



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:17 PM UTC

PDB ID : 6YMU / pdb_00006ymu
Title : Imidazole Glycerol Phosphate Synthase
Authors : Sterner, R.; Rajendran, C.; Andrea, K.
Deposited on : 2020-04-09
Resolution : 2.11 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

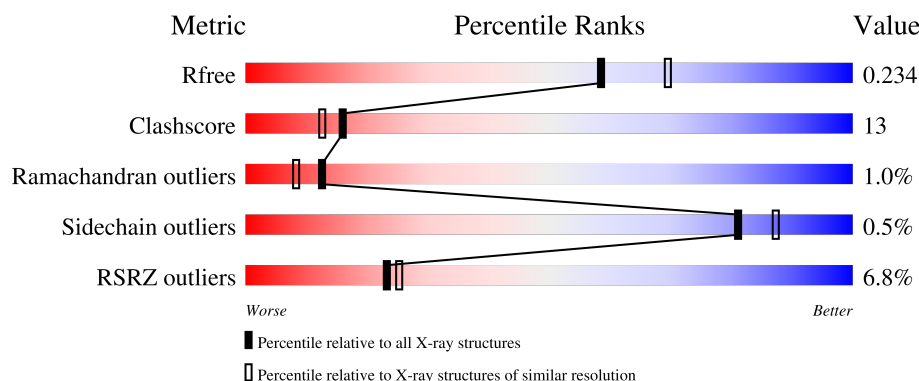
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	253	7% 75% 22% .
1	C	253	7% 74% 23% ..
1	E	253	7% 72% 23% ..
2	B	201	2% 82% 17%
2	D	201	% 79% 20% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	201	16% 69% 28% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10918 atoms, of which 14 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 Imidazole glycerol phosphate synthase subunit HisF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1867	1191	314	356	6			
1	C	251	Total	C	N	O	S	0	1	0
			1911	1218	319	368	6			
1	E	246	Total	C	N	O	S	0	1	0
			1875	1193	317	359	6			

- Molecule 2 is a protein called Imidazole glycerol phosphate synthase subunit HisH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	200	Total	C	H	N	O	S	0	0
			1625	1029	14	281	293	8		
2	D	200	Total	C	N	O	S	0	0	0
			1614	1030	282	294	8			
2	F	199	Total	C	N	O	S	0	0	0
			1581	1013	270	290	8			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	123	OZW	TRP	conflict	UNP Q9X0C8
D	123	OZW	TRP	conflict	UNP Q9X0C8
F	123	OZW	TRP	conflict	UNP Q9X0C8

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	88	Total	O	0	0
			88	88		
3	B	103	Total	O	0	0
			103	103		

Continued on next page...

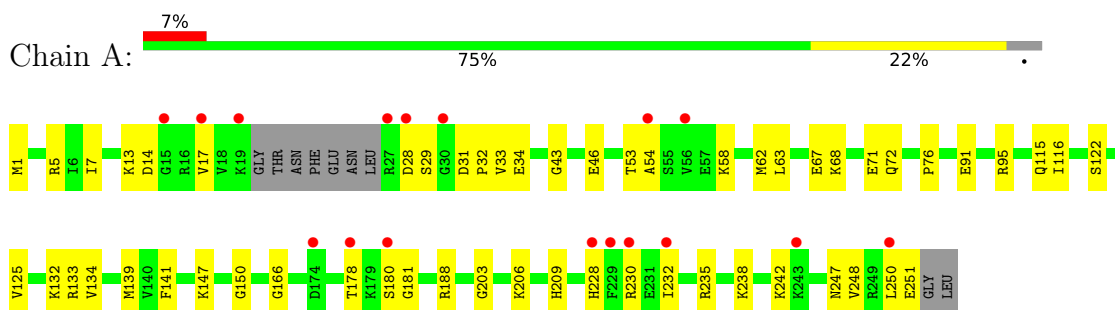
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	67	Total 67	O 67	0	0
3	D	104	Total 104	O 104	0	0
3	E	37	Total 37	O 37	0	0
3	F	46	Total 46	O 46	0	0

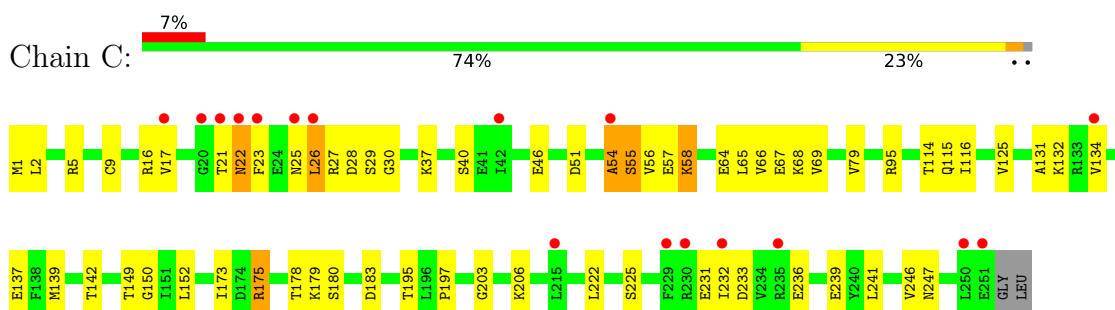
3 Residue-property plots [i](#)

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.

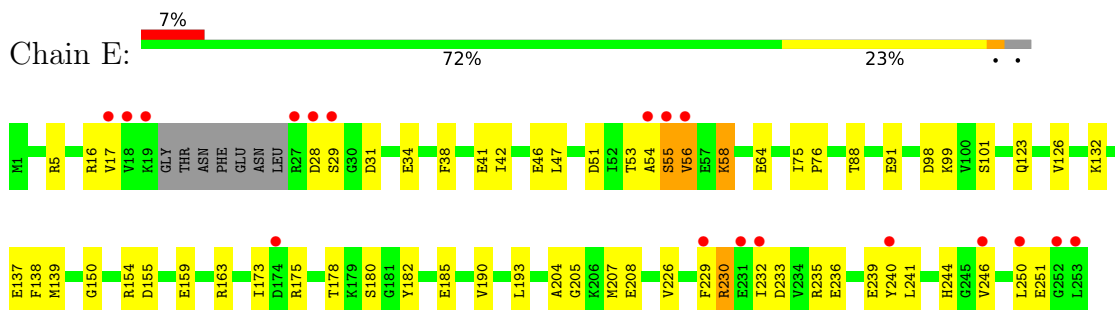
- Molecule 1: Imidazole glycerol phosphate synthase subunit HisF



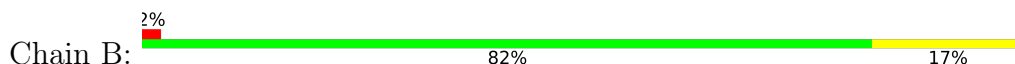
- Molecule 1: Imidazole glycerol phosphate synthase subunit HisF

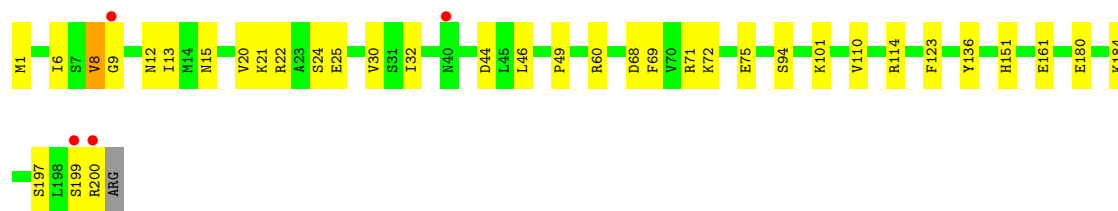


- Molecule 1: Imidazole glycerol phosphate synthase subunit HisF

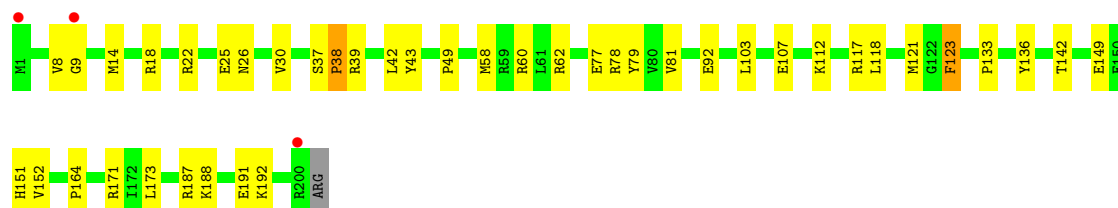
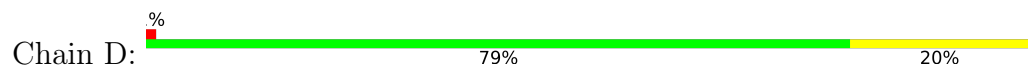


- Molecule 2: Imidazole glycerol phosphate synthase subunit HisH

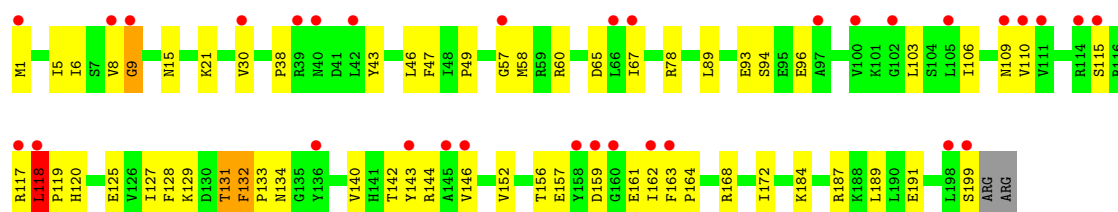




- Molecule 2: Imidazole glycerol phosphate synthase subunit HisH



- Molecule 2: Imidazole glycerol phosphate synthase subunit HisH



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.42Å 85.90Å 128.75Å 90.00° 108.24° 90.00°	Depositor
Resolution (Å)	40.00 – 2.11 40.00 – 2.11	Depositor EDS
% Data completeness (in resolution range)	99.0 (40.00-2.11) 93.3 (40.00-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.17	Depositor
R, R_{free}	0.210 , 0.250 (Not available) , 0.234	Depositor DCC
R_{free} test set	4786 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10918	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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

5.1 Standard geometry

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

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	0.33	0/1892	0.56	0/2551
1	C	0.54	2/1938 (0.1%)	0.69	6/2618 (0.2%)
1	E	0.50	0/1900	0.62	2/2565 (0.1%)
2	B	0.47	0/1623	0.60	0/2181
2	D	0.52	1/1626 (0.1%)	0.62	1/2185 (0.0%)
2	F	0.53	1/1593 (0.1%)	0.68	6/2145 (0.3%)
All	All	0.49	4/10572 (0.0%)	0.63	15/14245 (0.1%)

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
2	B	0	1
2	D	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	118	LEU	CA-C	-5.58	1.45	1.52
1	C	58	LYS	C-O	-5.36	1.18	1.24
1	C	175	ARG	C-O	-5.15	1.17	1.24
2	D	39	ARG	CA-C	-5.15	1.46	1.53

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	118	LEU	CA-C-N	8.20	130.09	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	118	LEU	C-N-CA	8.20	130.09	119.84
2	F	117	ARG	N-CA-C	-8.12	88.88	107.48
1	C	26	LEU	N-CA-C	6.97	120.78	110.46
1	C	25	ASN	N-CA-C	6.65	124.97	110.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	8	VAL	Peptide
2	D	38	PRO	Mainchain

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	1867	0	1904	46	0
1	C	1911	0	1919	59	0
1	E	1875	0	1888	56	0
2	B	1611	14	1586	32	0
2	D	1614	0	1589	34	0
2	F	1581	0	1538	56	0
3	A	88	0	0	10	0
3	B	103	0	0	4	0
3	C	67	0	0	12	0
3	D	104	0	0	10	0
3	E	37	0	0	7	0
3	F	46	0	0	14	0
All	All	10904	14	10424	275	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 13.

The worst 5 of 275 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)
2:F:118:LEU:HB3	2:F:119:PRO:CD	1.07	1.47
2:F:118:LEU:CB	2:F:119:PRO:HD3	1.29	1.40
2:F:118:LEU:CB	2:F:119:PRO:CD	1.90	1.11
1:E:230:ARG:HG2	1:E:230:ARG:HH11	1.20	1.03
1:C:16:ARG:NH1	3:C:301:HOH:O	1.91	1.02

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	240/253 (95%)	229 (95%)	9 (4%)	2 (1%)	16	12
1	C	250/253 (99%)	236 (94%)	12 (5%)	2 (1%)	16	12
1	E	243/253 (96%)	229 (94%)	12 (5%)	2 (1%)	16	12
2	B	197/201 (98%)	187 (95%)	9 (5%)	1 (0%)	24	22
2	D	197/201 (98%)	189 (96%)	7 (4%)	1 (0%)	24	22
2	F	196/201 (98%)	178 (91%)	13 (7%)	5 (3%)	4	1
All	All	1323/1362 (97%)	1248 (94%)	62 (5%)	13 (1%)	12	8

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	54	ALA
2	F	118	LEU
1	C	55	SER
2	F	131	THR
1	A	28	ASP

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	198/208 (95%)	198 (100%)	0	100	100
1	C	200/208 (96%)	197 (98%)	3 (2%)	57	65
1	E	196/208 (94%)	193 (98%)	3 (2%)	57	65
2	B	173/176 (98%)	173 (100%)	0	100	100
2	D	174/176 (99%)	174 (100%)	0	100	100
2	F	168/176 (96%)	168 (100%)	0	100	100
All	All	1109/1152 (96%)	1103 (100%)	6 (0%)	81	87

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	56	VAL
1	E	58	LYS
1	E	230	ARG
1	C	55	SER
1	C	22	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	HIS
2	D	151	HIS
1	E	115	GLN
1	E	118	GLN
2	F	53	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

3 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$
2	OZW	D	123	2	19,20,21	0.76	0	20,25,27	1.17	2 (10%)
2	OZW	B	123	2	19,20,21	0.73	0	20,25,27	0.87	1 (5%)
2	OZW	F	123	2	19,20,21	0.68	0	20,25,27	0.93	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
2	OZW	D	123	2	-	1/10/11/13	0/2/2/2
2	OZW	B	123	2	-	2/10/11/13	0/2/2/2
2	OZW	F	123	2	-	3/10/11/13	0/2/2/2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	123	OZW	CD2-CG-CD1	2.59	122.08	118.23
2	B	123	OZW	CD2-CG-CD1	2.09	121.34	118.23
2	D	123	OZW	CB-CG-CD2	-2.00	117.17	120.90

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	123	OZW	CE1-CZ-N2-N1
2	F	123	OZW	CE2-CZ-N2-N1
2	F	123	OZW	C6-N1-N2-CZ

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	123	OZW	C1-C6-N1-N2
2	D	123	OZW	C1-C6-N1-N2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	123	OZW	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	123:OZW	C	124:ASN	N	1.05

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	244/253 (96%)	0.54	17 (6%) 22 24	27, 46, 72, 90	0
1	C	251/253 (99%)	0.65	17 (6%) 23 25	21, 50, 75, 96	1 (0%)
1	E	246/253 (97%)	0.75	18 (7%) 21 23	20, 53, 82, 101	1 (0%)
2	B	199/201 (99%)	0.08	4 (2%) 65 68	30, 39, 58, 85	0
2	D	199/201 (99%)	0.04	3 (1%) 72 74	29, 39, 55, 86	0
2	F	198/201 (98%)	1.07	32 (16%) 4 5	39, 61, 85, 90	0
All	All	1337/1362 (98%)	0.53	91 (6%) 23 25	20, 48, 77, 101	2 (0%)

The worst 5 of 91 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	229	PHE	4.7
1	E	54	ALA	4.3
1	A	27	ARG	4.2
2	B	9	GLY	4.2
2	F	146	VAL	4.2

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, 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(Å ²)	Q<0.9
2	OZW	F	123	19/20	0.92	0.12	45,48,55,55	0
2	OZW	D	123	19/20	0.93	0.11	35,41,48,49	0
2	OZW	B	123	19/20	0.96	0.06	34,40,48,52	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.