



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 10:25 pm BST

PDB ID : 3RFY  
Title : Crystal structure of arabidopsis thaliana cyclophilin 38 (ATCYP38)  
Authors : Vasudevan, D.; Swaminathan, K.  
Deposited on : 2011-04-07  
Resolution : 2.39 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

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

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
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

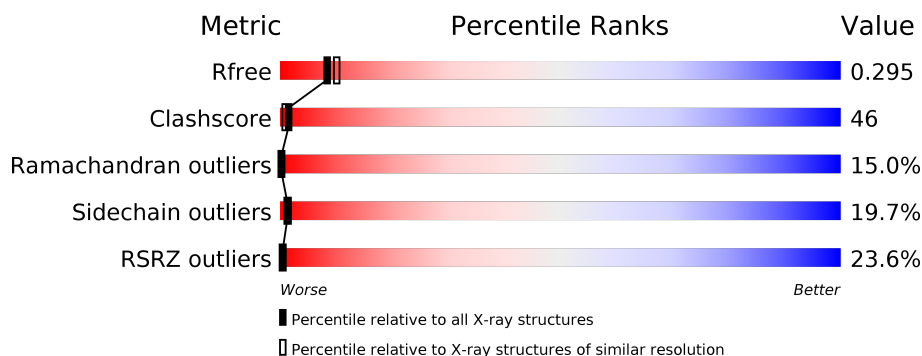
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	369	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2879 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 Peptidyl-prolyl cis-trans isomerase CYP38, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	0	0
			2765	1751	456	547	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	GLY	-	EXPRESSION TAG	UNP Q9SSA5
A	70	SER	-	EXPRESSION TAG	UNP Q9SSA5
A	71	PRO	-	EXPRESSION TAG	UNP Q9SSA5
A	72	GLY	-	EXPRESSION TAG	UNP Q9SSA5
A	73	ILE	-	EXPRESSION TAG	UNP Q9SSA5
A	74	SER	-	EXPRESSION TAG	UNP Q9SSA5
A	75	GLY	-	EXPRESSION TAG	UNP Q9SSA5
A	76	GLY	-	EXPRESSION TAG	UNP Q9SSA5
A	77	GLY	-	EXPRESSION TAG	UNP Q9SSA5
A	78	GLY	-	EXPRESSION TAG	UNP Q9SSA5
A	79	GLY	-	EXPRESSION TAG	UNP Q9SSA5
A	80	ILE	-	EXPRESSION TAG	UNP Q9SSA5
A	81	LEU	-	EXPRESSION TAG	UNP Q9SSA5
A	82	LEU	-	EXPRESSION TAG	UNP Q9SSA5

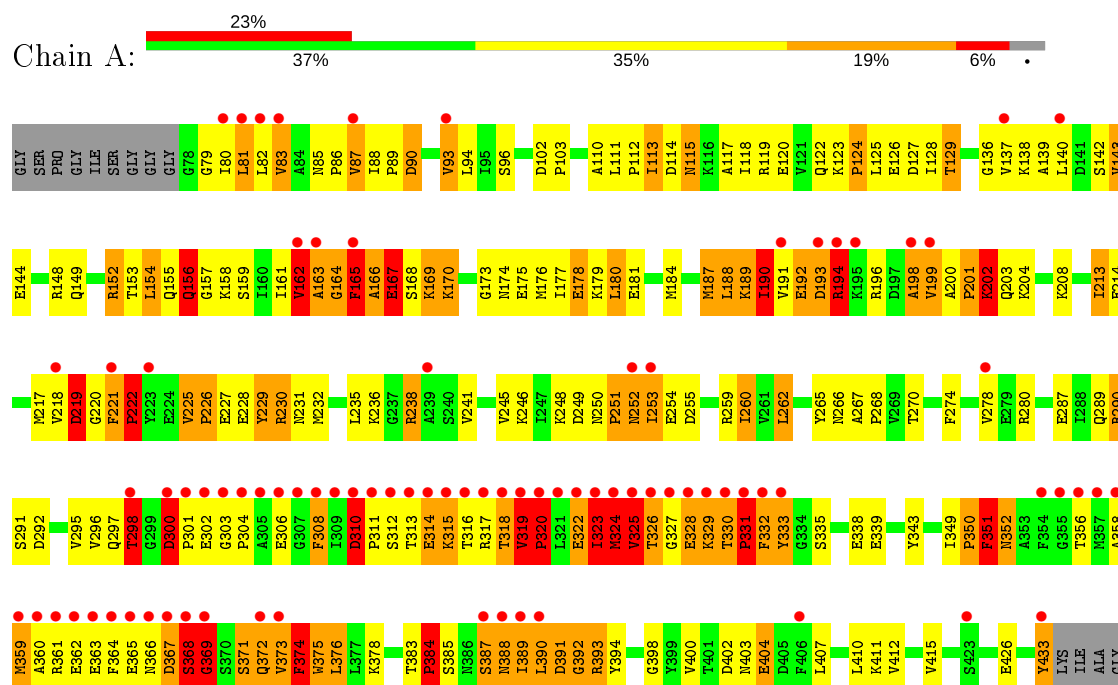
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	114	Total	O	0	0
			114	114		

### 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: Peptidyl-prolyl cis-trans isomerase CYP38, chloroplastic



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.69Å 96.72Å 166.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.89 – 2.39 41.84 – 2.39	Depositor EDS
% Data completeness (in resolution range)	86.9 (19.89-2.39) 87.0 (41.84-2.39)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.248 , 0.266 0.256 , 0.295	Depositor DCC
$R_{free}$ test set	836 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.7	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 78.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.032 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.043 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	2879	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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, 0.333 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	0.74	1/2814 (0.0%)	1.24	37/3810 (1.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	375	TRP	NE1-CE2	9.52	1.50	1.37

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	TRP	CE2-CD2-CG	9.67	115.04	107.30
1	A	297	GLN	N-CA-C	-8.62	87.71	111.00
1	A	375	TRP	CD2-CE2-CZ2	7.82	131.68	122.30
1	A	390	LEU	CA-CB-CG	7.69	132.98	115.30
1	A	164	GLY	N-CA-C	7.64	132.19	113.10
1	A	194	ARG	N-CA-C	-7.58	90.52	111.00
1	A	372	GLN	N-CA-C	7.50	131.26	111.00
1	A	391	ASP	N-CA-C	7.28	130.66	111.00
1	A	388	ASN	N-CA-C	6.89	129.62	111.00
1	A	202	LYS	N-CA-C	-6.87	92.44	111.00
1	A	298	THR	N-CA-C	6.53	128.63	111.00
1	A	165	PHE	N-CA-C	6.48	128.49	111.00
1	A	81	LEU	N-CA-C	6.40	128.27	111.00
1	A	191	VAL	N-CA-C	-6.38	93.78	111.00
1	A	367	ASP	N-CA-C	6.32	128.06	111.00
1	A	319	VAL	N-CA-C	-6.13	94.44	111.00
1	A	219	ASP	N-CA-C	-5.80	95.35	111.00
1	A	374	PHE	N-CA-C	5.79	126.62	111.00
1	A	251	PRO	N-CA-C	-5.74	97.17	112.10
1	A	433	TYR	N-CA-C	5.61	126.16	111.00
1	A	156	GLN	N-CA-C	-5.61	95.86	111.00
1	A	324	MET	N-CA-C	5.61	126.14	111.00
1	A	227	GLU	N-CA-C	5.60	126.11	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	ALA	N-CA-C	5.54	125.97	111.00
1	A	190	ILE	N-CA-C	-5.52	96.09	111.00
1	A	323	ILE	CG1-CB-CG2	-5.52	99.26	111.40
1	A	262	LEU	CA-CB-CG	-5.51	102.63	115.30
1	A	375	TRP	NE1-CE2-CD2	-5.50	101.80	107.30
1	A	331	PRO	N-CA-C	5.48	126.35	112.10
1	A	387	SER	N-CA-C	5.48	125.80	111.00
1	A	375	TRP	CE2-CD2-CE3	-5.28	112.36	118.70
1	A	300	ASP	N-CA-C	5.28	125.25	111.00
1	A	358	ALA	N-CA-C	5.21	125.07	111.00
1	A	238	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	325	VAL	N-CA-C	5.19	125.02	111.00
1	A	369	GLY	N-CA-C	5.18	126.06	113.10
1	A	371	SER	N-CA-C	5.06	124.66	111.00

There are no chirality outliers.

There are no planarity outliers.

## 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	2765	0	2753	255	1
2	A	114	0	0	30	2
All	All	2879	0	2753	255	2

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 46.

All (255) 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:319:VAL:H	1:A:320:PRO:CD	1.60	1.10
1:A:88:ILE:N	1:A:89:PRO:HD3	1.56	1.10
1:A:86:PRO:HB2	2:A:684:HOH:O	1.53	1.08
1:A:129:THR:HG22	1:A:203:GLN:HE22	1.12	1.08

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:VAL:H	1:A:320:PRO:HD2	1.19	1.06
1:A:260:ILE:HD13	1:A:400:VAL:HG22	1.38	1.02
1:A:158:LYS:O	1:A:162:VAL:HG23	1.58	1.01
1:A:157:GLY:HA3	2:A:674:HOH:O	1.63	0.98
1:A:308:PHE:HD1	1:A:308:PHE:H	1.10	0.98
1:A:80:ILE:HG23	1:A:96:SER:HB3	1.48	0.96
1:A:80:ILE:HD12	1:A:96:SER:HB2	1.47	0.96
1:A:125:LEU:N	2:A:671:HOH:O	1.98	0.96
1:A:280:ARG:HD3	2:A:683:HOH:O	1.64	0.95
1:A:80:ILE:HG21	1:A:407:LEU:CD1	1.98	0.93
1:A:88:ILE:N	1:A:89:PRO:CD	2.31	0.92
1:A:79:GLY:O	1:A:80:ILE:HD13	1.73	0.89
1:A:221:PHE:HB3	1:A:222:PRO:HD2	1.54	0.88
1:A:319:VAL:N	1:A:320:PRO:CD	2.36	0.88
1:A:169:LYS:HD3	1:A:219:ASP:OD2	1.73	0.88
1:A:218:VAL:HG21	2:A:670:HOH:O	1.71	0.87
1:A:314:GLU:O	1:A:315:LYS:HB2	1.71	0.87
1:A:190:ILE:HD11	1:A:199:VAL:CG1	2.05	0.86
1:A:330:THR:HG22	1:A:331:PRO:HD2	1.58	0.86
1:A:331:PRO:O	1:A:332:PHE:O	1.94	0.85
1:A:80:ILE:HB	1:A:400:VAL:HB	1.56	0.85
1:A:200:ALA:O	1:A:202:LYS:N	2.11	0.83
1:A:113:ILE:HD11	1:A:214:GLU:O	1.77	0.83
1:A:169:LYS:CD	1:A:219:ASP:OD2	2.27	0.83
1:A:129:THR:CG2	1:A:203:GLN:HE22	1.93	0.82
1:A:189:LYS:O	1:A:190:ILE:HG13	1.79	0.82
1:A:190:ILE:HA	1:A:192:GLU:HG2	1.61	0.82
1:A:129:THR:HG22	1:A:203:GLN:NE2	1.96	0.81
1:A:80:ILE:HG21	1:A:407:LEU:HD13	1.63	0.81
1:A:80:ILE:HG21	1:A:407:LEU:HD11	1.63	0.80
1:A:154:LEU:O	1:A:156:GLN:N	2.14	0.80
1:A:330:THR:CG2	1:A:331:PRO:HD2	2.12	0.79
1:A:159:SER:O	1:A:163:ALA:HB3	1.82	0.78
1:A:426:GLU:OE1	2:A:654:HOH:O	2.03	0.76
1:A:221:PHE:HB3	1:A:222:PRO:CD	2.15	0.76
1:A:177:ILE:O	1:A:181:GLU:HG3	1.86	0.76
1:A:80:ILE:HG23	1:A:96:SER:CB	2.16	0.76
1:A:140:LEU:N	1:A:140:LEU:HD12	2.00	0.75
1:A:80:ILE:CD1	1:A:96:SER:HB2	2.17	0.75
1:A:350:PRO:HB2	1:A:352:ASN:HD21	1.53	0.74
1:A:190:ILE:HD11	1:A:199:VAL:CB	2.17	0.74

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:ILE:O	1:A:390:LEU:HD22	1.87	0.74
1:A:426:GLU:OE1	2:A:605:HOH:O	2.04	0.74
1:A:190:ILE:HD11	1:A:199:VAL:HB	1.69	0.73
1:A:350:PRO:O	1:A:351:PHE:HB2	1.87	0.73
1:A:187:MET:HE1	1:A:200:ALA:HA	1.69	0.73
1:A:80:ILE:CG2	1:A:407:LEU:HD13	2.19	0.73
1:A:319:VAL:N	1:A:320:PRO:HD2	2.00	0.73
1:A:280:ARG:HB2	1:A:433:TYR:CG	2.24	0.73
1:A:350:PRO:O	1:A:351:PHE:CB	2.36	0.72
1:A:248:LYS:O	1:A:411:LYS:NZ	2.23	0.72
1:A:378:LYS:NZ	2:A:641:HOH:O	2.23	0.71
1:A:378:LYS:HE3	2:A:641:HOH:O	1.89	0.71
1:A:190:ILE:C	1:A:192:GLU:H	1.93	0.71
1:A:126:GLU:O	1:A:129:THR:HG23	1.90	0.70
1:A:87:VAL:C	1:A:89:PRO:HD3	2.11	0.70
1:A:175:GLU:O	1:A:179:LYS:HG3	1.91	0.70
1:A:290:ARG:NH2	1:A:292:ASP:OD1	2.25	0.69
1:A:378:LYS:CE	2:A:641:HOH:O	2.40	0.69
1:A:83:VAL:HG12	1:A:93:VAL:HB	1.74	0.69
1:A:251:PRO:O	1:A:252:ASN:HB2	1.94	0.68
1:A:199:VAL:O	1:A:202:LYS:HB3	1.94	0.68
1:A:313:THR:O	1:A:314:GLU:HB2	1.93	0.68
1:A:144:GLU:OE1	1:A:148:ARG:NH1	2.27	0.67
1:A:113:ILE:HG13	1:A:218:VAL:HB	1.75	0.67
1:A:392:GLY:O	1:A:393:ARG:HB2	1.94	0.67
1:A:308:PHE:CD1	1:A:308:PHE:N	2.62	0.67
1:A:225:VAL:HG12	1:A:226:PRO:HD2	1.75	0.67
1:A:222:PRO:HG2	1:A:236:LYS:HG2	1.76	0.67
1:A:289:GLN:NE2	1:A:349:ILE:HD11	2.09	0.67
1:A:322:GLU:HB3	1:A:324:MET:H	1.59	0.67
1:A:287:GLU:O	1:A:350:PRO:O	2.13	0.67
1:A:190:ILE:CA	1:A:192:GLU:HG2	2.24	0.67
1:A:140:LEU:H	1:A:140:LEU:HD12	1.58	0.67
1:A:162:VAL:O	1:A:163:ALA:C	2.34	0.66
1:A:252:ASN:O	1:A:253:ILE:HG22	1.96	0.66
1:A:86:PRO:C	1:A:88:ILE:H	1.99	0.66
1:A:190:ILE:HA	1:A:192:GLU:CG	2.26	0.66
1:A:190:ILE:C	1:A:192:GLU:N	2.48	0.65
1:A:178:GLU:HG2	2:A:628:HOH:O	1.97	0.65
1:A:129:THR:HB	2:A:692:HOH:O	1.97	0.64
1:A:124:PRO:O	1:A:126:GLU:N	2.29	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:GLN:HE22	1:A:349:ILE:HD11	1.62	0.64
1:A:122:GLN:O	1:A:124:PRO:O	2.16	0.63
1:A:176:MET:HB3	1:A:213:ILE:HD13	1.80	0.63
1:A:350:PRO:HB2	1:A:352:ASN:ND2	2.12	0.63
1:A:327:GLY:C	1:A:328:GLU:HG2	2.17	0.63
1:A:140:LEU:CD1	1:A:140:LEU:H	2.11	0.63
1:A:349:ILE:HB	1:A:350:PRO:HD2	1.79	0.63
1:A:310:ASP:HB3	1:A:311:PRO:CD	2.29	0.62
1:A:296:VAL:HG21	1:A:378:LYS:HD2	1.81	0.62
1:A:115:ASN:HD21	1:A:117:ALA:HB3	1.65	0.62
1:A:280:ARG:HB2	1:A:433:TYR:CD2	2.35	0.62
1:A:89:PRO:O	1:A:90:ASP:HB2	1.97	0.62
1:A:88:ILE:H	1:A:89:PRO:HD3	1.58	0.61
1:A:113:ILE:CD1	1:A:214:GLU:O	2.46	0.61
1:A:387:SER:OG	1:A:388:ASN:N	2.33	0.61
1:A:80:ILE:CG2	1:A:407:LEU:CD1	2.72	0.61
1:A:251:PRO:O	1:A:252:ASN:CB	2.48	0.60
1:A:123:LYS:C	1:A:124:PRO:O	2.38	0.60
1:A:88:ILE:HG22	1:A:88:ILE:O	2.02	0.60
1:A:222:PRO:HG3	2:A:604:HOH:O	2.01	0.59
1:A:280:ARG:HG2	2:A:643:HOH:O	2.01	0.59
1:A:260:ILE:CD1	1:A:400:VAL:HG22	2.22	0.59
1:A:157:GLY:O	1:A:161:ILE:HG13	2.03	0.58
1:A:103:PRO:HG3	1:A:404:GLU:OE2	2.04	0.58
1:A:349:ILE:HB	1:A:350:PRO:CD	2.33	0.58
1:A:140:LEU:CD1	1:A:140:LEU:N	2.67	0.58
1:A:119:ARG:HH11	1:A:122:GLN:HE22	1.50	0.58
1:A:296:VAL:CG2	1:A:378:LYS:HD2	2.34	0.58
1:A:266:ASN:O	1:A:384:PRO:HD2	2.04	0.58
1:A:220:GLY:N	2:A:707:HOH:O	2.33	0.58
1:A:87:VAL:C	1:A:89:PRO:CD	2.70	0.58
1:A:238:ARG:HH11	1:A:265:TYR:HD1	1.52	0.57
1:A:359:MET:HG2	1:A:360:ALA:H	1.69	0.56
1:A:193:ASP:O	1:A:194:ARG:HB2	2.05	0.56
1:A:198:ALA:O	1:A:199:VAL:HG23	2.05	0.56
1:A:189:LYS:O	1:A:190:ILE:CG1	2.53	0.56
1:A:80:ILE:HG13	1:A:407:LEU:CD1	2.36	0.56
1:A:164:GLY:HA3	2:A:611:HOH:O	2.06	0.56
1:A:200:ALA:C	1:A:202:LYS:H	2.07	0.55
1:A:120:GLU:O	1:A:124:PRO:HD2	2.06	0.55
1:A:300:ASP:OD1	2:A:610:HOH:O	2.18	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ILE:HD13	1:A:174:ASN:OD1	2.07	0.55
1:A:254:GLU:HA	2:A:703:HOH:O	2.05	0.54
1:A:196:ARG:O	1:A:196:ARG:HG2	2.08	0.54
1:A:123:LYS:HE3	1:A:127:ASP:OD2	2.08	0.54
1:A:153:THR:O	1:A:156:GLN:HB3	2.07	0.54
1:A:221:PHE:CB	1:A:222:PRO:HD2	2.33	0.54
1:A:115:ASN:C	1:A:115:ASN:HD22	2.12	0.54
1:A:124:PRO:O	1:A:125:LEU:HB2	2.08	0.54
1:A:323:ILE:O	1:A:323:ILE:CG2	2.55	0.53
1:A:187:MET:CE	1:A:200:ALA:HA	2.36	0.53
1:A:176:MET:CB	1:A:213:ILE:HD13	2.37	0.53
1:A:383:THR:O	1:A:385:SER:N	2.42	0.53
1:A:165:PHE:HB3	1:A:170:LYS:HG2	1.91	0.53
1:A:192:GLU:O	1:A:193:ASP:C	2.48	0.53
1:A:136:GLY:O	1:A:138:LYS:N	2.42	0.52
1:A:225:VAL:HG12	1:A:226:PRO:CD	2.38	0.52
1:A:81:LEU:O	1:A:94:LEU:HA	2.08	0.52
1:A:359:MET:HG2	1:A:360:ALA:N	2.25	0.52
1:A:245:VAL:O	1:A:255:ASP:HB2	2.10	0.52
1:A:89:PRO:O	1:A:90:ASP:CB	2.58	0.52
1:A:289:GLN:OE1	1:A:351:PHE:HA	2.10	0.52
1:A:83:VAL:HG13	1:A:394:TYR:CD2	2.45	0.51
1:A:79:GLY:C	1:A:80:ILE:HD13	2.30	0.51
1:A:201:PRO:HB2	2:A:609:HOH:O	2.09	0.51
1:A:349:ILE:HD12	2:A:679:HOH:O	2.10	0.51
1:A:260:ILE:HD13	1:A:400:VAL:CG2	2.27	0.51
1:A:322:GLU:O	1:A:323:ILE:HB	2.10	0.51
1:A:290:ARG:H	1:A:412:VAL:HG12	1.74	0.51
1:A:267:ALA:N	1:A:268:PRO:HD3	2.26	0.50
1:A:328:GLU:O	1:A:329:LYS:HB2	2.11	0.50
1:A:204:LYS:O	1:A:208:LYS:HG2	2.11	0.50
1:A:187:MET:HE3	1:A:200:ALA:O	2.12	0.50
1:A:402:ASP:O	1:A:403:ASN:HB2	2.11	0.50
1:A:200:ALA:C	1:A:202:LYS:N	2.65	0.49
1:A:176:MET:CB	1:A:213:ILE:CD1	2.89	0.49
1:A:322:GLU:HG2	1:A:324:MET:HA	1.94	0.49
1:A:139:ALA:O	1:A:142:SER:HB3	2.12	0.49
1:A:274:PHE:O	1:A:278:VAL:HG23	2.13	0.49
1:A:392:GLY:N	2:A:653:HOH:O	2.35	0.48
1:A:86:PRO:C	1:A:88:ILE:N	2.65	0.48
1:A:85:ASN:OD1	2:A:669:HOH:O	2.20	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ILE:CD1	1:A:174:ASN:OD1	2.62	0.48
1:A:190:ILE:HD11	1:A:199:VAL:HG11	1.91	0.48
1:A:300:ASP:CB	1:A:301:PRO:CD	2.92	0.47
1:A:266:ASN:C	1:A:268:PRO:HD3	2.35	0.47
1:A:426:GLU:CD	2:A:605:HOH:O	2.48	0.47
1:A:140:LEU:HA	1:A:143:VAL:HG13	1.96	0.47
1:A:167:GLU:HB2	1:A:168:SER:H	1.37	0.47
1:A:296:VAL:C	1:A:298:THR:N	2.66	0.47
1:A:374:PHE:O	1:A:375:TRP:CD1	2.68	0.47
1:A:124:PRO:C	1:A:126:GLU:H	2.18	0.47
1:A:80:ILE:CG1	1:A:407:LEU:CD1	2.92	0.47
1:A:124:PRO:C	1:A:126:GLU:N	2.67	0.47
1:A:120:GLU:HB3	1:A:153:THR:HG21	1.95	0.47
1:A:200:ALA:HB3	1:A:201:PRO:HD3	1.97	0.46
1:A:259:ARG:HB3	1:A:402:ASP:HB3	1.97	0.46
1:A:253:ILE:HG23	1:A:253:ILE:O	2.14	0.46
1:A:324:MET:O	1:A:325:VAL:O	2.33	0.46
1:A:152:ARG:CD	2:A:617:HOH:O	2.63	0.46
1:A:102:ASP:HA	1:A:103:PRO:HD2	1.79	0.46
1:A:364:PHE:HD1	1:A:364:PHE:O	1.98	0.46
1:A:249:ASP:HB3	2:A:697:HOH:O	2.15	0.46
1:A:176:MET:HB2	1:A:213:ILE:CD1	2.46	0.45
1:A:296:VAL:O	1:A:298:THR:N	2.49	0.45
1:A:388:ASN:O	1:A:389:ILE:HG13	2.16	0.45
1:A:329:LYS:O	1:A:330:THR:O	2.34	0.45
1:A:115:ASN:ND2	1:A:118:ILE:H	2.15	0.45
1:A:190:ILE:HD11	1:A:199:VAL:HG12	1.94	0.45
1:A:229:TYR:HB3	1:A:232:MET:SD	2.57	0.45
1:A:144:GLU:O	1:A:148:ARG:HG3	2.17	0.45
1:A:176:MET:HB3	1:A:213:ILE:CD1	2.45	0.45
1:A:250:ASN:OD1	1:A:252:ASN:O	2.35	0.45
1:A:318:THR:O	1:A:322:GLU:OE2	2.34	0.45
1:A:82:LEU:HB2	1:A:398:GLY:HA3	1.99	0.45
1:A:180:LEU:O	1:A:184:MET:HG3	2.16	0.44
1:A:221:PHE:CB	1:A:222:PRO:CD	2.88	0.44
1:A:333:TYR:CE2	1:A:339:GLU:OE1	2.70	0.44
1:A:359:MET:CG	1:A:360:ALA:H	2.28	0.44
1:A:114:ASP:C	1:A:114:ASP:OD1	2.56	0.44
1:A:253:ILE:CG2	1:A:253:ILE:O	2.66	0.44
1:A:287:GLU:HG2	1:A:415:VAL:HG22	2.00	0.44
1:A:310:ASP:CB	1:A:311:PRO:CD	2.93	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:VAL:N	1:A:89:PRO:HD3	2.33	0.44
1:A:169:LYS:HD2	1:A:219:ASP:OD2	2.14	0.44
1:A:328:GLU:O	1:A:329:LYS:CB	2.66	0.44
1:A:123:LYS:O	1:A:124:PRO:O	2.36	0.44
1:A:228:GLU:HB2	2:A:675:HOH:O	2.18	0.44
1:A:200:ALA:HB3	1:A:201:PRO:CD	2.49	0.43
1:A:364:PHE:CD1	1:A:364:PHE:O	2.71	0.43
1:A:368:SER:HB3	1:A:369:GLY:H	1.56	0.43
1:A:302:GLU:HB3	1:A:303:GLY:H	1.41	0.43
1:A:343:TYR:CD1	1:A:343:TYR:N	2.87	0.43
1:A:372:GLN:HG2	1:A:374:PHE:CE1	2.53	0.43
1:A:365:GLU:HG2	1:A:365:GLU:H	1.68	0.43
1:A:188:LEU:HA	1:A:188:LEU:HD22	1.86	0.43
1:A:164:GLY:CA	2:A:611:HOH:O	2.66	0.42
1:A:238:ARG:HD3	1:A:265:TYR:CE1	2.54	0.42
1:A:167:GLU:HG3	1:A:167:GLU:H	1.72	0.42
1:A:111:LEU:HA	1:A:112:PRO:HD3	1.90	0.42
1:A:193:ASP:O	1:A:194:ARG:CB	2.67	0.42
1:A:371:SER:O	1:A:372:GLN:HB2	2.20	0.42
1:A:165:PHE:CZ	1:A:173:GLY:HA3	2.54	0.42
1:A:199:VAL:O	1:A:202:LYS:CB	2.65	0.42
1:A:202:LYS:HG3	1:A:202:LYS:O	2.19	0.42
1:A:246:LYS:NZ	1:A:248:LYS:HE3	2.35	0.42
1:A:280:ARG:CB	1:A:433:TYR:CD2	3.01	0.42
1:A:373:VAL:O	1:A:374:PHE:HB2	2.20	0.42
1:A:188:LEU:O	1:A:190:ILE:N	2.53	0.41
1:A:200:ALA:CB	1:A:201:PRO:HD3	2.50	0.41
1:A:289:GLN:HA	1:A:412:VAL:HG12	2.01	0.41
1:A:290:ARG:O	1:A:291:SER:HB3	2.20	0.41
1:A:388:ASN:C	1:A:389:ILE:HG13	2.39	0.41
1:A:192:GLU:O	1:A:194:ARG:O	2.38	0.41
1:A:349:ILE:CB	1:A:350:PRO:CD	2.98	0.41
1:A:229:TYR:C	1:A:231:ASN:H	2.24	0.41
1:A:190:ILE:CD1	1:A:199:VAL:HB	2.45	0.41
1:A:326:THR:HG22	1:A:327:GLY:N	2.35	0.41
1:A:338:GLU:HG3	2:A:602:HOH:O	2.19	0.41
1:A:152:ARG:HD2	2:A:617:HOH:O	2.20	0.41
1:A:110:ALA:HB1	1:A:266:ASN:ND2	2.36	0.41
1:A:89:PRO:CG	2:A:687:HOH:O	2.68	0.41
1:A:128:ILE:HG23	1:A:143:VAL:HB	2.03	0.40
1:A:333:TYR:CD2	1:A:333:TYR:C	2.94	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LEU:HD12	1:A:184:MET:CE	2.51	0.40
1:A:323:ILE:HG22	1:A:323:ILE:O	2.21	0.40
1:A:198:ALA:O	1:A:199:VAL:CG2	2.70	0.40
1:A:245:VAL:HG11	1:A:410:LEU:HD22	2.03	0.40
1:A:280:ARG:HG2	1:A:433:TYR:CD2	2.57	0.40

All (2) 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)
2:A:605:HOH:O	2:A:605:HOH:O 3_555	2.15	0.05
1:A:375:TRP:O	2:A:602:HOH:O 4_566	2.19	0.01

## 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	354/369 (96%)	257 (73%)	44 (12%)	53 (15%)	<b>0</b> <b>0</b>

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	VAL
1	A	137	VAL
1	A	155	GLN
1	A	156	GLN
1	A	162	VAL
1	A	163	ALA
1	A	167	GLU
1	A	190	ILE
1	A	217	MET
1	A	222	PRO

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	314	GLU
1	A	315	LYS
1	A	320	PRO
1	A	323	ILE
1	A	324	MET
1	A	325	VAL
1	A	329	LYS
1	A	330	THR
1	A	332	PHE
1	A	335	SER
1	A	351	PHE
1	A	363	GLU
1	A	369	GLY
1	A	389	ILE
1	A	391	ASP
1	A	194	ARG
1	A	253	ILE
1	A	300	ASP
1	A	333	TYR
1	A	367	ASP
1	A	374	PHE
1	A	376	LEU
1	A	124	PRO
1	A	199	VAL
1	A	322	GLU
1	A	359	MET
1	A	366	ASN
1	A	393	ARG
1	A	166	ALA
1	A	221	PHE
1	A	230	ARG
1	A	326	THR
1	A	331	PRO
1	A	368	SER
1	A	193	ASP
1	A	198	ALA
1	A	252	ASN
1	A	310	ASP
1	A	319	VAL
1	A	392	GLY
1	A	304	PRO
1	A	373	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	384	PRO

### 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	305/311 (98%)	245 (80%)	60 (20%)	<b>1</b> <b>1</b>

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	VAL
1	A	90	ASP
1	A	93	VAL
1	A	113	ILE
1	A	115	ASN
1	A	129	THR
1	A	143	VAL
1	A	149	GLN
1	A	152	ARG
1	A	154	LEU
1	A	162	VAL
1	A	165	PHE
1	A	167	GLU
1	A	169	LYS
1	A	170	LYS
1	A	178	GLU
1	A	180	LEU
1	A	187	MET
1	A	188	LEU
1	A	189	LYS
1	A	192	GLU
1	A	194	ARG
1	A	201	PRO
1	A	202	LYS
1	A	213	ILE

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	219	ASP
1	A	222	PRO
1	A	225	VAL
1	A	226	PRO
1	A	229	TYR
1	A	230	ARG
1	A	235	LEU
1	A	241	VAL
1	A	260	ILE
1	A	262	LEU
1	A	270	THR
1	A	290	ARG
1	A	295	VAL
1	A	298	THR
1	A	306	GLU
1	A	308	PHE
1	A	310	ASP
1	A	312	SER
1	A	316	THR
1	A	317	ARG
1	A	318	THR
1	A	320	PRO
1	A	323	ILE
1	A	325	VAL
1	A	328	GLU
1	A	350	PRO
1	A	351	PHE
1	A	352	ASN
1	A	356	THR
1	A	361	ARG
1	A	362	GLU
1	A	368	SER
1	A	376	LEU
1	A	384	PRO
1	A	404	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
1	A	122	GLN
1	A	203	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	289	GLN
1	A	352	ASN
1	A	403	ASN

### 5.3.3 RNA [i](#)

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	356/369 (96%)	1.84	84 (23%) 0 0	31, 58, 148, 168	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	366	ASN	14.4
1	A	325	VAL	14.2
1	A	323	ILE	13.9
1	A	321	LEU	13.4
1	A	326	THR	12.0
1	A	330	THR	12.0
1	A	313	THR	11.3
1	A	357	MET	11.3
1	A	373	VAL	11.2
1	A	309	ILE	11.1
1	A	310	ASP	10.6
1	A	315	LYS	9.9
1	A	311	PRO	9.9
1	A	367	ASP	9.5
1	A	318	THR	9.4
1	A	303	GLY	9.0
1	A	329	LYS	9.0
1	A	358	ALA	9.0
1	A	359	MET	8.9
1	A	308	PHE	8.5
1	A	320	PRO	7.9
1	A	319	VAL	7.9
1	A	328	GLU	7.5
1	A	356	THR	7.2
1	A	324	MET	7.0
1	A	327	GLY	6.8
1	A	198	ALA	6.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	300	ASP	6.4
1	A	304	PRO	6.4
1	A	322	GLU	6.3
1	A	360	ALA	6.2
1	A	223	TYR	6.1
1	A	307	GLY	6.0
1	A	368	SER	5.7
1	A	194	ARG	5.6
1	A	355	GLY	5.5
1	A	305	ALA	5.5
1	A	316	THR	5.3
1	A	333	TYR	5.0
1	A	362	GLU	4.8
1	A	253	ILE	4.6
1	A	314	GLU	4.6
1	A	361	ARG	4.6
1	A	317	ARG	4.4
1	A	218	VAL	4.3
1	A	372	GLN	4.2
1	A	163	ALA	4.2
1	A	331	PRO	4.1
1	A	312	SER	4.1
1	A	364	PHE	4.0
1	A	387	SER	3.9
1	A	252	ASN	3.7
1	A	199	VAL	3.7
1	A	301	PRO	3.7
1	A	162	VAL	3.5
1	A	221	PHE	3.3
1	A	363	GLU	3.1
1	A	389	ILE	3.1
1	A	83	VAL	3.0
1	A	80	ILE	2.9
1	A	390	LEU	2.9
1	A	82	LEU	2.8
1	A	87	VAL	2.8
1	A	302	GLU	2.7
1	A	406	PHE	2.7
1	A	137	VAL	2.6
1	A	239	ALA	2.5
1	A	365	GLU	2.5
1	A	93	VAL	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	278	VAL	2.4
1	A	388	ASN	2.4
1	A	332	PHE	2.4
1	A	354	PHE	2.3
1	A	193	ASP	2.3
1	A	81	LEU	2.3
1	A	195	LYS	2.2
1	A	191	VAL	2.2
1	A	298	THR	2.1
1	A	369	GLY	2.1
1	A	433	TYR	2.1
1	A	423	SER	2.1
1	A	140	LEU	2.0
1	A	165	PHE	2.0
1	A	306	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.