



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 10:53 AM UTC

PDB ID : 3FEM / pdb_00003fem
Title : Structure of the synthase subunit Pdx1.1 (Snz1) of PLP synthase from *Saccharomyces cerevisiae*
Authors : Strohmeier, M.; Windeisen, V.; Sinning, I.; Tews, I.
Deposited on : 2008-11-30
Resolution : 3.02 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
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

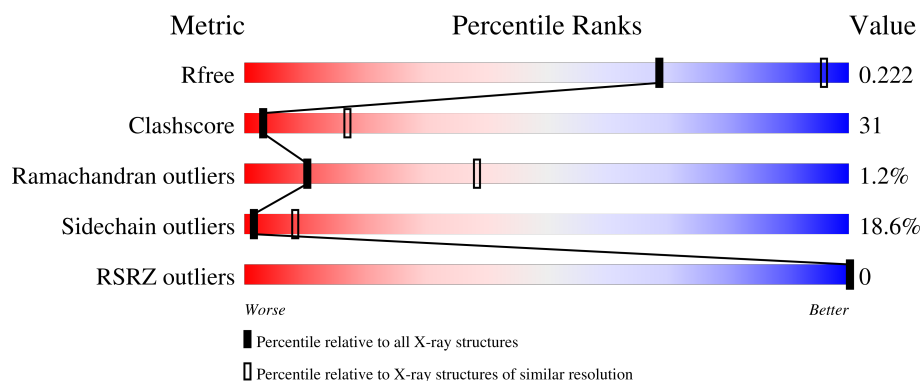
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.02 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	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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	297	
1	B	297	
1	C	297	
1	D	297	
1	E	297	

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Mol	Chain	Length	Quality of chain
1	F	297	45% 40% 9% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12600 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 Pyridoxine biosynthesis protein SNZ1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2099	1319	357	406	17			
1	B	281	Total	C	N	O	S	0	0	0
			2099	1319	357	406	17			
1	C	281	Total	C	N	O	S	0	0	0
			2099	1319	357	406	17			
1	D	281	Total	C	N	O	S	0	0	0
			2099	1319	357	406	17			
1	E	281	Total	C	N	O	S	0	0	0
			2099	1319	357	406	17			
1	F	281	Total	C	N	O	S	0	0	0
			2099	1319	357	406	17			

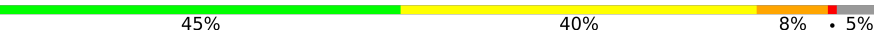
- Molecule 2 is water.

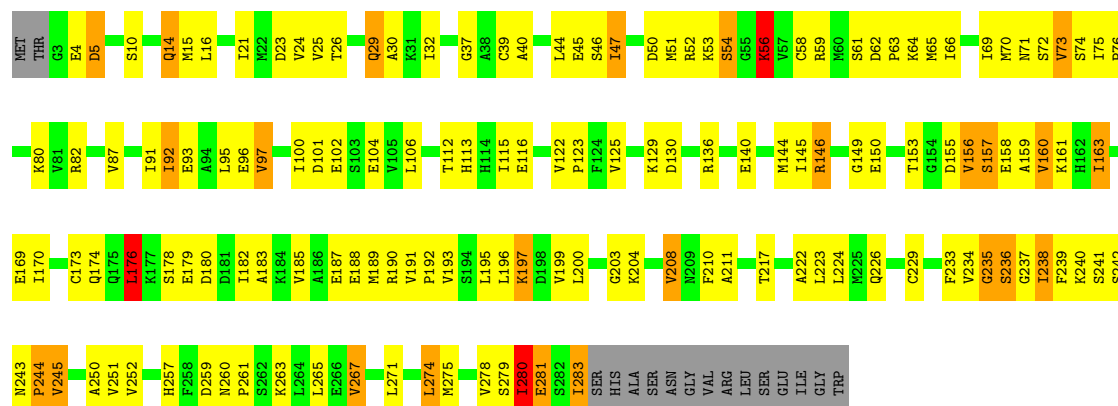
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O	0	0
			1	1		
2	B	1	Total	O	0	0
			1	1		
2	C	1	Total	O	0	0
			1	1		
2	D	1	Total	O	0	0
			1	1		
2	E	1	Total	O	0	0
			1	1		
2	F	1	Total	O	0	0
			1	1		

3 Residue-property plots

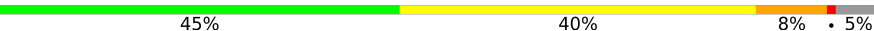
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

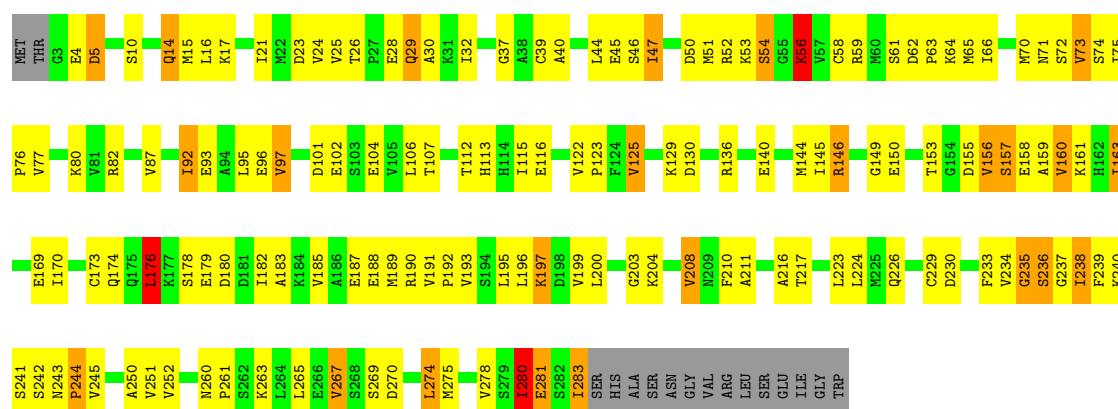
• Molecule 1: Pyridoxine biosynthesis protein SNZ1

Chain A: 

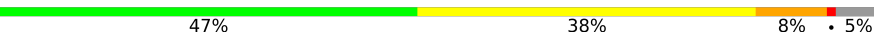


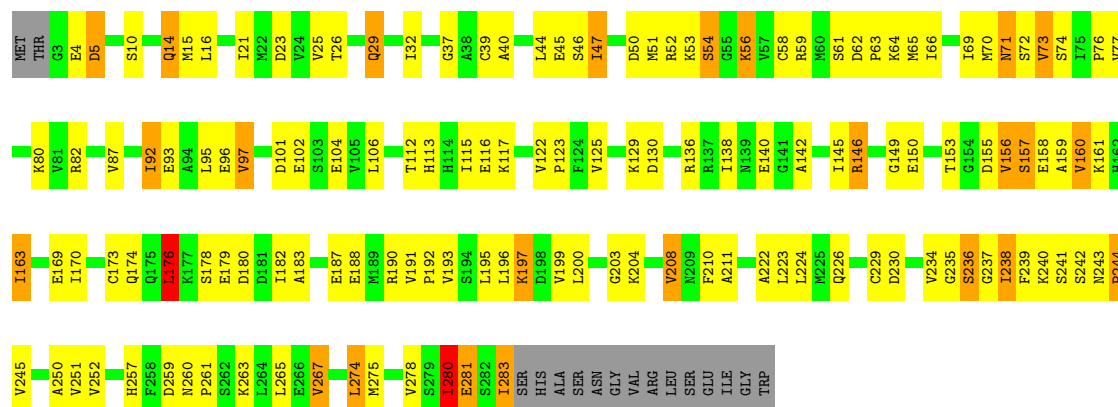
• Molecule 1: Pyridoxine biosynthesis protein SNZ1

Chain B: 



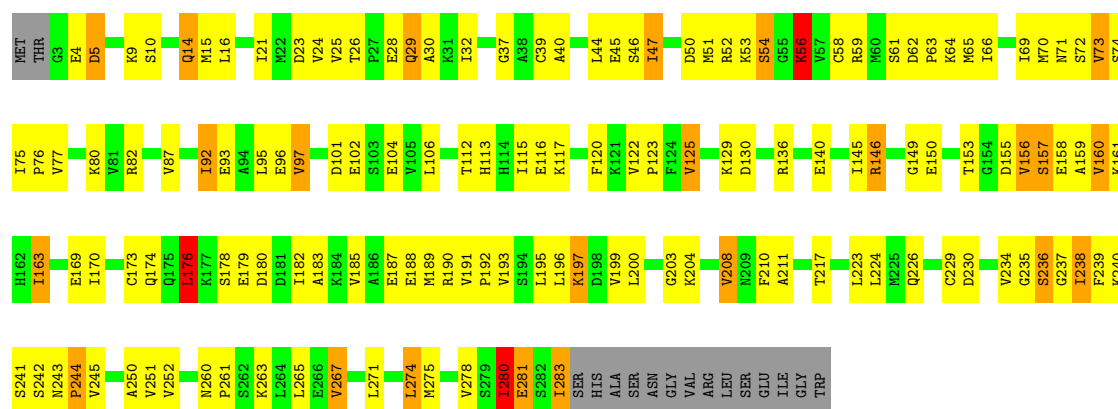
• Molecule 1: Pyridoxine biosynthesis protein SNZ1

Chain C: 



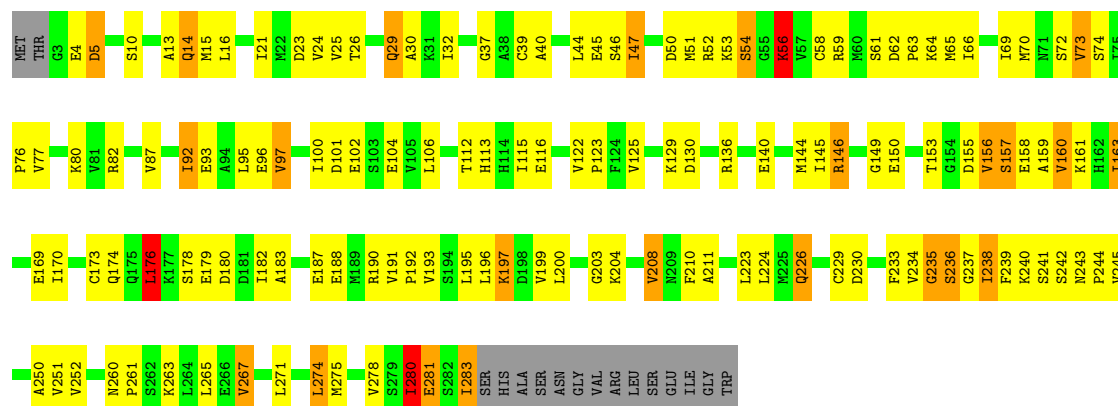
• Molecule 1: Pyridoxine biosynthesis protein SNZ1

Chain D: 46% 40% 8% • 5%



• Molecule 1: Pyridoxine biosynthesis protein SNZ1

Chain E: 47% 38% 8% • 5%



• Molecule 1: Pyridoxine biosynthesis protein SNZ1

Chain F: 45% 40% 9% • 5%

G237	I238	F239	K240	S241	S242	N243	P244	V245	A250	V251	V252	N260	P261	S262	K263	L264	L265	E266	V267	L274	M275	V278	S279	I280	E281	S282	I283	SER	HIS	ALA	ALA	SER	SER	ASN	GLY	GLY	VAL	ARG	LEU	SER	GLU	ILE	GLY	GLY	TRP							
V160	K161	H162	I163	E169	I170	C173	Q174	Q175	Q176	K177	S178	E179	D180	D181	I182	A183	K184	V185	A186	E187	E188	M189	R190	V191	P192	V193	S194	L195	L196	K197	D198	V199	L200	G203	K204	V208	N209	F210	A211	T217	A222	L223	L224	N225	Q226	C229	D230	F233	V234	G235	S236	
S74	I75	P76	V77	K80	H81	R82	V87	I92	E93	A94	L95	E96	V97	D101	E102	S103	E104	V105	L106	T112	H113	H114	I115	E116	K117	F120	K121	V122	P123	F124	V125	K129	D130	R136	E140	M144	I145	R146	G149	E150	T153	G154	D155	V156	S157	E158	A159					
MET	THR	G3	E4	D5	K9	Q14	M15	L16	I21	M22	D23	V24	V25	T26	P27	E28	Q29	A30	K31	I32	K35	S36	G37	A38	C39	A40	L44	E45	S46	I47	D50	M51	R52	K53	S54	G55	K56	V57	C58	R59	M60	S61	D62	P63	K64	M65	I66	I69	M70	N71	S72	V73

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	154.07Å 154.22Å 154.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.02 20.00 – 3.03	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-3.02) 99.2 (20.00-3.03)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 3.04Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.162 , 0.181 0.223 , 0.222	Depositor DCC
R_{free} test set	2009 reflections (2.81%)	wwPDB-VP
Wilson B-factor (Å ²)	71.4	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.149 for -h,l,k 0.149 for -l,-k,-h 0.149 for k,h,-l 0.348 for k,l,h 0.348 for l,h,k	Xtriage
Reported twinning fraction	0.470 for H,K,L 0.298 for K,-L,-H 0.231 for -L,-H,K	Depositor
Outliers	0 of 71521 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12600	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% 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

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	0.65	0/2125	0.94	3/2861 (0.1%)
1	B	0.70	0/2125	0.96	3/2861 (0.1%)
1	C	0.67	0/2125	0.95	1/2861 (0.0%)
1	D	0.71	0/2125	0.96	2/2861 (0.1%)
1	E	0.65	0/2125	0.94	3/2861 (0.1%)
1	F	0.69	0/2125	0.96	3/2861 (0.1%)
All	All	0.68	0/12750	0.95	15/17166 (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
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	6

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	197	LYS	N-CA-C	6.13	117.63	111.07
1	A	197	LYS	N-CA-C	6.12	117.95	111.28
1	C	197	LYS	N-CA-C	6.05	117.87	111.28
1	F	197	LYS	N-CA-C	5.87	117.35	111.07
1	E	197	LYS	N-CA-C	5.86	117.66	111.28

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	176	LEU	Peptide
1	B	176	LEU	Peptide
1	C	176	LEU	Peptide
1	D	176	LEU	Peptide
1	E	176	LEU	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	2099	0	2162	142	0
1	B	2099	0	2162	141	1
1	C	2099	0	2162	131	0
1	D	2099	0	2162	137	0
1	E	2099	0	2162	140	0
1	F	2099	0	2162	138	1
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
2	E	1	0	0	0	0
2	F	1	0	0	0	0
All	All	12600	0	12972	805	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 31.

The worst 5 of 805 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:173:CYS:O	1:B:176:LEU:HD22	1.29	1.32
1:F:173:CYS:O	1:F:176:LEU:HD22	1.31	1.29
1:D:173:CYS:O	1:D:176:LEU:HD22	1.28	1.26
1:A:173:CYS:O	1:A:176:LEU:HD22	1.31	1.25
1:C:173:CYS:O	1:C:176:LEU:HD22	1.29	1.23

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:76:PRO:CD	1:F:35:LYS:NZ[3_655]	2.05	0.15

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	279/297 (94%)	242 (87%)	33 (12%)	4 (1%)	9	34
1	B	279/297 (94%)	239 (86%)	37 (13%)	3 (1%)	11	41
1	C	279/297 (94%)	241 (86%)	35 (12%)	3 (1%)	11	41
1	D	279/297 (94%)	242 (87%)	34 (12%)	3 (1%)	11	41
1	E	279/297 (94%)	238 (85%)	38 (14%)	3 (1%)	11	41
1	F	279/297 (94%)	240 (86%)	35 (12%)	4 (1%)	9	34
All	All	1674/1782 (94%)	1442 (86%)	212 (13%)	20 (1%)	10	38

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	SER
1	B	236	SER
1	C	236	SER
1	D	236	SER
1	E	236	SER

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	229/242 (95%)	187 (82%)	42 (18%)	2	9
1	B	229/242 (95%)	186 (81%)	43 (19%)	1	8
1	C	229/242 (95%)	186 (81%)	43 (19%)	1	8
1	D	229/242 (95%)	185 (81%)	44 (19%)	1	8
1	E	229/242 (95%)	188 (82%)	41 (18%)	2	9
1	F	229/242 (95%)	186 (81%)	43 (19%)	1	8
All	All	1374/1452 (95%)	1118 (81%)	256 (19%)	1	8

5 of 256 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	145	ILE
1	F	178	SER
1	C	74	SER
1	C	56	LYS
1	F	204	LYS

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

Mol	Chain	Res	Type
1	E	243	ASN
1	F	257	HIS
1	E	257	HIS
1	F	139	ASN
1	C	90	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 [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](#)

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	281/297 (94%)	-1.70	0 100 100	7, 39, 56, 67	0
1	B	281/297 (94%)	-1.63	0 100 100	7, 39, 56, 67	0
1	C	281/297 (94%)	-1.61	0 100 100	7, 39, 56, 67	0
1	D	281/297 (94%)	-1.56	0 100 100	7, 39, 56, 67	0
1	E	281/297 (94%)	-1.61	0 100 100	7, 39, 56, 67	0
1	F	281/297 (94%)	-1.65	0 100 100	7, 39, 56, 67	0
All	All	1686/1782 (94%)	-1.63	0 100 100	7, 39, 57, 67	0

There are no RSRZ outliers to report.

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.