



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 05:33 AM UTC

PDB ID : 8QX3 / pdb_00008qx3
Title : Arabidopsis thaliana Phosphoenolpyruvate carboxylase PPC1 R886G mutant
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Deposited on : 2023-10-21
Resolution : 2.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

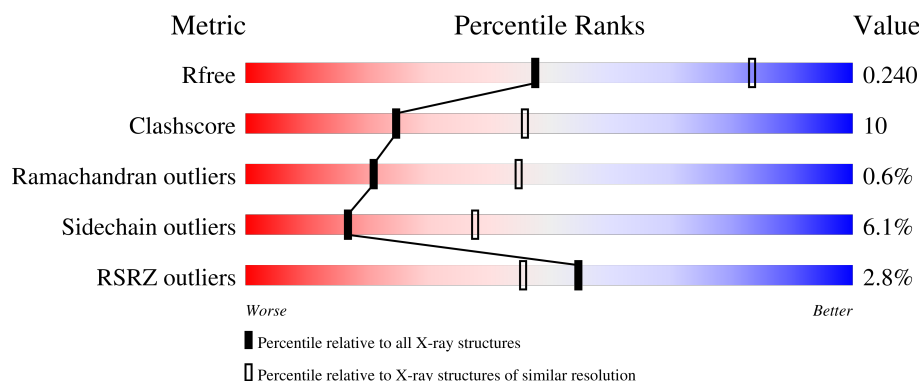
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	974	2% 67% 22% • 8%
1	B	974	2% 68% 22% • 8%
1	C	974	4% 68% 21% • 9%
1	D	974	3% 67% 21% • 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 28637 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 Phosphoenolpyruvate carboxylase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	897	Total	C	N	O	S	0	0	0
			7221	4581	1263	1348	29			
1	B	899	Total	C	N	O	S	0	0	0
			7233	4588	1263	1353	29			
1	C	883	Total	C	N	O	S	0	0	0
			7103	4507	1243	1324	29			
1	D	877	Total	C	N	O	S	0	0	0
			7052	4475	1228	1320	29			

There are 32 discrepancies between the modelled and reference sequences:

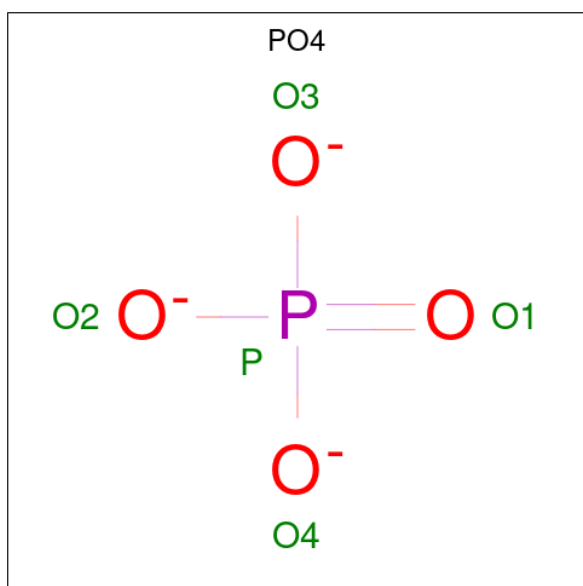
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP Q9MAH0
A	-5	HIS	-	expression tag	UNP Q9MAH0
A	-4	HIS	-	expression tag	UNP Q9MAH0
A	-3	HIS	-	expression tag	UNP Q9MAH0
A	-2	HIS	-	expression tag	UNP Q9MAH0
A	-1	HIS	-	expression tag	UNP Q9MAH0
A	0	HIS	-	expression tag	UNP Q9MAH0
A	886	GLY	ARG	engineered mutation	UNP Q9MAH0
B	-6	MET	-	initiating methionine	UNP Q9MAH0
B	-5	HIS	-	expression tag	UNP Q9MAH0
B	-4	HIS	-	expression tag	UNP Q9MAH0
B	-3	HIS	-	expression tag	UNP Q9MAH0
B	-2	HIS	-	expression tag	UNP Q9MAH0
B	-1	HIS	-	expression tag	UNP Q9MAH0
B	0	HIS	-	expression tag	UNP Q9MAH0
B	886	GLY	ARG	engineered mutation	UNP Q9MAH0
C	-6	MET	-	initiating methionine	UNP Q9MAH0
C	-5	HIS	-	expression tag	UNP Q9MAH0
C	-4	HIS	-	expression tag	UNP Q9MAH0
C	-3	HIS	-	expression tag	UNP Q9MAH0
C	-2	HIS	-	expression tag	UNP Q9MAH0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	HIS	-	expression tag	UNP Q9MAH0
C	0	HIS	-	expression tag	UNP Q9MAH0
C	886	GLY	ARG	engineered mutation	UNP Q9MAH0
D	-6	MET	-	initiating methionine	UNP Q9MAH0
D	-5	HIS	-	expression tag	UNP Q9MAH0
D	-4	HIS	-	expression tag	UNP Q9MAH0
D	-3	HIS	-	expression tag	UNP Q9MAH0
D	-2	HIS	-	expression tag	UNP Q9MAH0
D	-1	HIS	-	expression tag	UNP Q9MAH0
D	0	HIS	-	expression tag	UNP Q9MAH0
D	886	GLY	ARG	engineered mutation	UNP Q9MAH0

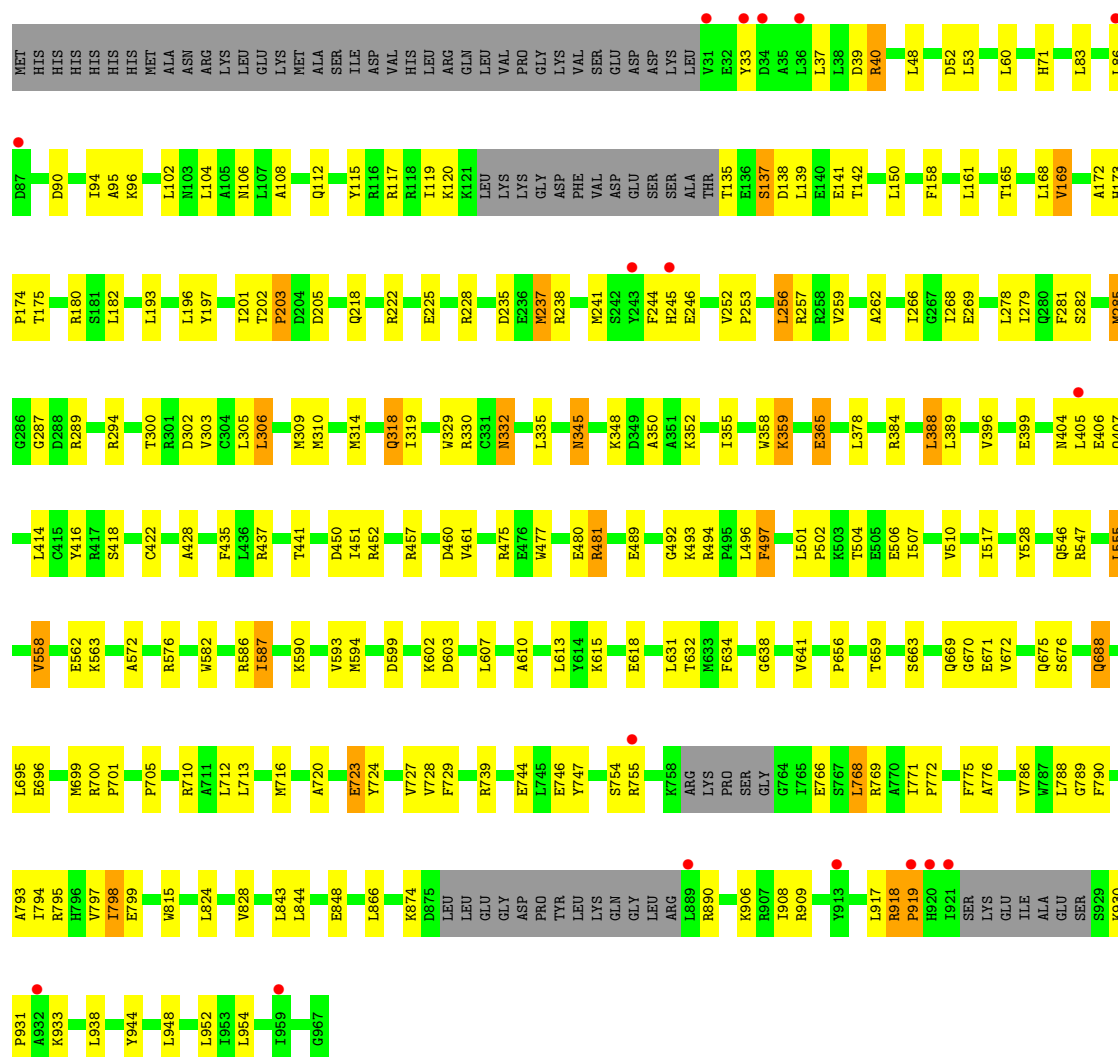
- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



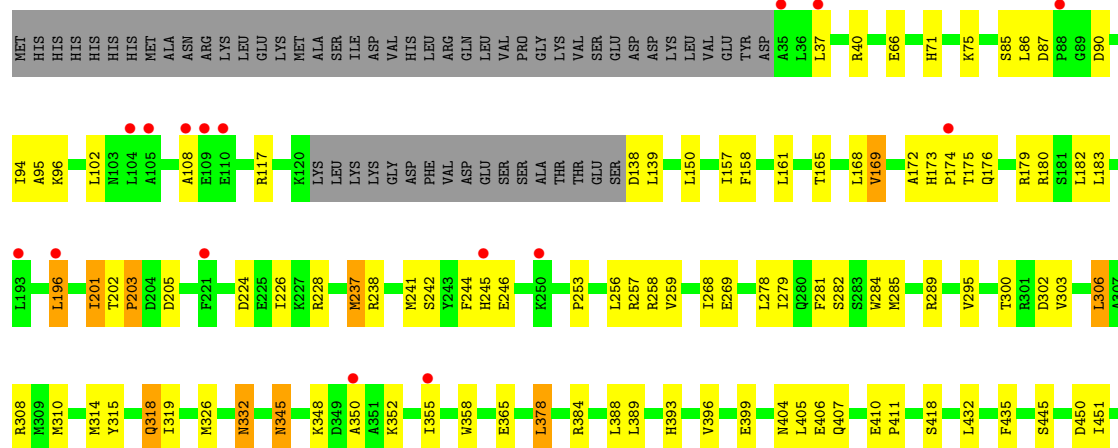
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

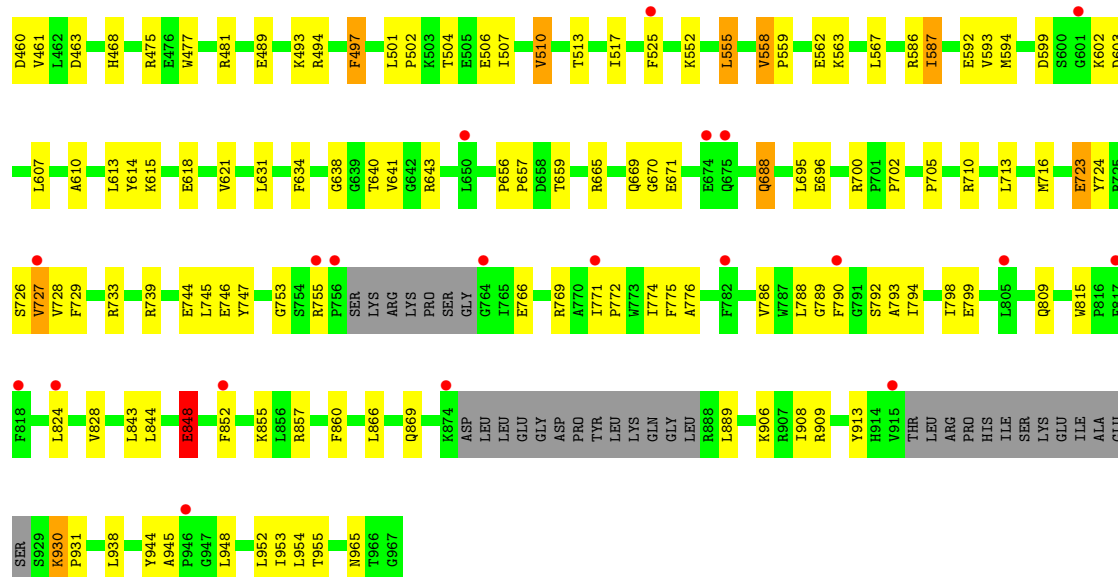
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total 5	O 5	0	0
3	B	3	Total 3	O 3	0	0

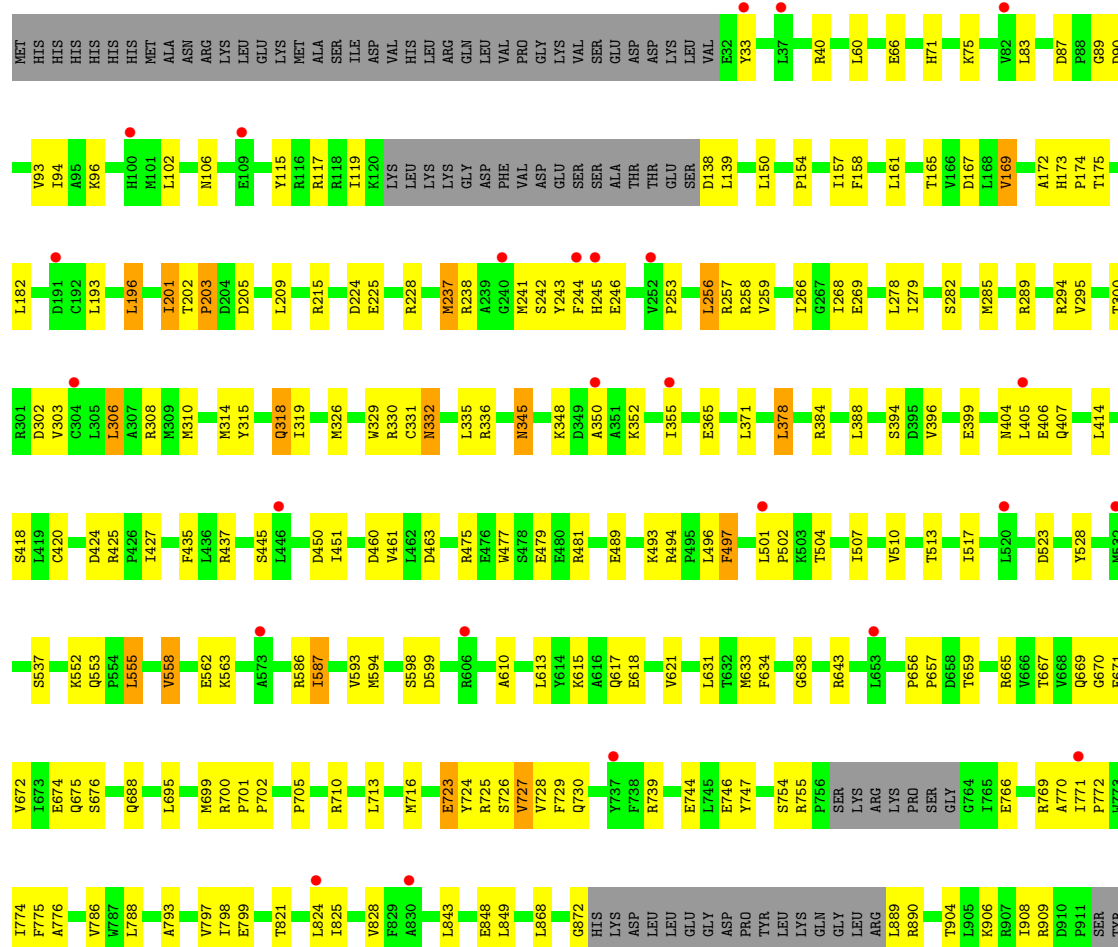


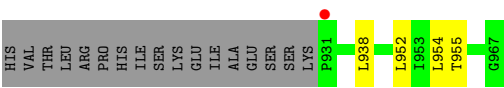
• Molecule 1: Phosphoenolpyruvate carboxylase 1





• Molecule 1: Phosphoenolpyruvate carboxylase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	127.67Å 159.16Å 140.99Å 90.00° 92.03° 90.00°	Depositor
Resolution (Å)	48.99 – 2.95 48.99 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.99-2.95) 99.7 (48.99-2.95)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.204 , 0.240 (Not available) , 0.240	Depositor DCC
R_{free} test set	5927 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	91.6	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 65.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.072 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28637	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: 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	0.20	0/7377	0.41	0/9985
1	B	0.20	0/7389	0.43	0/10001
1	C	0.16	0/7256	0.36	0/9820
1	D	0.15	0/7203	0.36	0/9750
All	All	0.18	0/29225	0.39	0/39556

There are no bond length outliers.

There are no bond angle outliers.

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	7221	0	7178	147	0
1	B	7233	0	7187	149	0
1	C	7103	0	7063	143	0
1	D	7052	0	7002	141	0
2	A	5	0	0	1	0
2	B	5	0	0	1	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	0	0	0
All	All	28637	0	28430	559	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.

The worst 5 of 559 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:404:ASN:HB2	1:A:407:GLN:HB2	1.63	0.81
1:D:460:ASP:OD1	1:D:475:ARG:NH1	2.14	0.79
1:A:173:HIS:ND1	1:A:669:GLN:OE1	2.15	0.79
1:A:638:GLY:HA2	1:A:669:GLN:HG3	1.64	0.77
1:B:638:GLY:HA2	1:B:669:GLN:HG3	1.67	0.76

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	887/974 (91%)	843 (95%)	37 (4%)	7 (1%)	16	36
1	B	889/974 (91%)	842 (95%)	40 (4%)	7 (1%)	16	36
1	C	873/974 (90%)	833 (95%)	36 (4%)	4 (0%)	24	49
1	D	867/974 (89%)	826 (95%)	38 (4%)	3 (0%)	36	59
All	All	3516/3896 (90%)	3344 (95%)	151 (4%)	21 (1%)	21	45

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	670	GLY

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Mol	Chain	Res	Type
1	A	919	PRO
1	B	670	GLY
1	B	919	PRO
1	C	670	GLY

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	780/848 (92%)	727 (93%)	53 (7%)	14	33
1	B	782/848 (92%)	734 (94%)	48 (6%)	17	38
1	C	766/848 (90%)	721 (94%)	45 (6%)	18	39
1	D	760/848 (90%)	717 (94%)	43 (6%)	18	41
All	All	3088/3392 (91%)	2899 (94%)	189 (6%)	17	38

5 of 189 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	279	ILE
1	C	799	GLU
1	C	332	ASN
1	C	504	THR
1	D	165	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	515	HIS
1	C	814	HIS
1	D	332	ASN
1	B	163	ASN
1	B	112	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	PO4	B	1001	-	4,4,4	0.96	0	6,6,6	0.48	0
2	PO4	D	1001	-	4,4,4	0.96	0	6,6,6	0.45	0
2	PO4	A	1001	-	4,4,4	0.91	0	6,6,6	0.49	0
2	PO4	C	1001	-	4,4,4	0.95	0	6,6,6	0.49	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	PO4	1	0
2	A	1001	PO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1001	PO4	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 [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	897/974 (92%)	-0.10	22 (2%)	58	49	49, 80, 131, 214	0
1	B	899/974 (92%)	-0.12	17 (1%)	66	58	51, 82, 135, 216	0
1	C	883/974 (90%)	0.20	36 (4%)	41	33	76, 140, 217, 268	0
1	D	877/974 (90%)	0.12	26 (2%)	52	44	78, 133, 196, 277	0
All	All	3556/3896 (91%)	0.02	101 (2%)	55	46	49, 105, 193, 277	0

The worst 5 of 101 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	196	LEU	6.1
1	B	245	HIS	5.3
1	A	245	HIS	4.6
1	A	31	VAL	4.6
1	C	105	ALA	3.9

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
2	PO4	D	1001	5/5	0.90	0.09	99,124,131,141	0
2	PO4	C	1001	5/5	0.91	0.08	119,125,133,135	0
2	PO4	A	1001	5/5	0.95	0.09	57,71,112,127	0
2	PO4	B	1001	5/5	0.98	0.06	57,89,98,105	0

6.5 Other polymers [i](#)

There are no such residues in this entry.