



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 3, 2024 – 02:54 am GMT

PDB ID : 4UPH  
Title : Crystal Structure of Phosphonate Monoester Hydrolase of Agrobacterium radiobacter  
Authors : Fischer, G.; Loo, B.v.; Hyvonen, M.; Hollfelder, F.  
Deposited on : 2014-06-17  
Resolution : 2.50 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](mailto:validation@mail.wwpdb.org)

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<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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

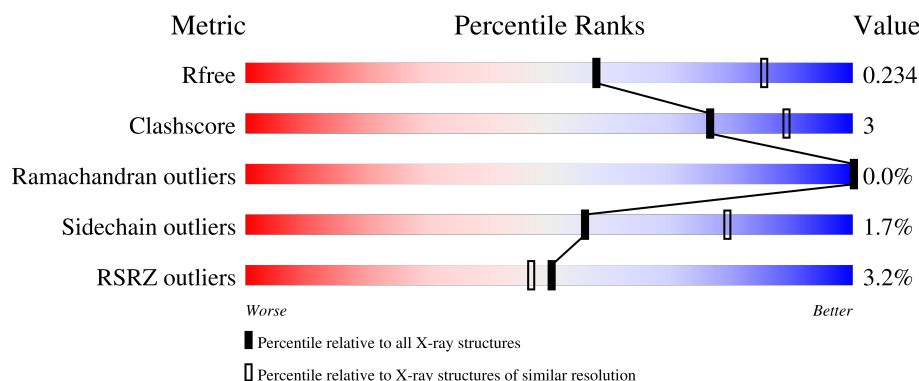
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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  $\geq 3$ , 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	547	 85% 7% • 8%
1	B	547	 84% 8% 8%
1	C	547	 85% 7% • 8%
1	D	547	 83% 8% • 8%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16052 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 SULFATASE (SULFURIC ESTER HYDROLASE) PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	0	0
			3926	2495	688	731	12			
1	B	504	Total	C	N	O	S	0	0	0
			3926	2495	688	731	12			
1	C	504	Total	C	N	O	S	0	0	0
			3926	2495	688	731	12			
1	D	504	Total	C	N	O	S	0	0	0
			3926	2495	688	731	12			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	MET	-	expression tag	UNP B9JE48
A	-27	ALA	-	expression tag	UNP B9JE48
A	-26	SER	-	expression tag	UNP B9JE48
A	-25	TRP	-	expression tag	UNP B9JE48
A	-24	SER	-	expression tag	UNP B9JE48
A	-23	HIS	-	expression tag	UNP B9JE48
A	-22	PRO	-	expression tag	UNP B9JE48
A	-21	GLN	-	expression tag	UNP B9JE48
A	-20	PHE	-	expression tag	UNP B9JE48
A	-19	GLU	-	expression tag	UNP B9JE48
A	-18	LYS	-	expression tag	UNP B9JE48
A	-17	GLY	-	expression tag	UNP B9JE48
A	-16	ALA	-	expression tag	UNP B9JE48
A	-15	GLU	-	expression tag	UNP B9JE48
A	-14	THR	-	expression tag	UNP B9JE48
A	-13	ALA	-	expression tag	UNP B9JE48
A	-12	VAL	-	expression tag	UNP B9JE48
A	-11	PRO	-	expression tag	UNP B9JE48
A	-10	ASN	-	expression tag	UNP B9JE48
A	-9	SER	-	expression tag	UNP B9JE48
A	-8	SER	-	expression tag	UNP B9JE48

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	SER	-	expression tag	UNP B9JE48
A	-6	VAL	-	expression tag	UNP B9JE48
A	-5	PRO	-	expression tag	UNP B9JE48
A	-4	GLY	-	expression tag	UNP B9JE48
A	-3	ASP	-	expression tag	UNP B9JE48
A	-2	PRO	-	expression tag	UNP B9JE48
A	-1	SER	-	expression tag	UNP B9JE48
A	0	SER	-	expression tag	UNP B9JE48
B	-28	MET	-	expression tag	UNP B9JE48
B	-27	ALA	-	expression tag	UNP B9JE48
B	-26	SER	-	expression tag	UNP B9JE48
B	-25	TRP	-	expression tag	UNP B9JE48
B	-24	SER	-	expression tag	UNP B9JE48
B	-23	HIS	-	expression tag	UNP B9JE48
B	-22	PRO	-	expression tag	UNP B9JE48
B	-21	GLN	-	expression tag	UNP B9JE48
B	-20	PHE	-	expression tag	UNP B9JE48
B	-19	GLU	-	expression tag	UNP B9JE48
B	-18	LYS	-	expression tag	UNP B9JE48
B	-17	GLY	-	expression tag	UNP B9JE48
B	-16	ALA	-	expression tag	UNP B9JE48
B	-15	GLU	-	expression tag	UNP B9JE48
B	-14	THR	-	expression tag	UNP B9JE48
B	-13	ALA	-	expression tag	UNP B9JE48
B	-12	VAL	-	expression tag	UNP B9JE48
B	-11	PRO	-	expression tag	UNP B9JE48
B	-10	ASN	-	expression tag	UNP B9JE48
B	-9	SER	-	expression tag	UNP B9JE48
B	-8	SER	-	expression tag	UNP B9JE48
B	-7	SER	-	expression tag	UNP B9JE48
B	-6	VAL	-	expression tag	UNP B9JE48
B	-5	PRO	-	expression tag	UNP B9JE48
B	-4	GLY	-	expression tag	UNP B9JE48
B	-3	ASP	-	expression tag	UNP B9JE48
B	-2	PRO	-	expression tag	UNP B9JE48
B	-1	SER	-	expression tag	UNP B9JE48
B	0	SER	-	expression tag	UNP B9JE48
C	-28	MET	-	expression tag	UNP B9JE48
C	-27	ALA	-	expression tag	UNP B9JE48
C	-26	SER	-	expression tag	UNP B9JE48
C	-25	TRP	-	expression tag	UNP B9JE48
C	-24	SER	-	expression tag	UNP B9JE48

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-23	HIS	-	expression tag	UNP B9JE48
C	-22	PRO	-	expression tag	UNP B9JE48
C	-21	GLN	-	expression tag	UNP B9JE48
C	-20	PHE	-	expression tag	UNP B9JE48
C	-19	GLU	-	expression tag	UNP B9JE48
C	-18	LYS	-	expression tag	UNP B9JE48
C	-17	GLY	-	expression tag	UNP B9JE48
C	-16	ALA	-	expression tag	UNP B9JE48
C	-15	GLU	-	expression tag	UNP B9JE48
C	-14	THR	-	expression tag	UNP B9JE48
C	-13	ALA	-	expression tag	UNP B9JE48
C	-12	VAL	-	expression tag	UNP B9JE48
C	-11	PRO	-	expression tag	UNP B9JE48
C	-10	ASN	-	expression tag	UNP B9JE48
C	-9	SER	-	expression tag	UNP B9JE48
C	-8	SER	-	expression tag	UNP B9JE48
C	-7	SER	-	expression tag	UNP B9JE48
C	-6	VAL	-	expression tag	UNP B9JE48
C	-5	PRO	-	expression tag	UNP B9JE48
C	-4	GLY	-	expression tag	UNP B9JE48
C	-3	ASP	-	expression tag	UNP B9JE48
C	-2	PRO	-	expression tag	UNP B9JE48
C	-1	SER	-	expression tag	UNP B9JE48
C	0	SER	-	expression tag	UNP B9JE48
D	-28	MET	-	expression tag	UNP B9JE48
D	-27	ALA	-	expression tag	UNP B9JE48
D	-26	SER	-	expression tag	UNP B9JE48
D	-25	TRP	-	expression tag	UNP B9JE48
D	-24	SER	-	expression tag	UNP B9JE48
D	-23	HIS	-	expression tag	UNP B9JE48
D	-22	PRO	-	expression tag	UNP B9JE48
D	-21	GLN	-	expression tag	UNP B9JE48
D	-20	PHE	-	expression tag	UNP B9JE48
D	-19	GLU	-	expression tag	UNP B9JE48
D	-18	LYS	-	expression tag	UNP B9JE48
D	-17	GLY	-	expression tag	UNP B9JE48
D	-16	ALA	-	expression tag	UNP B9JE48
D	-15	GLU	-	expression tag	UNP B9JE48
D	-14	THR	-	expression tag	UNP B9JE48
D	-13	ALA	-	expression tag	UNP B9JE48
D	-12	VAL	-	expression tag	UNP B9JE48
D	-11	PRO	-	expression tag	UNP B9JE48

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	ASN	-	expression tag	UNP B9JE48
D	-9	SER	-	expression tag	UNP B9JE48
D	-8	SER	-	expression tag	UNP B9JE48
D	-7	SER	-	expression tag	UNP B9JE48
D	-6	VAL	-	expression tag	UNP B9JE48
D	-5	PRO	-	expression tag	UNP B9JE48
D	-4	GLY	-	expression tag	UNP B9JE48
D	-3	ASP	-	expression tag	UNP B9JE48
D	-2	PRO	-	expression tag	UNP B9JE48
D	-1	SER	-	expression tag	UNP B9JE48
D	0	SER	-	expression tag	UNP B9JE48

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	121	Total O 121 121	0	0

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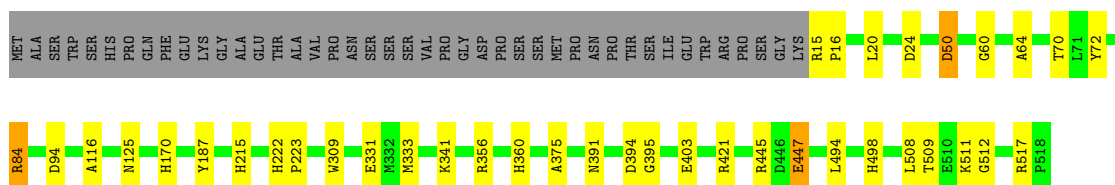
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	84	Total 84	O 84	0	0
4	C	81	Total 81	O 81	0	0
4	D	54	Total 54	O 54	0	0

### 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.

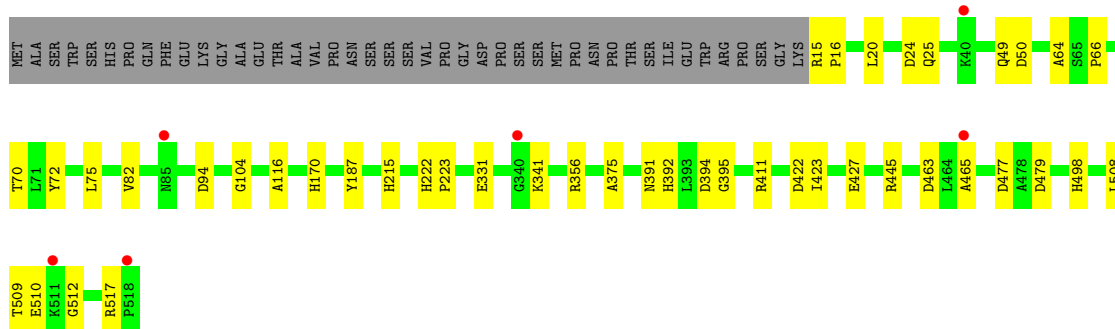
- Molecule 1: SULFATASE (SULFURIC ESTER HYDROLASE) PROTEIN

Chain A:



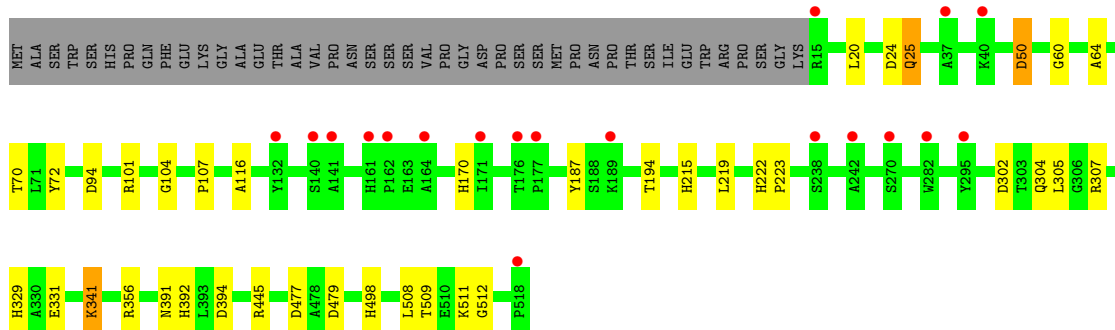
- Molecule 1: SULFATASE (SULFURIC ESTER HYDROLASE) PROTEIN

Chain B:



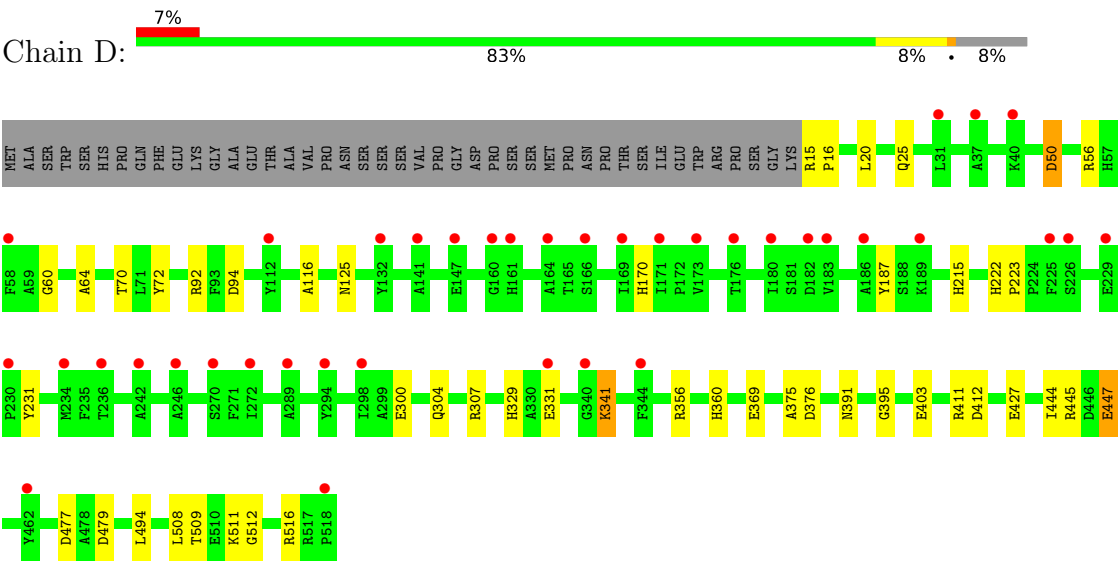
- Molecule 1: SULFATASE (SULFURIC ESTER HYDROLASE) PROTEIN

Chain C:





● Molecule 1: SULFATASE (SULFURIC ESTER HYDROLASE) PROTEIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	232.69Å 232.69Å 112.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.17 – 2.50 58.17 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (58.17-2.50) 100.0 (58.17-2.50)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, $R_{free}$	0.196 , 0.225 0.207 , 0.234	Depositor DCC
$R_{free}$ test set	5295 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.3	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16052	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.35 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.7999e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: DDZ, MG, CL

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	0.53	0/4037	0.67	0/5503
1	B	0.51	0/4037	0.67	0/5503
1	C	0.51	0/4037	0.66	0/5503
1	D	0.51	0/4037	0.67	0/5503
All	All	0.52	0/16148	0.67	0/22012

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	3926	0	3741	20	0
1	B	3926	0	3741	25	0
1	C	3926	0	3741	23	0
1	D	3926	0	3741	26	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	121	0	0	1	0
4	B	84	0	0	2	0
4	C	81	0	0	0	0
4	D	54	0	0	1	0
All	All	16052	0	14964	86	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 3.

The worst 5 of 86 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:94:ASP:H	1:B:391:ASN:HD21	1.24	0.86
1:A:94:ASP:H	1:A:391:ASN:HD21	1.25	0.82
1:D:94:ASP:H	1:D:391:ASN:HD21	1.24	0.81
1:B:509:THR:HG22	1:B:512:GLY:O	1.83	0.79
1:A:84:ARG:HD2	1:A:421:ARG:O	1.83	0.79

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	501/547 (92%)	490 (98%)	11 (2%)	0	100	100
1	B	501/547 (92%)	489 (98%)	12 (2%)	0	100	100
1	C	501/547 (92%)	489 (98%)	12 (2%)	0	100	100
1	D	501/547 (92%)	489 (98%)	11 (2%)	1 (0%)	44	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2004/2188 (92%)	1957 (98%)	46 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	231	TYR

### 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	400/438 (91%)	392 (98%)	8 (2%)	50	75
1	B	400/438 (91%)	394 (98%)	6 (2%)	60	82
1	C	400/438 (91%)	395 (99%)	5 (1%)	65	85
1	D	400/438 (91%)	392 (98%)	8 (2%)	50	75
All	All	1600/1752 (91%)	1573 (98%)	27 (2%)	56	79

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	25	GLN
1	C	341	LYS
1	D	445	ARG
1	C	194	THR
1	C	445	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	161	HIS
1	D	391	ASN
1	C	304	GLN
1	D	215	HIS

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Mol	Chain	Res	Type
1	C	215	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	DDZ	C	64	1,2	4,6,7	1.69	2 (50%)	3,7,9	1.75	1 (33%)
1	DDZ	B	64	1,2	4,6,7	1.57	1 (25%)	3,7,9	1.62	1 (33%)
1	DDZ	D	64	1,2	4,6,7	1.38	1 (25%)	3,7,9	1.78	1 (33%)
1	DDZ	A	64	1,2	4,6,7	1.40	1 (25%)	3,7,9	1.73	1 (33%)

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	DDZ	C	64	1,2	-	0/2/6/8	-
1	DDZ	B	64	1,2	-	0/2/6/8	-
1	DDZ	D	64	1,2	-	0/2/6/8	-
1	DDZ	A	64	1,2	-	0/2/6/8	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	DDZ	OG1-CB	2.42	1.45	1.40
1	C	64	DDZ	OG2-CB	2.31	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	64	DDZ	OG1-CB	2.26	1.45	1.40
1	A	64	DDZ	OG2-CB	2.06	1.45	1.40
1	D	64	DDZ	OG2-CB	2.04	1.44	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	64	DDZ	O-C-CA	-2.99	116.93	124.78
1	C	64	DDZ	O-C-CA	-2.94	117.07	124.78
1	B	64	DDZ	O-C-CA	-2.76	117.54	124.78
1	A	64	DDZ	O-C-CA	-2.64	117.87	124.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	503/547 (91%)	-0.16	0 100 100	32, 49, 73, 99	0
1	B	503/547 (91%)	0.30	6 (1%) 76 73	38, 60, 84, 115	0
1	C	503/547 (91%)	0.29	19 (3%) 44 41	34, 58, 88, 112	0
1	D	503/547 (91%)	0.70	39 (7%) 20 19	37, 65, 97, 120	0
All	All	2012/2188 (91%)	0.28	64 (3%) 50 47	32, 57, 89, 120	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	340	GLY	4.2
1	D	225	PHE	3.7
1	D	518	PRO	3.7
1	C	518	PRO	3.6
1	B	518	PRO	3.3

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	DDZ	C	64	7/8	0.91	0.10	52,54,61,65	0
1	DDZ	B	64	7/8	0.92	0.08	52,54,56,58	0
1	DDZ	D	64	7/8	0.92	0.09	50,51,58,59	0
1	DDZ	A	64	7/8	0.96	0.07	44,46,52,58	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> 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	C	1549	1/1	0.84	0.14	98,98,98,98	0
3	CL	D	1549	1/1	0.86	0.23	100,100,100,100	0
3	CL	A	1549	1/1	0.89	0.16	81,81,81,81	0
3	CL	B	1549	1/1	0.92	0.18	85,85,85,85	0
2	MG	B	1001	1/1	0.98	0.05	44,44,44,44	0
2	MG	C	1001	1/1	0.99	0.03	35,35,35,35	0
2	MG	D	1001	1/1	0.99	0.05	56,56,56,56	0
2	MG	A	1001	1/1	0.99	0.06	36,36,36,36	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.