



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 03:05 pm BST

PDB ID : 2ZE8  
Title : Crystal Structure of adenosine phosphate-isopentenyltransferase complexed with diphosphate  
Authors : Sakakibara, H.  
Deposited on : 2007-12-06  
Resolution : 2.80 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)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

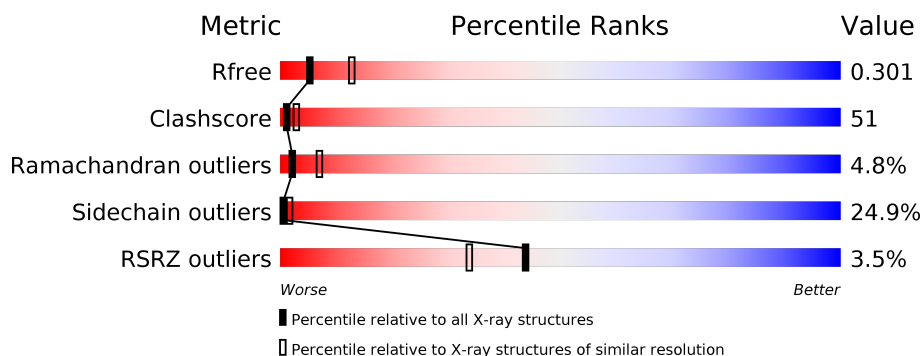
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on 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	253	<div> <div>3%</div> <div>24% 43% 20% • 11%</div> </div>
1	B	253	<div> <div>4%</div> <div>25% 40% 22% • 11%</div> </div>
1	C	253	<div> <div>3%</div> <div>24% 39% 22% • 11%</div> </div>
1	D	253	<div> <div>3%</div> <div>28% 41% 18% • 11%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	POP	D	301	-	X	-	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7296 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 Isopentenyl transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1815	1146	327	333	9			
1	B	226	Total	C	N	O	S	0	0	0
			1815	1146	327	333	9			
1	C	226	Total	C	N	O	S	0	0	0
			1815	1146	327	333	9			
1	D	226	Total	C	N	O	S	0	0	0
			1815	1146	327	333	9			

There are 40 discrepancies between the modelled and reference sequences:

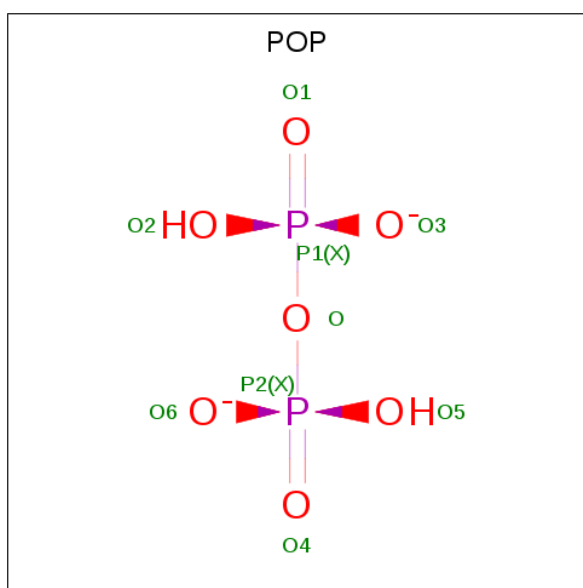
Chain	Residue	Modelled	Actual	Comment	Reference
A	244	GLY	-	EXPRESSION TAG	UNP P58758
A	245	SER	-	EXPRESSION TAG	UNP P58758
A	246	ARG	-	EXPRESSION TAG	UNP P58758
A	247	SER	-	EXPRESSION TAG	UNP P58758
A	248	HIS	-	EXPRESSION TAG	UNP P58758
A	249	HIS	-	EXPRESSION TAG	UNP P58758
A	250	HIS	-	EXPRESSION TAG	UNP P58758
A	251	HIS	-	EXPRESSION TAG	UNP P58758
A	252	HIS	-	EXPRESSION TAG	UNP P58758
A	253	HIS	-	EXPRESSION TAG	UNP P58758
B	244	GLY	-	EXPRESSION TAG	UNP P58758
B	245	SER	-	EXPRESSION TAG	UNP P58758
B	246	ARG	-	EXPRESSION TAG	UNP P58758
B	247	SER	-	EXPRESSION TAG	UNP P58758
B	248	HIS	-	EXPRESSION TAG	UNP P58758
B	249	HIS	-	EXPRESSION TAG	UNP P58758
B	250	HIS	-	EXPRESSION TAG	UNP P58758
B	251	HIS	-	EXPRESSION TAG	UNP P58758
B	252	HIS	-	EXPRESSION TAG	UNP P58758
B	253	HIS	-	EXPRESSION TAG	UNP P58758
C	244	GLY	-	EXPRESSION TAG	UNP P58758

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Chain	Residue	Modelled	Actual	Comment	Reference
C	245	SER	-	EXPRESSION TAG	UNP P58758
C	246	ARG	-	EXPRESSION TAG	UNP P58758
C	247	SER	-	EXPRESSION TAG	UNP P58758
C	248	HIS	-	EXPRESSION TAG	UNP P58758
C	249	HIS	-	EXPRESSION TAG	UNP P58758
C	250	HIS	-	EXPRESSION TAG	UNP P58758
C	251	HIS	-	EXPRESSION TAG	UNP P58758
C	252	HIS	-	EXPRESSION TAG	UNP P58758
C	253	HIS	-	EXPRESSION TAG	UNP P58758
D	244	GLY	-	EXPRESSION TAG	UNP P58758
D	245	SER	-	EXPRESSION TAG	UNP P58758
D	246	ARG	-	EXPRESSION TAG	UNP P58758
D	247	SER	-	EXPRESSION TAG	UNP P58758
D	248	HIS	-	EXPRESSION TAG	UNP P58758
D	249	HIS	-	EXPRESSION TAG	UNP P58758
D	250	HIS	-	EXPRESSION TAG	UNP P58758
D	251	HIS	-	EXPRESSION TAG	UNP P58758
D	252	HIS	-	EXPRESSION TAG	UNP P58758
D	253	HIS	-	EXPRESSION TAG	UNP P58758

- Molecule 2 is PYROPHOSPHATE 2- (three-letter code: POP) (formula:  $\text{H}_2\text{O}_7\text{P}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			9	7	2		
2	B	1	Total	O	P	0	0
			9	7	2		

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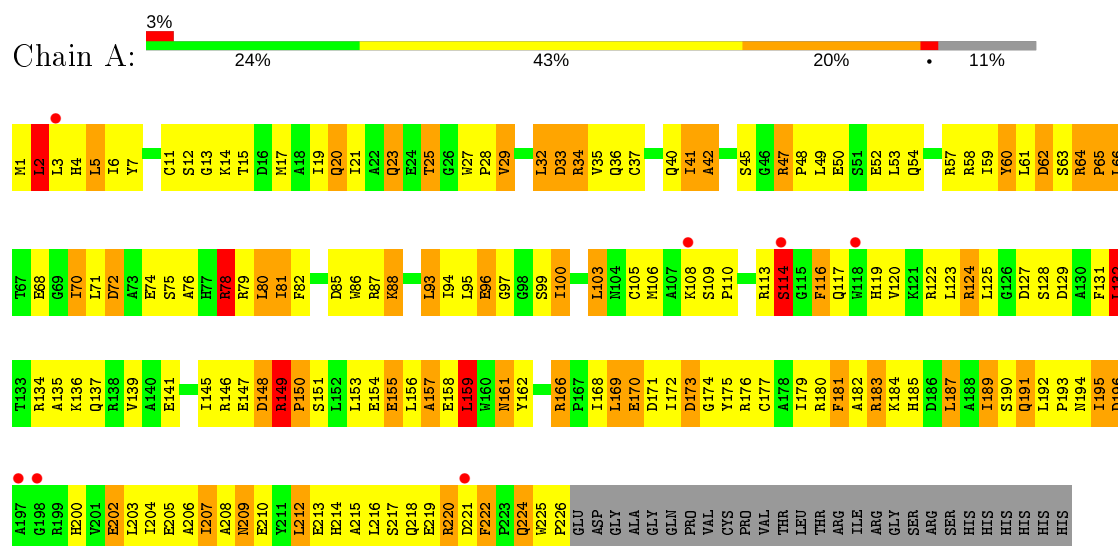
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	P	0	0
			9	7	2		
2	D	1	Total	O	P	0	0
			9	7	2		

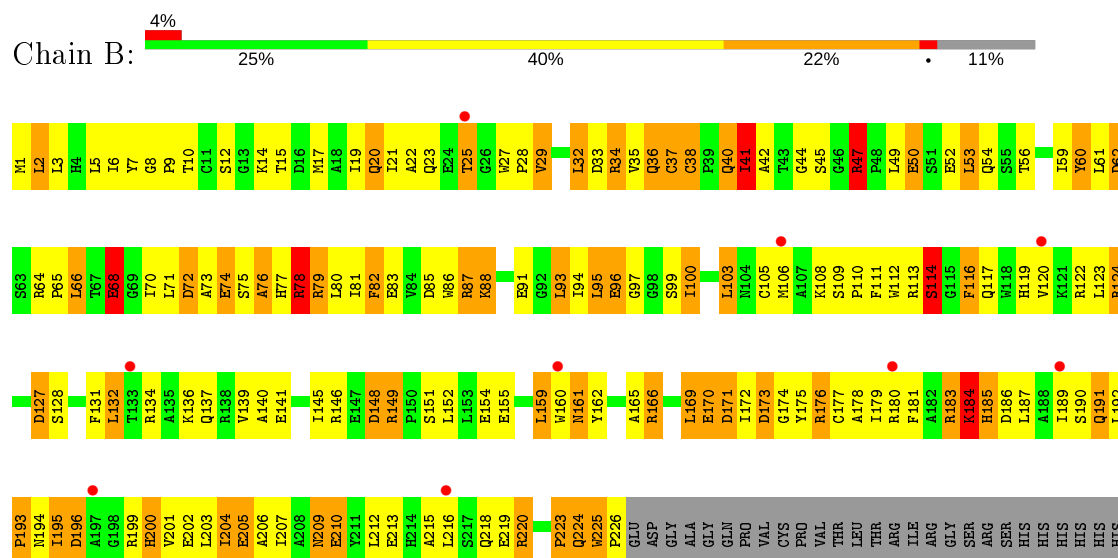
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

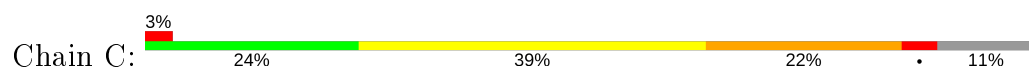
#### • Molecule 1: Isopentenyl transferase

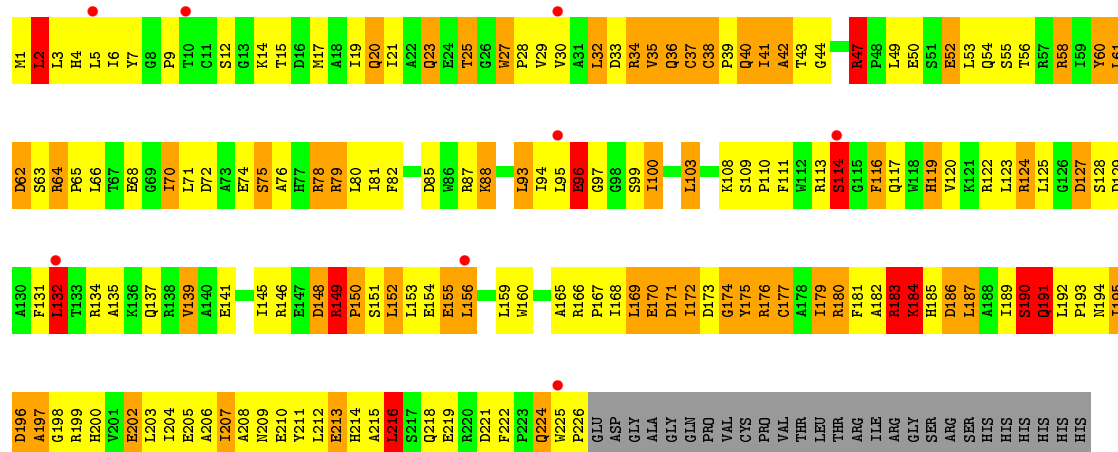


#### • Molecule 1: Isopentenyl transferase

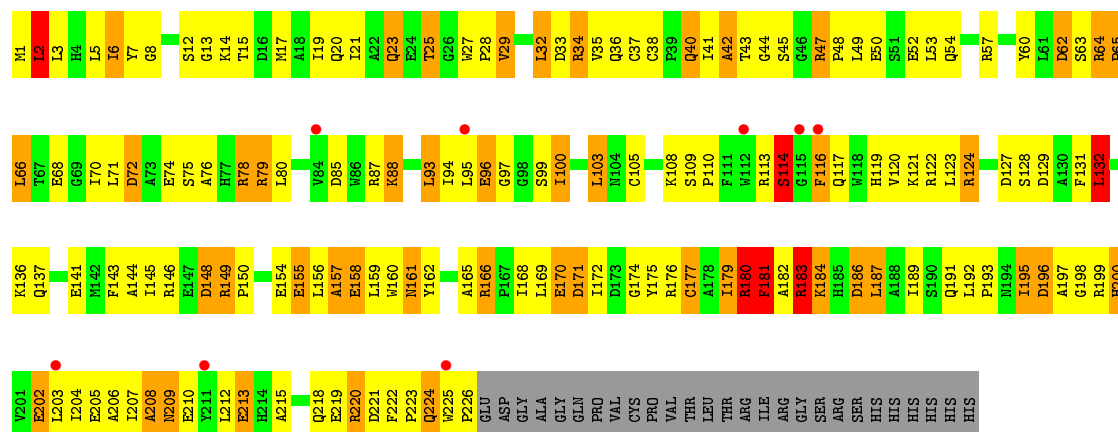


#### • Molecule 1: Isopentenyl transferase





• Molecule 1: Isopentenyl transferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.51Å 97.57Å 131.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	131.31 – 2.80 47.52 – 2.77	Depositor EDS
% Data completeness (in resolution range)	97.8 (131.31-2.80) 96.6 (47.52-2.77)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.230 , 0.302 0.231 , 0.301	Depositor DCC
$R_{free}$ test set	1594 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.8	Xtriage
Anisotropy	0.645	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 90.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.459 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7296	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	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 75.01 % 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 1.3713e-06. 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: POP

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	1.50	15/1856 (0.8%)	1.52	25/2514 (1.0%)
1	B	1.59	21/1856 (1.1%)	1.44	20/2514 (0.8%)
1	C	1.70	30/1856 (1.6%)	1.61	31/2514 (1.2%)
1	D	1.31	6/1856 (0.3%)	1.36	17/2514 (0.7%)
All	All	1.53	72/7424 (1.0%)	1.49	93/10056 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	186	ASP	CG-OD1	11.22	1.51	1.25
1	C	183	ARG	CZ-NH1	10.84	1.47	1.33
1	B	177	CYS	CB-SG	-10.70	1.64	1.82
1	C	175	TYR	CD1-CE1	10.62	1.55	1.39
1	C	184	LYS	CE-NZ	10.05	1.74	1.49

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	186	ASP	CB-CG-OD1	-12.32	107.21	118.30
1	C	183	ARG	NE-CZ-NH2	-11.94	114.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	64	ARG	NE-CZ-NH1	-11.36	114.62	120.30
1	A	93	LEU	CB-CG-CD1	-11.11	92.11	111.00
1	A	64	ARG	NE-CZ-NH1	-10.38	115.11	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	41	ILE	Peptide
1	C	190	SER	Peptide

## 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	1815	0	1798	172	0
1	B	1815	0	1798	189	1
1	C	1815	0	1797	197	0
1	D	1815	0	1798	191	0
2	A	9	0	0	0	0
2	B	9	0	0	2	0
2	C	9	0	0	1	0
2	D	9	0	0	1	0
All	All	7296	0	7191	746	1

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 51.

The worst 5 of 746 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:184:LYS:CE	1:C:184:LYS:NZ	1.74	1.48
1:B:176:ARG:HB3	1:B:176:ARG:NH1	1.38	1.38
1:B:176:ARG:CB	1:B:176:ARG:HH11	1.44	1.28
1:B:176:ARG:CB	1:B:176:ARG:NH1	2.07	1.12
1:C:34:ARG:HH11	1:C:34:ARG:HG2	1.15	1.11

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:GLU:OE1	1:B:185:HIS:ND1[4_545]	2.11	0.09

## 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	224/253 (88%)	185 (83%)	31 (14%)	8 (4%)	3	11
1	B	224/253 (88%)	180 (80%)	30 (13%)	14 (6%)	1	3
1	C	224/253 (88%)	183 (82%)	32 (14%)	9 (4%)	3	9
1	D	224/253 (88%)	191 (85%)	21 (9%)	12 (5%)	2	5
All	All	896/1012 (88%)	739 (82%)	114 (13%)	43 (5%)	2	7

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	SER
1	A	150	PRO
1	A	174	GLY
1	A	196	ASP
1	B	42	ALA

### 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	192/215 (89%)	144 (75%)	48 (25%)	0	2
1	B	192/215 (89%)	143 (74%)	49 (26%)	0	1
1	C	192/215 (89%)	144 (75%)	48 (25%)	0	2
1	D	192/215 (89%)	146 (76%)	46 (24%)	0	2
All	All	768/860 (89%)	577 (75%)	191 (25%)	0	2

5 of 191 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	191	GLN
1	C	47	ARG
1	D	161	ASN
1	B	195	ILE
1	B	225	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	224	GLN
1	C	40	GLN
1	D	200	HIS
1	C	20	GLN
1	C	191	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 carbohydrates 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	POP	A	301	-	6,8,8	1.10	0	13,13,13	1.51	2 (15%)
2	POP	C	301	-	6,8,8	1.60	2 (33%)	13,13,13	2.18	4 (30%)
2	POP	B	301	-	6,8,8	1.59	1 (16%)	13,13,13	1.44	2 (15%)
2	POP	D	301	-	6,8,8	1.53	1 (16%)	13,13,13	2.10	6 (46%)

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
2	POP	A	301	-	-	0/6/6/6	-
2	POP	C	301	-	-	0/6/6/6	-
2	POP	B	301	-	-	1/6/6/6	-
2	POP	D	301	-	-	5/6/6/6	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	POP	P1-O1	3.10	1.60	1.50
2	D	301	POP	P1-O1	2.95	1.60	1.50
2	C	301	POP	P1-O1	2.27	1.57	1.50
2	C	301	POP	P2-O6	-2.03	1.47	1.54

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	POP	O2-P1-O	5.00	121.41	104.64
2	C	301	POP	O3-P1-O2	4.15	123.49	107.64
2	D	301	POP	O6-P2-O	3.77	117.29	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	POP	O3-P1-O	3.65	116.87	104.64
2	B	301	POP	O6-P2-O	3.53	116.47	104.64

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	POP	P2-O-P1-O3
2	D	301	POP	P1-O-P2-O6
2	B	301	POP	P1-O-P2-O5
2	D	301	POP	P1-O-P2-O5
2	D	301	POP	P1-O-P2-O4

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	POP	1	0
2	B	301	POP	2	0
2	D	301	POP	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, 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	226/253 (89%)	0.31	7 (3%)	49	39	65, 85, 105, 112	0
1	B	226/253 (89%)	0.26	9 (3%)	38	28	65, 85, 104, 111	0
1	C	226/253 (89%)	0.24	8 (3%)	44	34	65, 85, 105, 111	0
1	D	226/253 (89%)	0.16	8 (3%)	44	34	65, 85, 104, 112	0
All	All	904/1012 (89%)	0.24	32 (3%)	44	34	65, 85, 105, 112	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	198	GLY	5.2
1	C	95	LEU	4.1
1	A	108	LYS	3.9
1	D	112	TRP	3.8
1	A	3	LEU	3.7

### 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 carbohydrates 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
2	POP	C	301	9/9	0.92	0.12	92,94,98,99	0
2	POP	B	301	9/9	0.93	0.10	89,89,92,92	0
2	POP	D	301	9/9	0.95	0.12	83,86,87,88	0
2	POP	A	301	9/9	0.96	0.11	89,90,91,92	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.