



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:58 AM GMT

PDB ID : 2VHH  
Title : CRYSTAL STRUCTURE OF A PYRIMIDINE DEGRADING ENZYME  
FROM DROSOPHILA MELANOGASTER  
Authors : Lundgren, S.; Lohkamp, B.; Andersen, B.; Piskur, J.; Dobritsch, D.  
Deposited on : 2007-11-21  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

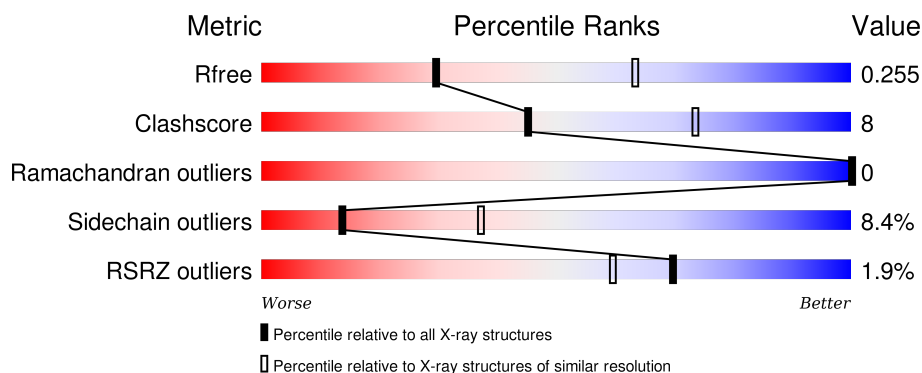
# 1 Overall quality at a glance

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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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. 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	<div> <div>4%</div> <div>65% 18% • 15%</div> </div>
1	B	405	<div> <div>%</div> <div>71% 20% • 6%</div> </div>
1	C	405	<div> <div>73% 19% • 6%</div> </div>
1	D	405	<div> <div>%</div> <div>75% 17% • 6%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11865 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.

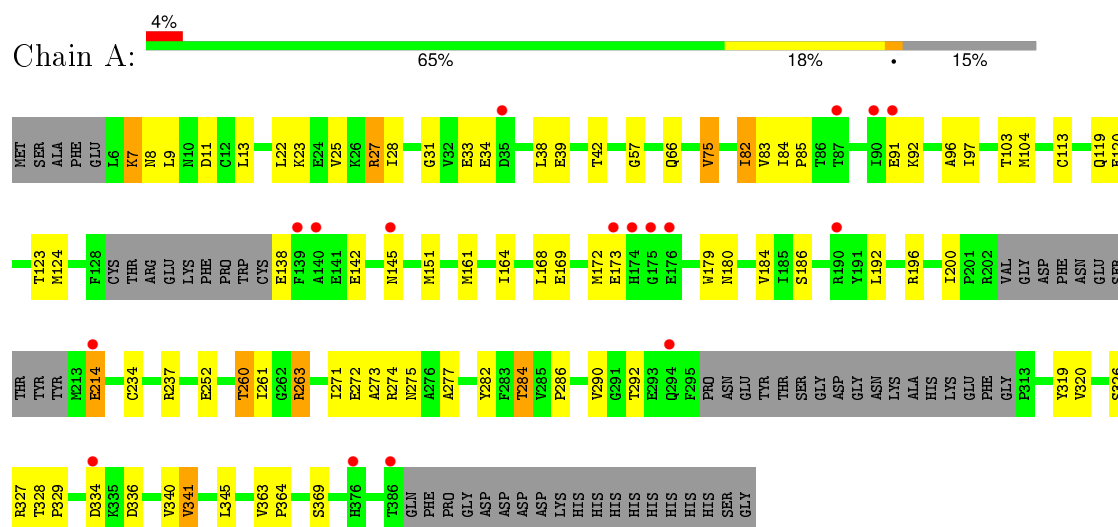
- Molecule 1 is a protein called CG3027-PA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	0	0
			2750	1743	485	508	14			
1	B	379	Total	C	N	O	S	0	0	0
			3027	1916	530	565	16			
1	C	382	Total	C	N	O	S	0	1	0
			3061	1937	536	572	16			
1	D	379	Total	C	N	O	S	0	0	0
			3027	1916	530	565	16			

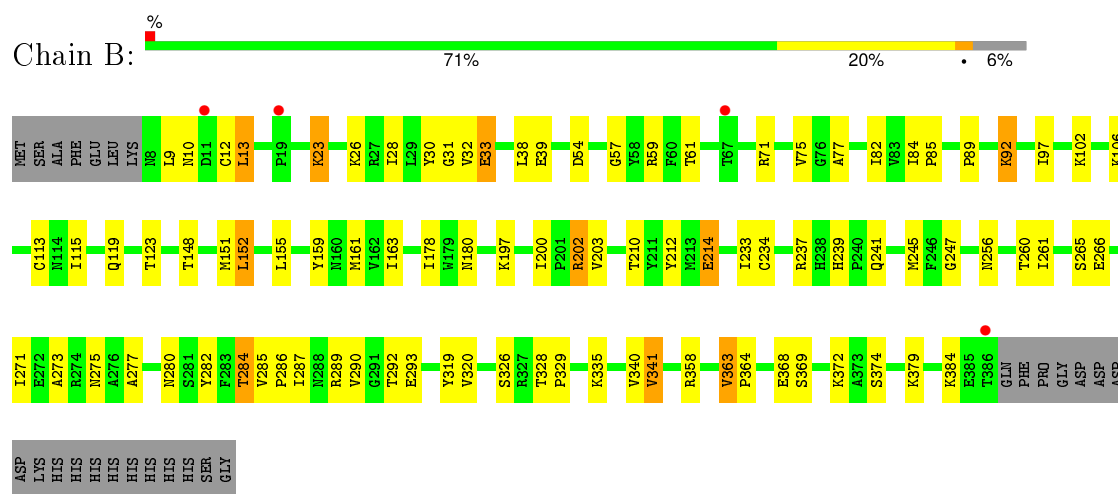
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

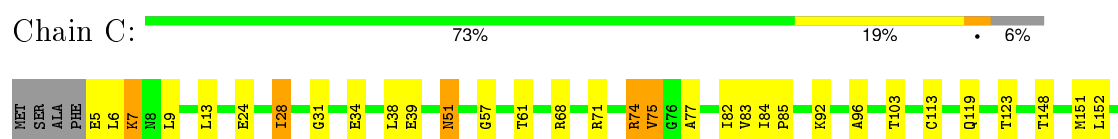
#### • Molecule 1: CG3027-PA

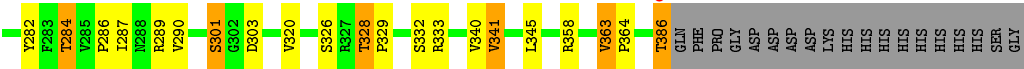


#### • Molecule 1: CG3027-PA

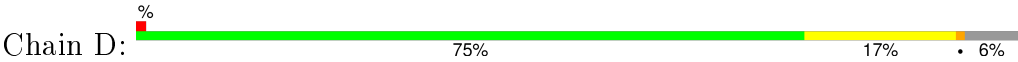


#### • Molecule 1: CG3027-PA





● Molecule 1: CG3027-PA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.04Å 197.88Å 97.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.80 56.16 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.8 (35.00-2.80) 94.8 (56.16-2.80)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.215 , 0.255 0.217 , 0.255	Depositor DCC
$R_{free}$ test set	2235 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.1	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 23.8	EDS
Estimated twinning fraction	0.025 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 43921 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11865	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.49	0/2810	0.59	0/3796
1	B	0.45	0/3101	0.62	0/4197
1	C	0.43	0/3135	0.62	0/4242
1	D	0.46	0/3101	0.59	0/4197
All	All	0.46	0/12147	0.61	0/16432

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	2
1	B	0	1
1	C	0	2
1	D	0	1
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	261	ILE	Peptide
1	A	82	ILE	Peptide
1	B	261	ILE	Peptide
1	C	261	ILE	Peptide
1	C	82	ILE	Peptide
1	D	261	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	2750	0	2726	53	0
1	B	3027	0	2958	56	0
1	C	3061	0	2993	51	0
1	D	3027	0	2958	41	0
All	All	11865	0	11635	183	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 8.

All (183) 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:A:82:ILE:HG12	1:A:83:VAL:H	1.32	0.95
1:C:205:ASP:OD1	1:C:301:SER:HB3	1.70	0.90
1:B:320:VAL:HG21	1:B:341:VAL:HG11	1.60	0.83
1:C:84:ILE:HB	1:C:85:PRO:HD2	1.64	0.79
1:D:84:ILE:HB	1:D:85:PRO:HD2	1.66	0.78
1:C:320:VAL:HG21	1:C:341:VAL:HG11	1.67	0.77
1:A:328:THR:HG22	1:A:329:PRO:O	1.87	0.74
1:B:84:ILE:HB	1:B:85:PRO:HD2	1.71	0.73
1:A:82:ILE:HG12	1:A:83:VAL:N	2.05	0.70
1:B:363:VAL:HG23	1:B:364:PRO:HD3	1.73	0.69
1:C:74:ARG:HB3	1:C:113:CYS:HA	1.74	0.68
1:D:320:VAL:HG21	1:D:341:VAL:HG11	1.76	0.67
1:C:200:ILE:HD13	1:C:214:GLU:HA	1.77	0.65
1:B:23:LYS:HG3	1:B:33:GLU:HB2	1.79	0.65
1:A:234:CYS:O	1:A:237:ARG:HB2	1.97	0.64
1:D:284:THR:HG22	1:D:286:PRO:HD3	1.81	0.63
1:A:273:ALA:O	1:A:284:THR:HG21	1.98	0.62
1:B:54:ASP:OD1	1:B:335:LYS:HE3	1.98	0.62
1:C:273:ALA:O	1:C:284:THR:HG21	1.98	0.62
1:A:31:GLY:HA3	1:A:326:SER:HA	1.81	0.62
1:B:280:ASN:O	1:B:358:ARG:NH1	2.33	0.62
1:C:363:VAL:HG23	1:C:364:PRO:HD3	1.81	0.62
1:C:234:CYS:O	1:C:237:ARG:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:VAL:HG11	1:D:96:ALA:HB1	1.82	0.61
1:C:275:ASN:HD22	1:D:275:ASN:CB	2.14	0.61
1:A:57:GLY:HA2	1:A:340:VAL:O	2.01	0.60
1:A:120:GLU:OE1	1:A:234:CYS:SG	2.59	0.60
1:C:31:GLY:HA3	1:C:326:SER:HA	1.83	0.60
1:B:31:GLY:HA3	1:B:326:SER:HA	1.85	0.59
1:C:164:ILE:HG12	1:C:184:VAL:HG22	1.86	0.58
1:D:31:GLY:HA3	1:D:326:SER:HA	1.85	0.58
1:D:23:LYS:HG3	1:D:33:GLU:HB2	1.86	0.58
1:B:200:ILE:HD13	1:B:214:GLU:HA	1.85	0.58
1:B:113:CYS:O	1:B:161:MET:HE2	2.04	0.57
1:C:275:ASN:HD22	1:D:275:ASN:HB3	1.70	0.57
1:A:82:ILE:HG13	1:A:97:ILE:HD11	1.85	0.57
1:A:200:ILE:HD13	1:A:214:GLU:HA	1.86	0.57
1:C:7:LYS:HE3	1:C:7:LYS:N	2.19	0.56
1:D:197:LYS:HG3	1:D:233:ILE:HB	1.87	0.56
1:A:84:ILE:HB	1:A:85:PRO:CD	2.35	0.56
1:A:272:GLU:HG2	1:B:275:ASN:HD21	1.71	0.55
1:A:83:VAL:HG11	1:A:96:ALA:HB1	1.89	0.55
1:A:28:ILE:HG22	1:B:266:GLU:HG2	1.87	0.55
1:A:271:ILE:HG22	1:B:275:ASN:HD22	1.72	0.55
1:A:33:GLU:CD	1:A:33:GLU:H	2.09	0.55
1:B:9:LEU:O	1:B:12:CYS:HB3	2.07	0.54
1:A:28:ILE:HD11	1:B:9:LEU:HD13	1.90	0.54
1:C:275:ASN:ND2	1:D:275:ASN:HB3	2.22	0.54
1:C:206:PHE:HE2	1:C:259:ALA:O	1.90	0.54
1:A:320:VAL:HG21	1:A:341:VAL:HG11	1.90	0.54
1:C:75:VAL:HG22	1:C:341:VAL:HG13	1.89	0.53
1:A:364:PRO:HG3	1:B:374:SER:HB2	1.90	0.53
1:C:119:GLN:OE1	1:C:289:ARG:HA	2.09	0.53
1:B:328:THR:HG22	1:B:329:PRO:O	2.08	0.53
1:D:273:ALA:HB1	1:D:284:THR:HG21	1.91	0.53
1:C:6:LEU:HB2	1:D:24:GLU:HG2	1.91	0.53
1:A:22:LEU:HA	1:A:25:VAL:HG12	1.90	0.52
1:B:89:PRO:HB2	1:B:92:LYS:HD2	1.91	0.52
1:C:57:GLY:HA2	1:C:340:VAL:O	2.09	0.52
1:A:272:GLU:HG2	1:B:275:ASN:ND2	2.25	0.52
1:B:286:PRO:HD2	1:B:319:TYR:O	2.10	0.52
1:A:9:LEU:HD13	1:B:28:ILE:HD11	1.92	0.52
1:D:8:ASN:HD21	1:D:10:ASN:HB3	1.75	0.52
1:A:164:ILE:HG12	1:A:184:VAL:HG22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:ASN:HD22	1:C:51:ASN:N	2.07	0.51
1:D:230:ALA:HB3	1:D:254:VAL:HG22	1.92	0.51
1:B:148:THR:O	1:B:152:LEU:HB2	2.10	0.51
1:D:33:GLU:CD	1:D:33:GLU:H	2.15	0.50
1:B:285:VAL:HG22	1:B:320:VAL:HG22	1.94	0.50
1:B:77:ALA:HB1	1:B:287:ILE:HG12	1.93	0.50
1:B:289:ARG:HD3	1:B:293:GLU:OE2	2.12	0.50
1:C:328:THR:HG22	1:C:329:PRO:O	2.12	0.50
1:D:30:TYR:CD1	1:D:30:TYR:N	2.79	0.50
1:A:8:ASN:HB3	1:A:11:ASP:HB2	1.93	0.50
1:D:57:GLY:HA2	1:D:340:VAL:O	2.11	0.50
1:B:102:LYS:HG2	1:B:155:LEU:HD11	1.94	0.49
1:D:368:GLU:OE2	1:D:372:LYS:HE2	2.12	0.49
1:A:169:GLU:HB3	1:A:179:TRP:HB2	1.94	0.49
1:A:75:VAL:HG22	1:A:341:VAL:HG13	1.95	0.49
1:A:363:VAL:HG23	1:A:364:PRO:HD3	1.95	0.49
1:A:9:LEU:O	1:A:13:LEU:HG	2.13	0.49
1:C:268:LEU:HD22	1:D:278:ILE:HD13	1.94	0.49
1:B:368:GLU:OE2	1:B:372:LYS:HE2	2.13	0.48
1:B:247:GLY:O	1:B:358:ARG:NH2	2.46	0.48
1:B:197:LYS:HG3	1:B:233:ILE:HB	1.95	0.48
1:C:214:GLU:H	1:C:214:GLU:CD	2.17	0.48
1:C:5:GLU:O	1:C:7:LYS:HE2	2.13	0.48
1:B:30:TYR:N	1:B:30:TYR:CD1	2.81	0.48
1:C:386:THR:C	1:D:190:ARG:HH22	2.16	0.48
1:B:9:LEU:HG	1:B:13:LEU:HD21	1.96	0.48
1:D:286:PRO:HD2	1:D:319:TYR:O	2.14	0.48
1:A:237:ARG:HH12	1:A:260:THR:HG21	1.78	0.47
1:D:284:THR:CG2	1:D:286:PRO:HD3	2.43	0.47
1:C:277:ALA:HB2	1:C:284:THR:HB	1.96	0.47
1:C:197:LYS:HG3	1:C:233:ILE:HB	1.95	0.47
1:B:57:GLY:HA2	1:B:340:VAL:O	2.14	0.47
1:A:273:ALA:HB1	1:A:284:THR:CG2	2.43	0.47
1:A:84:ILE:HB	1:A:85:PRO:HD2	1.97	0.47
1:B:368:GLU:HA	1:B:368:GLU:OE1	2.15	0.47
1:C:252:GLU:HB3	1:C:345:LEU:HD22	1.97	0.47
1:C:24:GLU:O	1:C:28:ILE:HG23	2.14	0.47
1:A:277:ALA:HB2	1:A:284:THR:HB	1.96	0.47
1:C:180:ASN:HB2	1:C:212:TYR:CE2	2.49	0.47
1:D:77:ALA:HB1	1:D:287:ILE:HG12	1.96	0.47
1:B:178:ILE:O	1:B:212:TYR:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:THR:CG2	1:D:329:PRO:O	2.63	0.47
1:C:7:LYS:HE3	1:C:7:LYS:H	1.79	0.46
1:B:273:ALA:HB1	1:B:284:THR:CG2	2.46	0.46
1:C:263:ARG:H	1:C:263:ARG:HD2	1.79	0.46
1:A:172:MET:HA	1:A:172:MET:HE2	1.97	0.46
1:A:275:ASN:HD22	1:B:271:ILE:HG22	1.80	0.46
1:A:263:ARG:H	1:A:263:ARG:HD2	1.81	0.46
1:D:113:CYS:O	1:D:161:MET:HE2	2.16	0.45
1:B:239:HIS:HD2	1:B:241:GLN:HE22	1.63	0.45
1:C:83:VAL:HG11	1:C:96:ALA:HB1	1.98	0.45
1:A:27:ARG:NH1	1:A:28:ILE:HG23	2.32	0.45
1:A:363:VAL:CG2	1:A:364:PRO:HD3	2.47	0.45
1:D:273:ALA:HB1	1:D:284:THR:CG2	2.47	0.44
1:C:157:LYS:HG3	1:C:188:SER:O	2.17	0.44
1:C:272:GLU:HA	1:D:275:ASN:ND2	2.33	0.44
1:D:200:ILE:HD13	1:D:214:GLU:HA	2.00	0.44
1:B:273:ALA:HB1	1:B:284:THR:HG21	1.99	0.44
1:B:75:VAL:HG12	1:B:115:ILE:HD12	2.00	0.44
1:A:186:SER:HB2	1:A:192:LEU:HG	2.00	0.44
1:B:320:VAL:HG21	1:B:341:VAL:CG1	2.40	0.44
1:D:239:HIS:HD2	1:D:241:GLN:HE22	1.64	0.44
1:B:9:LEU:CD1	1:B:13:LEU:HD21	2.48	0.43
1:C:284:THR:HG23	1:C:286:PRO:HD3	2.00	0.43
1:A:252:GLU:HB3	1:A:345:LEU:HD22	1.99	0.43
1:A:286:PRO:HD2	1:A:319:TYR:O	2.18	0.43
1:D:11:ASP:HA	1:D:14:GLU:HG2	2.00	0.43
1:A:113:CYS:O	1:A:161:MET:HE2	2.19	0.43
1:C:238:HIS:HD1	1:C:272:GLU:CD	2.20	0.43
1:B:82:ILE:HG22	1:B:97:ILE:HD11	2.01	0.43
1:C:152:LEU:HG	1:C:163:ILE:HG21	2.01	0.43
1:D:290:VAL:HG22	1:D:334:ASP:HA	2.01	0.43
1:C:180:ASN:HB2	1:C:212:TYR:CZ	2.54	0.43
1:C:239:HIS:HD2	1:C:241:GLN:HE22	1.67	0.43
1:A:124:MET:SD	1:A:168:LEU:HD12	2.59	0.43
1:B:273:ALA:O	1:B:284:THR:HG21	2.17	0.43
1:A:104:MET:HE1	1:A:336:ASP:HB3	2.01	0.43
1:B:277:ALA:HB2	1:B:284:THR:HB	2.01	0.43
1:B:13:LEU:H	1:B:13:LEU:HG	1.61	0.43
1:B:256:ASN:HB3	1:B:286:PRO:HA	2.00	0.43
1:B:180:ASN:HB2	1:B:212:TYR:CE2	2.54	0.42
1:C:9:LEU:O	1:C:13:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:THR:O	1:C:152:LEU:HB2	2.19	0.42
1:D:148:THR:O	1:D:152:LEU:HB2	2.18	0.42
1:D:214:GLU:CD	1:D:214:GLU:H	2.23	0.42
1:D:357:PHE:O	1:D:361:GLN:HG3	2.19	0.42
1:D:295:PHE:HB3	1:D:296:PRO:HD2	2.01	0.42
1:C:303:ASP:N	1:C:303:ASP:OD1	2.51	0.42
1:D:201:PRO:HB3	1:D:235:TYR:CD1	2.54	0.42
1:D:247:GLY:O	1:D:358:ARG:NH2	2.49	0.42
1:A:320:VAL:H	1:A:328:THR:HB	1.85	0.42
1:A:284:THR:HG22	1:A:286:PRO:HD3	2.01	0.42
1:B:234:CYS:O	1:B:237:ARG:HB2	2.20	0.42
1:A:23:LYS:HD3	1:A:33:GLU:HB2	2.00	0.42
1:B:202:ARG:HB2	1:C:210:THR:HA	2.01	0.42
1:D:269:TRP:CH2	1:D:288:ASN:HB2	2.55	0.42
1:D:178:ILE:O	1:D:212:TYR:HB3	2.20	0.42
1:C:247:GLY:O	1:C:358:ARG:NH2	2.43	0.42
1:A:142:GLU:OE2	1:A:172:MET:HG3	2.20	0.41
1:C:214:GLU:N	1:C:214:GLU:CD	2.72	0.41
1:D:197:LYS:NZ	1:D:234:CYS:HB3	2.35	0.41
1:B:284:THR:CG2	1:B:286:PRO:HD3	2.50	0.41
1:C:178:ILE:O	1:C:212:TYR:HB3	2.19	0.41
1:B:210:THR:HA	1:C:202:ARG:HB2	2.02	0.41
1:A:274:ARG:HD3	1:A:327:ARG:HD2	2.01	0.41
1:B:320:VAL:CG2	1:B:341:VAL:HG11	2.42	0.41
1:A:237:ARG:HH22	1:A:260:THR:HG23	1.85	0.41
1:B:119:GLN:OE1	1:B:289:ARG:HA	2.21	0.41
1:A:273:ALA:HB1	1:A:284:THR:HG21	2.02	0.41
1:C:284:THR:CG2	1:C:286:PRO:HD3	2.50	0.41
1:B:152:LEU:HG	1:B:163:ILE:HG21	2.03	0.41
1:D:328:THR:HG22	1:D:329:PRO:O	2.20	0.41
1:A:179:TRP:CE3	1:A:196:ARG:HD3	2.56	0.41
1:A:7:LYS:N	1:A:7:LYS:HD2	2.36	0.41
1:C:77:ALA:HB1	1:C:287:ILE:HG12	2.02	0.41
1:A:369:SER:HB3	1:B:245:MET:SD	2.61	0.41
1:B:106:LYS:HG3	1:B:159:TYR:OH	2.21	0.41
1:B:10:ASN:OD1	1:B:26:LYS:HE2	2.22	0.40
1:C:192:LEU:HD23	1:C:192:LEU:HA	1.90	0.40

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	337/405 (83%)	322 (96%)	15 (4%)	0	100	100
1	B	377/405 (93%)	364 (97%)	13 (3%)	0	100	100
1	C	381/405 (94%)	370 (97%)	11 (3%)	0	100	100
1	D	377/405 (93%)	366 (97%)	11 (3%)	0	100	100
All	All	1472/1620 (91%)	1422 (97%)	50 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	294/346 (85%)	267 (91%)	27 (9%)	11	32
1	B	323/346 (93%)	296 (92%)	27 (8%)	14	37
1	C	327/346 (94%)	297 (91%)	30 (9%)	11	32
1	D	323/346 (93%)	301 (93%)	22 (7%)	20	49
All	All	1267/1384 (92%)	1161 (92%)	106 (8%)	14	37

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	27	ARG

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Mol	Chain	Res	Type
1	A	34	GLU
1	A	38	LEU
1	A	39	GLU
1	A	42	THR
1	A	66	GLN
1	A	75	VAL
1	A	91	GLU
1	A	92	LYS
1	A	103	THR
1	A	119	GLN
1	A	123	THR
1	A	138	GLU
1	A	145	ASN
1	A	151	MET
1	A	173	GLU
1	A	180	ASN
1	A	214	GLU
1	A	260	THR
1	A	263	ARG
1	A	282	TYR
1	A	284	THR
1	A	290	VAL
1	A	292	THR
1	A	334	ASP
1	A	341	VAL
1	B	13	LEU
1	B	23	LYS
1	B	32	VAL
1	B	33	GLU
1	B	38	LEU
1	B	39	GLU
1	B	59	ARG
1	B	61	THR
1	B	71	ARG
1	B	92	LYS
1	B	123	THR
1	B	151	MET
1	B	152	LEU
1	B	202	ARG
1	B	203	VAL
1	B	214	GLU
1	B	260	THR

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Mol	Chain	Res	Type
1	B	265	SER
1	B	282	TYR
1	B	284	THR
1	B	290	VAL
1	B	292	THR
1	B	341	VAL
1	B	363	VAL
1	B	369	SER
1	B	379	LYS
1	B	384	LYS
1	C	7	LYS
1	C	28	ILE
1	C	34	GLU
1	C	38	LEU
1	C	39	GLU
1	C	51	ASN
1	C	61	THR
1	C	68	ARG
1	C	71	ARG
1	C	74	ARG
1	C	75	VAL
1	C	92	LYS
1	C	103	THR
1	C	123	THR
1	C	151	MET
1	C	168	LEU
1	C	202	ARG
1	C	203	VAL
1	C	214	GLU
1	C	260	THR
1	C	282	TYR
1	C	284	THR
1	C	290	VAL
1	C	301	SER
1	C	328	THR
1	C	332	SER
1	C	333	ARG
1	C	341	VAL
1	C	363	VAL
1	C	386	THR
1	D	12	CYS
1	D	24	GLU

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Mol	Chain	Res	Type
1	D	34	GLU
1	D	38	LEU
1	D	39	GLU
1	D	63	ARG
1	D	90	ILE
1	D	92	LYS
1	D	123	THR
1	D	151	MET
1	D	152	LEU
1	D	168	LEU
1	D	202	ARG
1	D	258	SER
1	D	261	ILE
1	D	282	TYR
1	D	284	THR
1	D	290	VAL
1	D	292	THR
1	D	328	THR
1	D	335	LYS
1	D	386	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	HIS
1	A	242	ASN
1	A	275	ASN
1	B	239	HIS
1	B	256	ASN
1	B	275	ASN
1	C	51	ASN
1	C	239	HIS
1	C	275	ASN
1	D	8	ASN
1	D	239	HIS
1	D	275	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 carbohydrates 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	345/405 (85%)	0.05	17 (4%) 33 22	20, 33, 55, 61	0
1	B	379/405 (93%)	-0.09	4 (1%) 82 74	20, 33, 55, 61	0
1	C	382/405 (94%)	-0.17	1 (0%) 94 92	20, 33, 55, 62	0
1	D	379/405 (93%)	-0.07	6 (1%) 74 66	20, 33, 54, 61	0
All	All	1485/1620 (91%)	-0.07	28 (1%) 70 59	20, 33, 55, 62	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	386	THR	5.0
1	B	67	THR	4.6
1	B	386	THR	4.1
1	A	294	GLN	3.5
1	A	176	GLU	3.4
1	A	90	ILE	3.4
1	A	376	HIS	3.3
1	B	19	PRO	3.3
1	A	173	GLU	3.1
1	A	190	ARG	3.0
1	D	386	THR	2.9
1	A	386	THR	2.8
1	A	145	ASN	2.7
1	A	174	HIS	2.7
1	D	306	LYS	2.6
1	B	11	ASP	2.5
1	A	140	ALA	2.4
1	A	334	ASP	2.4
1	D	303	ASP	2.3
1	A	214	GLU	2.3
1	A	139	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	302	GLY	2.2
1	D	308	HIS	2.2
1	A	87	THR	2.1
1	D	130	THR	2.1
1	A	35	ASP	2.0
1	A	175	GLY	2.0
1	A	91	GLU	2.0

## 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 carbohydrates 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.