYS	2.5
1	C	33	MET	2.4
1	A	298	ASN	2.3
1	A	295	ILE	2.1
1	B	252	GLY	2.1

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 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
4	KIK	C	403	7/8	0.78	0.17	45,46,51,51	0
4	KIK	A	403	7/8	0.84	0.13	32,35,37,40	0
4	KIK	D	403	7/8	0.86	0.13	31,42,45,45	0
4	KIK	B	403	7/8	0.87	0.12	27,37,43,44	0
2	PO4	C	401	5/5	0.96	0.07	39,40,45,46	0
2	PO4	B	401	5/5	0.97	0.07	32,34,37,41	0
2	PO4	D	401	5/5	0.97	0.06	38,42,42,45	0
2	PO4	A	401	5/5	0.98	0.06	27,27,32,32	0
3	SO4	B	402	5/5	0.99	0.05	25,26,31,34	0
3	SO4	D	402	5/5	0.99	0.06	27,28,31,35	0
3	SO4	A	402	5/5	0.99	0.06	24,26,29,31	0
3	SO4	C	402	5/5	1.00	0.04	24,26,32,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.