



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 09:29 AM UTC

PDB ID : 2VHI / pdb_00002vhi
Title : Crystal structure of a pyrimidine degrading enzyme from *Drosophila melanogaster*
Authors : Lundgren, S.; Lohkamp, B.; Andersen, B.; Piskur, J.; Dobritzsch, D.
Deposited on : 2007-11-21
Resolution : 3.30 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

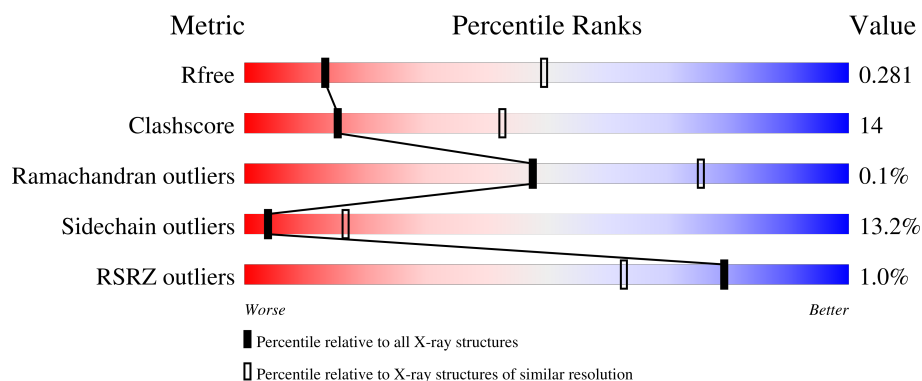
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	405	2% 52% 29% 5% 14%
1	B	405	59% 30% 6%
1	C	405	59% 31% 6%
1	D	405	60% 28% 6% 6%
1	E	405	2% 60% 29% 6%

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Mol	Chain	Length	Quality of chain
1	F	405	63%26%•6%
1	G	405	61%28%••6%
1	H	405	% 54%26%•16%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23689 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.

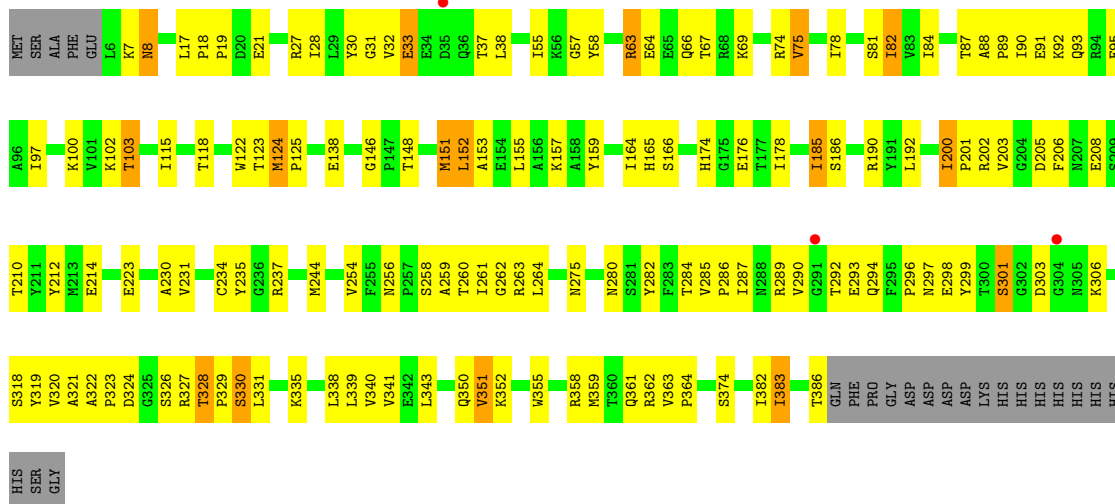
- Molecule 1 is a protein called CG3027-PA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	1	0
			2774	1756	487	516	15			
1	B	379	Total	C	N	O	S	0	0	0
			3027	1916	530	565	16			
1	C	381	Total	C	N	O	S	0	0	0
			3044	1928	533	567	16			
1	D	379	Total	C	N	O	S	0	0	0
			3027	1916	530	565	16			
1	E	380	Total	C	N	O	S	0	0	0
			3036	1922	532	566	16			
1	F	379	Total	C	N	O	S	0	0	0
			3027	1916	530	565	16			
1	G	381	Total	C	N	O	S	0	0	0
			3044	1928	533	567	16			
1	H	342	Total	C	N	O	S	0	0	0
			2710	1712	478	505	15			

HIS
HIS
HIS
HIS
HIS
HIS
SER
GLY

• Molecule 1: CG3027-PA

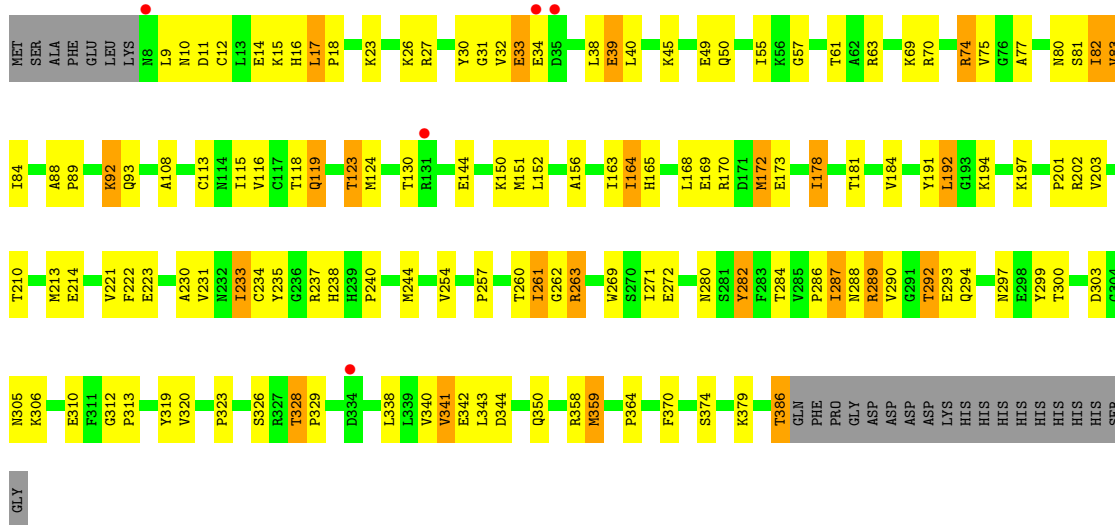
Chain C:  %



HIS
SER
GLY

• Molecule 1: CG3027-PA

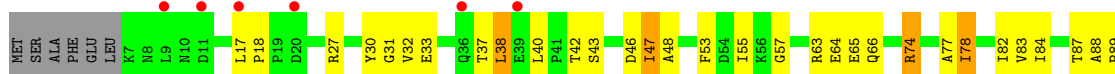
Chain D:  %

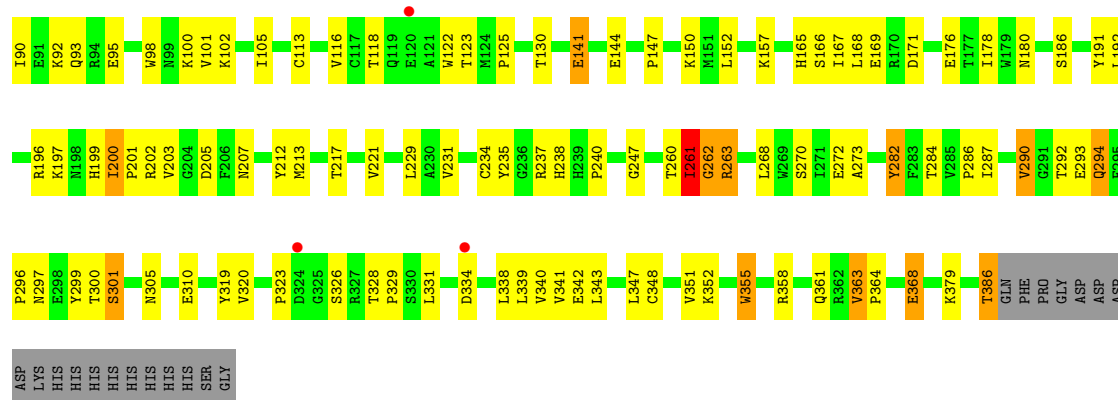


GLY

• Molecule 1: CG3027-PA

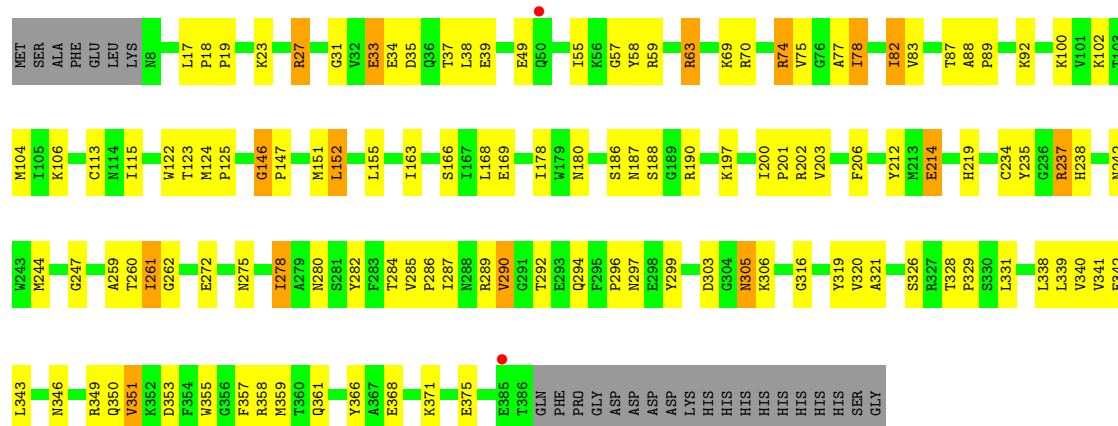
Chain E:  %





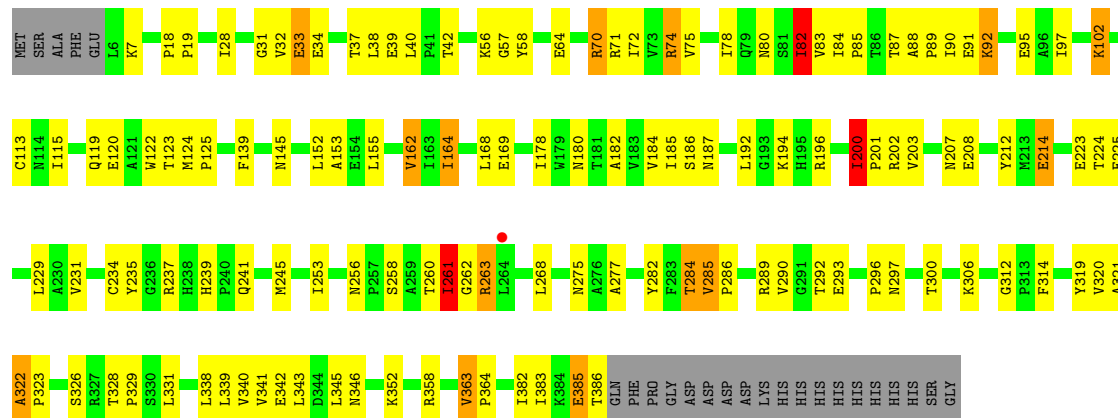
• Molecule 1: CG3027-PA

Chain F: 63% 26% 6%



• Molecule 1: CG3027-PA

Chain G: 61% 28% 6%



• Molecule 1: CG3027-PA

Chain H: 54% 26% 16%

1382	PHE	GLY	N99	MET
1383	PRO	ASP	K100	SER
K384	ASN	PHE	V101	ALA
E385	GLU	ASN	K102	PHE
T386	THR	GLU	T103	GLU
	SER	THR	M104	LEU
	GLY	TYR	I105	LYS
	ASP	TYR	V116	N8
	GLY	M213		L9
	ASN	E214	Q119	N10
	LYS		E120	D11
	ALA	T217	A121	P18
	HIS			F19
	LYS	F222	A127	D20
	GLU	E223	PHE	E21
	GLU		CYS	L22
	PHE	V231	THR	Y30
		N232	ARG	G31
		I233	GLU	V32
	S318	C234	LYS	E33
	Y319	Y235	PHE	E34
	V320	G236	PRO	
		R237	TRP	L38
	S326	H238	C137	
	R327	H239		M51
	T328	P240	E142	
	S329	Q241		K56
	L331		M145	G57
	S332	M244	K150	Y58
	R333	N245	M151	R59
	D334		L152	
	K335	L248	A153	R63
	D336		E154	E64
		N256		K69
	L339	T260	I164	
	V340	I261		V73
	V341	G262	L168	R74
	E342	R263	E169	V75
	L343		R170	G76
		E266	D171	A77
	V351	P267	M172	I78
	K355		E173	
		E272	H174	S81
	T360	A273	G176	I82
			E176	V83
	V363	N280		I84
		S281	A182	
	S369	Y282	V183	A88
		F283	V184	P89
	A373	T284		
	S374	V285	R190	K92
	E375	P286		Q93
	H376	I287	R196	E94
	G377	N288	K197	E95
	F378	R289		A96
	K379	V290	P201	I97
	P380		ARG	
	Q381	Q294	VAL	W98

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	278.86Å 95.05Å 199.31Å 90.00° 125.82° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 30.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	85.6 (30.00-3.30) 85.4 (30.00-3.30)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.226 , 0.282 0.229 , 0.281	Depositor DCC
R_{free} test set	2766 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	45.8	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	23689	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.82% 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	0.60	1/2835 (0.0%)	0.95	3/3833 (0.1%)
1	B	0.55	0/3101	0.92	5/4197 (0.1%)
1	C	0.58	0/3118	0.98	6/4219 (0.1%)
1	D	0.57	0/3101	0.92	2/4197 (0.0%)
1	E	0.59	0/3110	0.96	4/4208 (0.1%)
1	F	0.56	0/3101	0.92	4/4197 (0.1%)
1	G	0.59	0/3118	0.94	5/4219 (0.1%)
1	H	0.60	1/2768 (0.0%)	0.92	0/3742
All	All	0.58	2/24252 (0.0%)	0.94	29/32812 (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	2
1	D	0	2
1	E	0	1
1	F	0	1
1	G	0	2
1	H	0	1
All	All	0	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	363	VAL	CA-CB	5.39	1.56	1.54
1	H	363	VAL	CA-CB	5.05	1.56	1.54

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	ILE	N-CA-C	-7.88	101.46	110.05
1	A	262	GLY	N-CA-C	-6.88	101.57	110.38
1	E	262	GLY	N-CA-C	-6.80	101.22	110.20
1	G	262	GLY	N-CA-C	-6.67	101.39	110.20
1	D	305	ASN	N-CA-C	6.60	118.52	110.41

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	261	ILE	Peptide
1	B	261	ILE	Peptide
1	C	261	ILE	Peptide
1	C	82	ILE	Peptide
1	D	82	ILE	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	2774	0	2738	89	0
1	B	3027	0	2958	93	0
1	C	3044	0	2982	95	0
1	D	3027	0	2958	91	0
1	E	3036	0	2971	85	0
1	F	3027	0	2958	72	0
1	G	3044	0	2982	83	0
1	H	2710	0	2678	92	0
All	All	23689	0	23225	634	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 14.

The worst 5 of 634 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:63:ARG:HG3	1:C:350:GLN:OE1	1.58	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ARG:HB2	1:B:63:ARG:HH11	1.17	1.04
1:A:172:MET:HE3	1:A:176:GLU:HG2	1.42	1.01
1:H:197:LYS:HA	1:H:233:ILE:HD13	1.42	1.01
1:G:87:THR:HG22	1:G:296:PRO:HG3	1.43	0.97

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	341/405 (84%)	317 (93%)	24 (7%)	0	100	100
1	B	377/405 (93%)	363 (96%)	14 (4%)	0	100	100
1	C	379/405 (94%)	362 (96%)	17 (4%)	0	100	100
1	D	377/405 (93%)	362 (96%)	14 (4%)	1 (0%)	36	65
1	E	378/405 (93%)	360 (95%)	18 (5%)	0	100	100
1	F	377/405 (93%)	360 (96%)	17 (4%)	0	100	100
1	G	379/405 (94%)	362 (96%)	16 (4%)	1 (0%)	36	65
1	H	334/405 (82%)	313 (94%)	20 (6%)	1 (0%)	36	65
All	All	2942/3240 (91%)	2799 (95%)	140 (5%)	3 (0%)	48	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	234	CYS
1	D	83	VAL
1	G	83	VAL

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	297/346 (86%)	257 (86%)	40 (14%)	4	16
1	B	323/346 (93%)	281 (87%)	42 (13%)	4	17
1	C	325/346 (94%)	282 (87%)	43 (13%)	4	17
1	D	323/346 (93%)	280 (87%)	43 (13%)	4	17
1	E	324/346 (94%)	278 (86%)	46 (14%)	3	14
1	F	323/346 (93%)	286 (88%)	37 (12%)	5	21
1	G	325/346 (94%)	281 (86%)	44 (14%)	4	16
1	H	290/346 (84%)	251 (87%)	39 (13%)	4	16
All	All	2530/2768 (91%)	2196 (87%)	334 (13%)	4	17

5 of 334 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	123	THR
1	G	282	TYR
1	F	237	ARG
1	G	56	LYS
1	H	51	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	66	GLN
1	F	308	HIS
1	E	239	HIS
1	F	51	ASN
1	G	180	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	348/405 (85%)	0.02	5 (1%) 73 55	18, 40, 65, 70	1 (0%)
1	B	379/405 (93%)	-0.02	0 100 100	23, 40, 62, 70	0
1	C	381/405 (94%)	0.14	3 (0%) 82 68	23, 40, 63, 70	0
1	D	379/405 (93%)	0.16	5 (1%) 75 56	23, 40, 62, 70	0
1	E	380/405 (93%)	0.19	9 (2%) 59 40	23, 40, 63, 70	0
1	F	379/405 (93%)	0.13	2 (0%) 87 76	23, 40, 62, 70	0
1	G	381/405 (94%)	0.02	1 (0%) 90 82	23, 40, 63, 70	0
1	H	342/405 (84%)	0.06	4 (1%) 76 58	23, 39, 63, 70	0
All	All	2969/3240 (91%)	0.09	29 (0%) 79 63	18, 40, 64, 70	1 (0%)

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	213	MET	3.7
1	C	304	GLY	3.1
1	E	334	ASP	3.1
1	F	50	GLN	3.1
1	C	291	GLY	3.0

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.