



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:35 AM UTC

PDB ID : 2Q43 / pdb_00002q43
Title : Ensemble refinement of the protein crystal structure of IAA-aminoacid hydrolase from Arabidopsis thaliana gene At5g56660
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2007-05-31
Resolution : 2.00 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

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

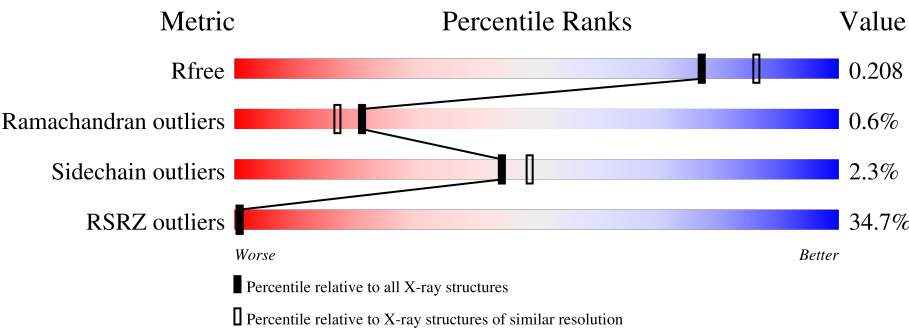
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	1-A	418	31% 88% 10%
1	10-A	418	88% 10%
1	11-A	418	87% 10%
1	12-A	418	88% 10%
1	13-A	418	87% 10%
1	14-A	418	87% 10%
1	15-A	418	88% 10%

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Mol	Chain	Length	Quality of chain
1	16-A	418	 86% • 10%
1	2-A	418	 88% • 10%
1	3-A	418	 87% • 10%
1	4-A	418	 88% • 10%
1	5-A	418	 88% • 10%
1	6-A	418	 88% • 10%
1	7-A	418	 88% • 10%
1	8-A	418	 88% • 10%
1	9-A	418	 88% • 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 50784 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 IAA-amino acid hydrolase ILR1-like 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			
1	2-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			
1	3-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			
1	4-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			
1	5-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			
1	6-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			
1	7-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			
1	8-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			
1	9-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			
1	10-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			
1	11-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			
1	12-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			
1	13-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			
1	14-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			
1	15-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			
1	16-A	375	Total	C	N	O	S	0	0	0
			2889	1841	501	536	11			

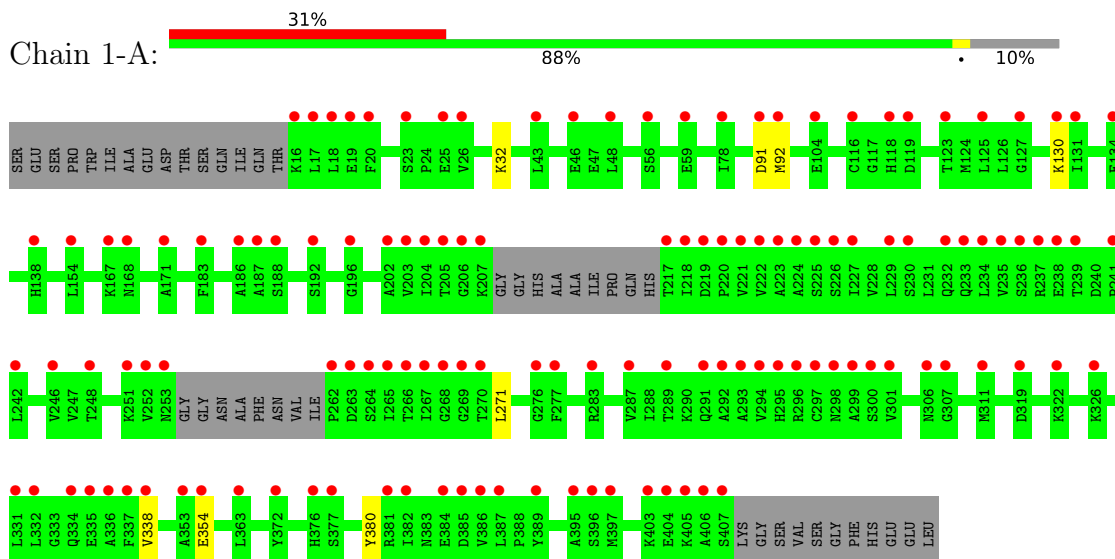
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1-A	285	Total O 285 285	0	0
2	2-A	285	Total O 285 285	0	0
2	3-A	285	Total O 285 285	0	0
2	4-A	285	Total O 285 285	0	0
2	5-A	285	Total O 285 285	0	0
2	6-A	285	Total O 285 285	0	0
2	7-A	285	Total O 285 285	0	0
2	8-A	285	Total O 285 285	0	0
2	9-A	285	Total O 285 285	0	0
2	10-A	285	Total O 285 285	0	0
2	11-A	285	Total O 285 285	0	0
2	12-A	285	Total O 285 285	0	0
2	13-A	285	Total O 285 285	0	0
2	14-A	285	Total O 285 285	0	0
2	15-A	285	Total O 285 285	0	0
2	16-A	285	Total O 285 285	0	0

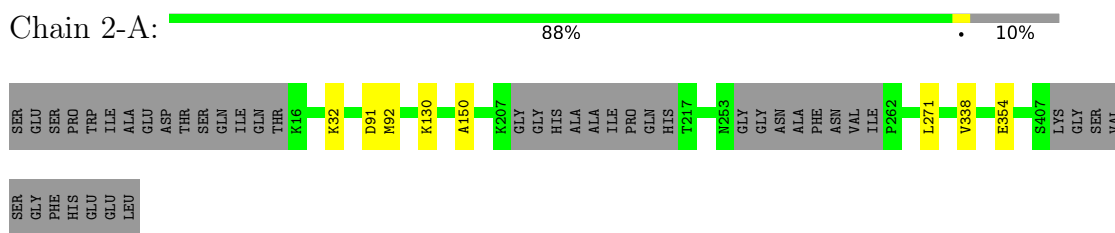
3 Residue-property plots [i](#)

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.

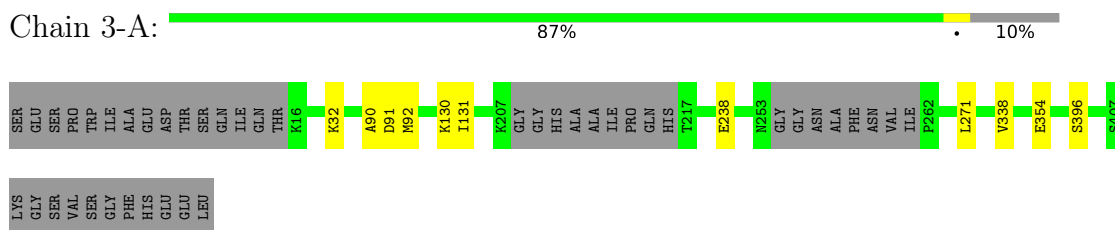
- Molecule 1: IAA-amino acid hydrolase ILR1-like 2



- Molecule 1: IAA-amino acid hydrolase ILR1-like 2

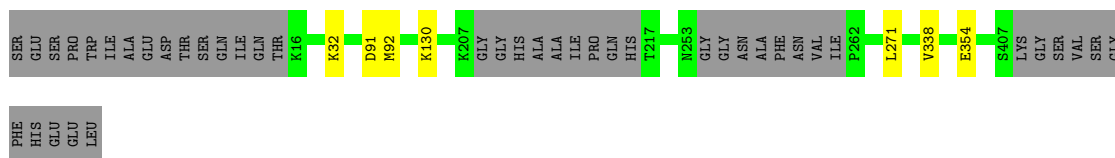


- Molecule 1: IAA-amino acid hydrolase ILR1-like 2



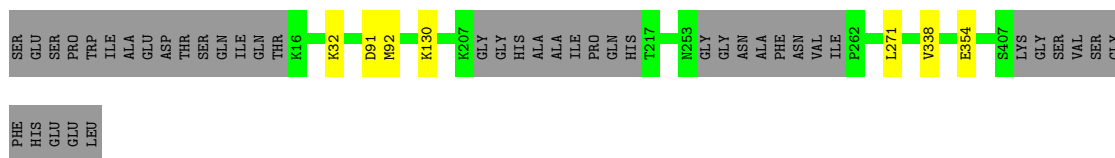
- Molecule 1: IAA-amino acid hydrolase ILR1-like 2

Chain 4-A:  88% 10%



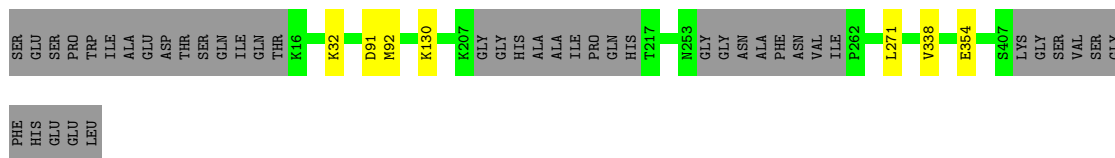
- Molecule 1: IAA-amino acid hydrolase ILR1-like 2

Chain 5-A:  88% 10%



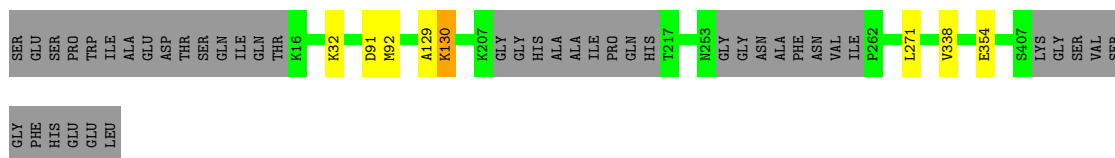
- Molecule 1: IAA-amino acid hydrolase ILR1-like 2

Chain 6-A:  88% 10%



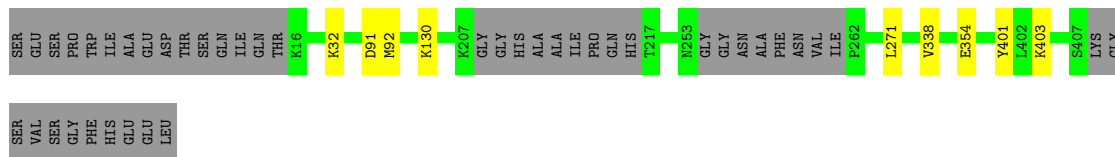
- Molecule 1: IAA-amino acid hydrolase ILR1-like 2

Chain 7-A:  88% 10%



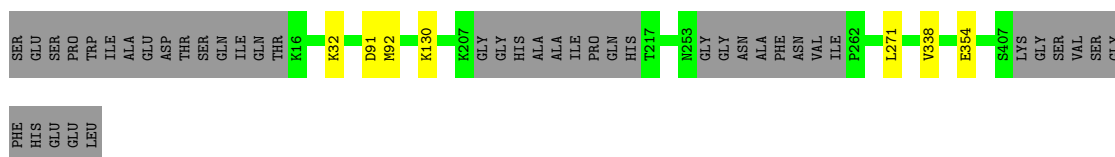
- Molecule 1: IAA-amino acid hydrolase ILR1-like 2

Chain 8-A:  88% 10%



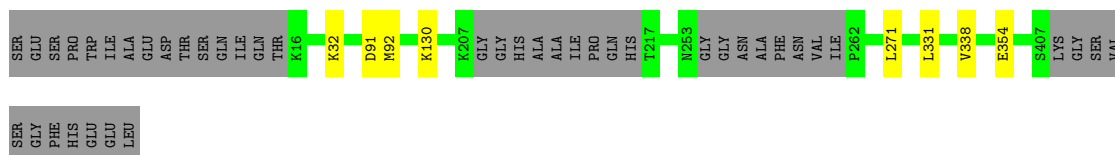
- Molecule 1: IAA-amino acid hydrolase ILR1-like 2

Chain 9-A:  88% 10%



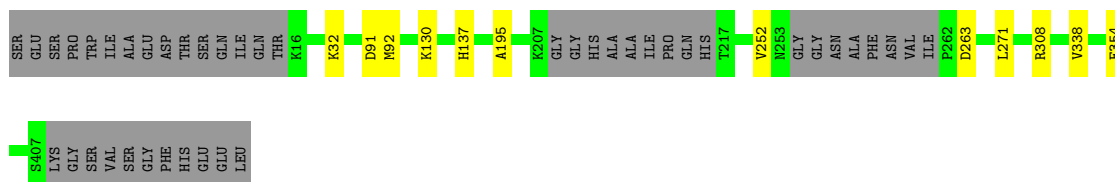
- Molecule 1: IAA-amino acid hydrolase ILR1-like 2

Chain 10-A: 88% 10%



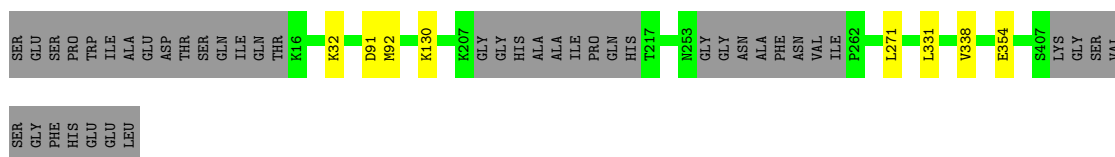
- Molecule 1: IAA-amino acid hydrolase ILR1-like 2

Chain 11-A: 87% 10%



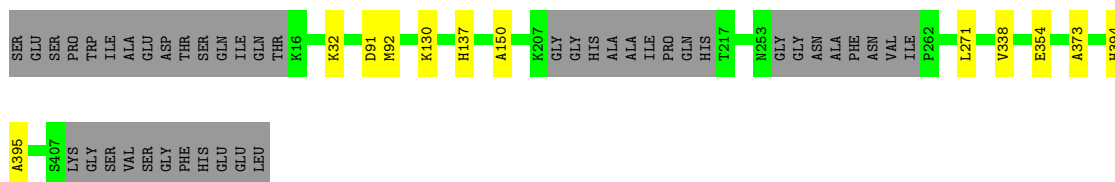
- Molecule 1: IAA-amino acid hydrolase ILR1-like 2

Chain 12-A: 88% 10%



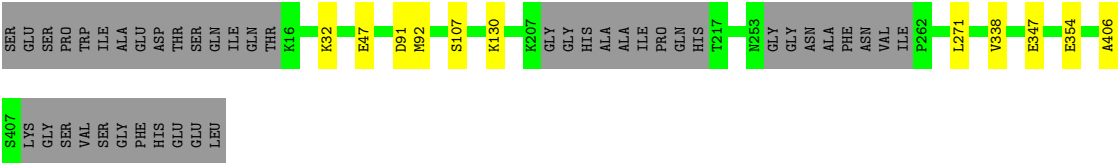
- Molecule 1: IAA-amino acid hydrolase ILR1-like 2

Chain 13-A: 87% 10%



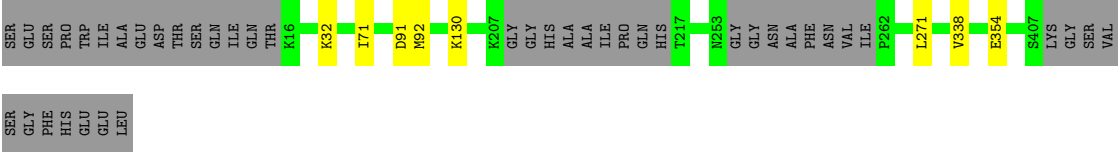
- Molecule 1: IAA-amino acid hydrolase ILR1-like 2

Chain 14-A: 87% 10%



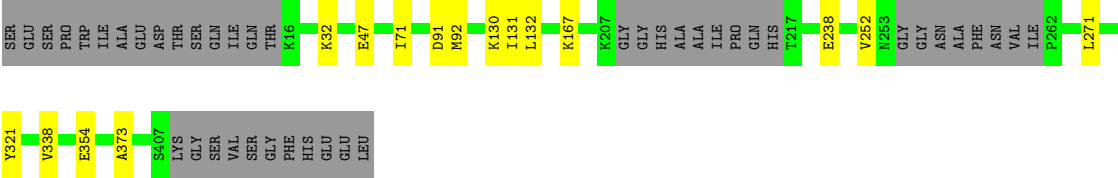
● Molecule 1: IAA-amino acid hydrolase ILR1-like 2

Chain 15-A: 88% 10%



● Molecule 1: IAA-amino acid hydrolase ILR1-like 2

Chain 16-A: 86% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	75.26Å 75.26Å 130.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	23.09 – 2.00 23.09 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (23.09-2.00) 99.8 (23.09-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 1.99Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.149 , 0.204 0.157 , 0.208	Depositor DCC
R_{free} test set	1504 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.02 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	50784	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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 [i](#)

5.1 Standard geometry [i](#)

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	1-A	0.28	0/2948	0.40	0/3984
1	2-A	0.28	0/2948	0.40	0/3984
1	3-A	0.28	0/2948	0.40	0/3984
1	4-A	0.28	0/2948	0.40	0/3984
1	5-A	0.28	0/2948	0.40	0/3984
1	6-A	0.28	0/2948	0.40	0/3984
1	7-A	0.28	0/2948	0.40	0/3984
1	8-A	0.28	0/2948	0.40	0/3984
1	9-A	0.28	0/2948	0.40	0/3984
1	10-A	0.28	0/2948	0.40	0/3984
1	11-A	0.28	0/2948	0.40	0/3984
1	12-A	0.28	0/2948	0.40	0/3984
1	13-A	0.28	0/2948	0.40	0/3984
1	14-A	0.28	0/2948	0.40	0/3984
1	15-A	0.28	0/2948	0.40	0/3984
1	16-A	0.28	0/2948	0.40	0/3984
All	All	0.28	0/47168	0.40	0/63744

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	16-A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	16-A	321	TYR	Sidechain

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	1-A	2889	0	2919	0	0
1	2-A	2889	0	2919	0	0
1	3-A	2889	0	2919	0	0
1	4-A	2889	0	2919	0	0
1	5-A	2889	0	2919	0	0
1	6-A	2889	0	2919	0	0
1	7-A	2889	0	2919	0	0
1	8-A	2889	0	2919	0	0
1	9-A	2889	0	2919	0	0
1	10-A	2889	0	2919	0	0
1	11-A	2889	0	2919	0	0
1	12-A	2889	0	2919	0	0
1	13-A	2889	0	2919	0	0
1	14-A	2889	0	2919	0	0
1	15-A	2889	0	2919	0	0
1	16-A	2889	0	2919	0	0
2	1-A	285	0	0	0	0
2	2-A	285	0	0	0	0
2	3-A	285	0	0	0	0
2	4-A	285	0	0	0	0
2	5-A	285	0	0	0	0
2	6-A	285	0	0	0	0
2	7-A	285	0	0	0	0
2	8-A	285	0	0	0	0
2	9-A	285	0	0	0	0
2	10-A	285	0	0	0	0
2	11-A	285	0	0	0	0
2	12-A	285	0	0	0	0
2	13-A	285	0	0	0	0
2	14-A	285	0	0	0	0
2	15-A	285	0	0	0	0
2	16-A	285	0	0	0	0
All	All	50784	0	46704	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	1-A	369/418 (88%)	348 (94%)	20 (5%)	1 (0%)	36	35
1	2-A	369/418 (88%)	348 (94%)	20 (5%)	1 (0%)	36	35
1	3-A	369/418 (88%)	338 (92%)	27 (7%)	4 (1%)	11	7
1	4-A	369/418 (88%)	354 (96%)	15 (4%)	0	100	100
1	5-A	369/418 (88%)	357 (97%)	12 (3%)	0	100	100
1	6-A	369/418 (88%)	352 (95%)	17 (5%)	0	100	100
1	7-A	369/418 (88%)	340 (92%)	27 (7%)	2 (0%)	24	21
1	8-A	369/418 (88%)	354 (96%)	13 (4%)	2 (0%)	24	21
1	9-A	369/418 (88%)	356 (96%)	13 (4%)	0	100	100
1	10-A	369/418 (88%)	355 (96%)	13 (4%)	1 (0%)	36	35
1	11-A	369/418 (88%)	348 (94%)	16 (4%)	5 (1%)	9	4
1	12-A	369/418 (88%)	345 (94%)	23 (6%)	1 (0%)	36	35
1	13-A	369/418 (88%)	341 (92%)	23 (6%)	5 (1%)	9	4
1	14-A	369/418 (88%)	349 (95%)	16 (4%)	4 (1%)	11	7
1	15-A	369/418 (88%)	347 (94%)	21 (6%)	1 (0%)	36	35
1	16-A	369/418 (88%)	340 (92%)	21 (6%)	8 (2%)	5	2
All	All	5904/6688 (88%)	5572 (94%)	297 (5%)	35 (1%)	21	17

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2-A	150	ALA
1	11-A	195	ALA
1	11-A	263	ASP
1	11-A	308	ARG
1	13-A	373	ALA
1	15-A	71	ILE
1	16-A	131	ILE
1	3-A	238	GLU
1	7-A	130	LYS
1	12-A	331	LEU
1	13-A	394	HIS
1	13-A	395	ALA
1	14-A	107	SER
1	16-A	132	LEU
1	16-A	238	GLU
1	3-A	90	ALA
1	8-A	403	LYS
1	10-A	331	LEU
1	11-A	137	HIS
1	13-A	137	HIS
1	14-A	47	GLU
1	14-A	406	ALA
1	16-A	373	ALA
1	1-A	380	TYR
1	3-A	396	SER
1	7-A	129	ALA
1	16-A	167	LYS
1	8-A	401	TYR
1	13-A	150	ALA
1	16-A	47	GLU
1	14-A	347	GLU
1	16-A	71	ILE
1	3-A	131	ILE
1	16-A	252	VAL
1	11-A	252	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	1-A	308/341 (90%)	301 (98%)	7 (2%)	44	49
1	2-A	308/341 (90%)	301 (98%)	7 (2%)	44	49
1	3-A	308/341 (90%)	301 (98%)	7 (2%)	44	49
1	4-A	308/341 (90%)	301 (98%)	7 (2%)	44	49
1	5-A	308/341 (90%)	301 (98%)	7 (2%)	44	49
1	6-A	308/341 (90%)	301 (98%)	7 (2%)	44	49
1	7-A	308/341 (90%)	301 (98%)	7 (2%)	44	49
1	8-A	308/341 (90%)	301 (98%)	7 (2%)	44	49
1	9-A	308/341 (90%)	301 (98%)	7 (2%)	44	49
1	10-A	308/341 (90%)	301 (98%)	7 (2%)	44	49
1	11-A	308/341 (90%)	301 (98%)	7 (2%)	44	49
1	12-A	308/341 (90%)	301 (98%)	7 (2%)	44	49
1	13-A	308/341 (90%)	301 (98%)	7 (2%)	44	49
1	14-A	308/341 (90%)	301 (98%)	7 (2%)	44	49
1	15-A	308/341 (90%)	301 (98%)	7 (2%)	44	49
1	16-A	308/341 (90%)	301 (98%)	7 (2%)	44	49
All	All	4928/5456 (90%)	4816 (98%)	112 (2%)	44	49

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	32	LYS
1	1-A	91	ASP
1	1-A	92	MET
1	1-A	130	LYS
1	1-A	271	LEU
1	1-A	338	VAL
1	1-A	354	GLU
1	2-A	32	LYS
1	2-A	91	ASP
1	2-A	92	MET
1	2-A	130	LYS
1	2-A	271	LEU
1	2-A	338	VAL
1	2-A	354	GLU
1	3-A	32	LYS
1	3-A	91	ASP

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Mol	Chain	Res	Type
1	3-A	92	MET
1	3-A	130	LYS
1	3-A	271	LEU
1	3-A	338	VAL
1	3-A	354	GLU
1	4-A	32	LYS
1	4-A	91	ASP
1	4-A	92	MET
1	4-A	130	LYS
1	4-A	271	LEU
1	4-A	338	VAL
1	4-A	354	GLU
1	5-A	32	LYS
1	5-A	91	ASP
1	5-A	92	MET
1	5-A	130	LYS
1	5-A	271	LEU
1	5-A	338	VAL
1	5-A	354	GLU
1	6-A	32	LYS
1	6-A	91	ASP
1	6-A	92	MET
1	6-A	130	LYS
1	6-A	271	LEU
1	6-A	338	VAL
1	6-A	354	GLU
1	7-A	32	LYS
1	7-A	91	ASP
1	7-A	92	MET
1	7-A	130	LYS
1	7-A	271	LEU
1	7-A	338	VAL
1	7-A	354	GLU
1	8-A	32	LYS
1	8-A	91	ASP
1	8-A	92	MET
1	8-A	130	LYS
1	8-A	271	LEU
1	8-A	338	VAL
1	8-A	354	GLU
1	9-A	32	LYS
1	9-A	91	ASP

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Mol	Chain	Res	Type
1	9-A	92	MET
1	9-A	130	LYS
1	9-A	271	LEU
1	9-A	338	VAL
1	9-A	354	GLU
1	10-A	32	LYS
1	10-A	91	ASP
1	10-A	92	MET
1	10-A	130	LYS
1	10-A	271	LEU
1	10-A	338	VAL
1	10-A	354	GLU
1	11-A	32	LYS
1	11-A	91	ASP
1	11-A	92	MET
1	11-A	130	LYS
1	11-A	271	LEU
1	11-A	338	VAL
1	11-A	354	GLU
1	12-A	32	LYS
1	12-A	91	ASP
1	12-A	92	MET
1	12-A	130	LYS
1	12-A	271	LEU
1	12-A	338	VAL
1	12-A	354	GLU
1	13-A	32	LYS
1	13-A	91	ASP
1	13-A	92	MET
1	13-A	130	LYS
1	13-A	271	LEU
1	13-A	338	VAL
1	13-A	354	GLU
1	14-A	32	LYS
1	14-A	91	ASP
1	14-A	92	MET
1	14-A	130	LYS
1	14-A	271	LEU
1	14-A	338	VAL
1	14-A	354	GLU
1	15-A	32	LYS
1	15-A	91	ASP

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Mol	Chain	Res	Type
1	15-A	92	MET
1	15-A	130	LYS
1	15-A	271	LEU
1	15-A	338	VAL
1	15-A	354	GLU
1	16-A	32	LYS
1	16-A	91	ASP
1	16-A	92	MET
1	16-A	130	LYS
1	16-A	271	LEU
1	16-A	338	VAL
1	16-A	354	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (144) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	133	HIS
1	1-A	232	GLN
1	1-A	233	GLN
1	1-A	281	GLN
1	1-A	298	ASN
1	1-A	316	ASN
1	1-A	317	ASN
1	1-A	376	HIS
1	2-A	114	HIS
1	2-A	133	HIS
1	2-A	140	GLN
1	2-A	233	GLN
1	2-A	281	GLN
1	2-A	298	ASN
1	2-A	316	ASN
1	2-A	334	GLN
1	2-A	359	HIS
1	2-A	370	ASN
1	2-A	400	GLN
1	3-A	114	HIS
1	3-A	176	HIS
1	3-A	233	GLN
1	3-A	281	GLN
1	3-A	298	ASN
1	3-A	302	ASN
1	3-A	306	ASN

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Mol	Chain	Res	Type
1	3-A	316	ASN
1	3-A	334	GLN
1	3-A	370	ASN
1	4-A	133	HIS
1	4-A	176	HIS
1	4-A	232	GLN
1	4-A	281	GLN
1	4-A	282	GLN
1	4-A	298	ASN
1	4-A	317	ASN
1	4-A	334	GLN
1	4-A	370	ASN
1	4-A	400	GLN
1	5-A	98	GLN
1	5-A	137	HIS
1	5-A	233	GLN
1	5-A	298	ASN
1	5-A	334	GLN
1	5-A	370	ASN
1	5-A	400	GLN
1	6-A	133	HIS
1	6-A	137	HIS
1	6-A	233	GLN
1	6-A	279	GLN
1	6-A	298	ASN
1	6-A	334	GLN
1	6-A	370	ASN
1	7-A	137	HIS
1	7-A	232	GLN
1	7-A	233	GLN
1	7-A	282	GLN
1	7-A	298	ASN
1	7-A	334	GLN
1	7-A	370	ASN
1	7-A	376	HIS
1	8-A	281	GLN
1	8-A	298	ASN
1	8-A	334	GLN
1	8-A	400	GLN
1	9-A	281	GLN
1	9-A	298	ASN
1	9-A	317	ASN

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Mol	Chain	Res	Type
1	9-A	334	GLN
1	9-A	370	ASN
1	9-A	400	GLN
1	10-A	133	HIS
1	10-A	140	GLN
1	10-A	176	HIS
1	10-A	232	GLN
1	10-A	233	GLN
1	10-A	253	ASN
1	10-A	298	ASN
1	10-A	306	ASN
1	10-A	323	GLN
1	10-A	370	ASN
1	11-A	133	HIS
1	11-A	138	HIS
1	11-A	233	GLN
1	11-A	298	ASN
1	11-A	316	ASN
1	11-A	334	GLN
1	11-A	370	ASN
1	11-A	400	GLN
1	12-A	105	HIS
1	12-A	140	GLN
1	12-A	168	ASN
1	12-A	232	GLN
1	12-A	233	GLN
1	12-A	282	GLN
1	12-A	298	ASN
1	12-A	306	ASN
1	12-A	359	HIS
1	12-A	370	ASN
1	13-A	40	ASN
1	13-A	98	GLN
1	13-A	114	HIS
1	13-A	133	HIS
1	13-A	137	HIS
1	13-A	176	HIS
1	13-A	232	GLN
1	13-A	281	GLN
1	13-A	298	ASN
1	13-A	323	GLN
1	13-A	334	GLN

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Mol	Chain	Res	Type
1	13-A	376	HIS
1	13-A	400	GLN
1	14-A	133	HIS
1	14-A	232	GLN
1	14-A	233	GLN
1	14-A	282	GLN
1	14-A	291	GLN
1	14-A	298	ASN
1	14-A	316	ASN
1	14-A	334	GLN
1	14-A	376	HIS
1	15-A	140	GLN
1	15-A	168	ASN
1	15-A	233	GLN
1	15-A	282	GLN
1	15-A	295	HIS
1	15-A	298	ASN
1	15-A	334	GLN
1	15-A	376	HIS
1	15-A	400	GLN
1	16-A	98	GLN
1	16-A	140	GLN
1	16-A	168	ASN
1	16-A	232	GLN
1	16-A	233	GLN
1	16-A	281	GLN
1	16-A	295	HIS
1	16-A	298	ASN
1	16-A	302	ASN
1	16-A	316	ASN
1	16-A	317	ASN
1	16-A	323	GLN
1	16-A	334	GLN
1	16-A	400	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 ⓘ

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, 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	1-A	375/418 (89%)	1.75	130 (34%) ⓘ ⓘ	1, 1, 3, 4	375 (100%)
1	2-A	0/418	-	-	-	-
1	3-A	0/418	-	-	-	-
1	4-A	0/418	-	-	-	-
1	5-A	0/418	-	-	-	-
1	6-A	0/418	-	-	-	-
1	7-A	0/418	-	-	-	-
1	8-A	0/418	-	-	-	-
1	9-A	0/418	-	-	-	-
1	10-A	0/418	-	-	-	-
1	11-A	0/418	-	-	-	-
1	12-A	0/418	-	-	-	-
1	13-A	0/418	-	-	-	-
1	14-A	0/418	-	-	-	-
1	15-A	0/418	-	-	-	-
1	16-A	0/418	-	-	-	-
All	All	375/6688 (5%)	1.75	130 (34%) ⓘ ⓘ	1, 1, 3, 4	375 (100%)

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	292	ALA	7.1
1	1-A	338	VAL	6.7
1	1-A	20	PHE	6.0
1	1-A	264	SER	6.0
1	1-A	381	ARG	6.0
1	1-A	119	ASP	5.9
1	1-A	382	ILE	5.9
1	1-A	354	GLU	5.8
1	1-A	332	LEU	5.7
1	1-A	17	LEU	5.5
1	1-A	206	GLY	5.3

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Mol	Chain	Res	Type	RSRZ
1	1-A	205	THR	5.2
1	1-A	134	GLU	5.2
1	1-A	131	ILE	5.2
1	1-A	265	ILE	4.9
1	1-A	224	ALA	4.8
1	1-A	223	ALA	4.7
1	1-A	337	PHE	4.7
1	1-A	293	ALA	4.7
1	1-A	307	GLY	4.7
1	1-A	298	ASN	4.6
1	1-A	268	GLY	4.5
1	1-A	221	VAL	4.5
1	1-A	116	CYS	4.5
1	1-A	219	ASP	4.4
1	1-A	222	VAL	4.4
1	1-A	291	GLN	4.4
1	1-A	207	LYS	4.3
1	1-A	220	PRO	4.2
1	1-A	218	ILE	4.2
1	1-A	229	LEU	4.2
1	1-A	127	GLY	4.1
1	1-A	294	VAL	4.1
1	1-A	204	ILE	4.1
1	1-A	130	LYS	4.0
1	1-A	301	VAL	4.0
1	1-A	125	LEU	4.0
1	1-A	297	CYS	4.0
1	1-A	236	SER	3.9
1	1-A	296	ARG	3.9
1	1-A	203	VAL	3.9
1	1-A	18	LEU	3.9
1	1-A	267	ILE	3.9
1	1-A	192	SER	3.8
1	1-A	289	THR	3.8
1	1-A	16	LYS	3.8
1	1-A	406	ALA	3.8
1	1-A	353	ALA	3.7
1	1-A	377	SER	3.6
1	1-A	386	VAL	3.5
1	1-A	217	THR	3.5
1	1-A	277	PHE	3.5
1	1-A	331	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	1-A	225	SER	3.3
1	1-A	300	SER	3.3
1	1-A	385	ASP	3.3
1	1-A	266	THR	3.2
1	1-A	376	HIS	3.2
1	1-A	262	PRO	3.1
1	1-A	251	LYS	3.1
1	1-A	227	ILE	3.1
1	1-A	389	TYR	3.0
1	1-A	306	ASN	3.0
1	1-A	334	GLN	2.9
1	1-A	202	ALA	2.9
1	1-A	48	LEU	2.8
1	1-A	91	ASP	2.8
1	1-A	104	GLU	2.8
1	1-A	226	SER	2.8
1	1-A	230	SER	2.8
1	1-A	395	ALA	2.8
1	1-A	59	GLU	2.8
1	1-A	26	VAL	2.8
1	1-A	246	VAL	2.8
1	1-A	237	ARG	2.8
1	1-A	295	HIS	2.8
1	1-A	319	ASP	2.8
1	1-A	25	GLU	2.8
1	1-A	403	LYS	2.8
1	1-A	299	ALA	2.7
1	1-A	263	ASP	2.7
1	1-A	335	GLU	2.7
1	1-A	404	GLU	2.7
1	1-A	372	TYR	2.7
1	1-A	56	SER	2.7
1	1-A	405	LYS	2.7
1	1-A	92	MET	2.6
1	1-A	253	ASN	2.6
1	1-A	23	SER	2.6
1	1-A	322	LYS	2.6
1	1-A	19	GLU	2.6
1	1-A	269	GLY	2.5
1	1-A	233	GLN	2.5
1	1-A	78	ILE	2.5
1	1-A	287	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	1-A	238	GLU	2.5
1	1-A	239	THR	2.5
1	1-A	387	LEU	2.5
1	1-A	336	ALA	2.4
1	1-A	252	VAL	2.4
1	1-A	168	ASN	2.4
1	1-A	241	PRO	2.4
1	1-A	46	GLU	2.4
1	1-A	397	MET	2.4
1	1-A	188	SER	2.4
1	1-A	311	MET	2.3
1	1-A	396	SER	2.3
1	1-A	270	THR	2.3
1	1-A	171	ALA	2.3
1	1-A	242	LEU	2.3
1	1-A	235	VAL	2.3
1	1-A	234	LEU	2.3
1	1-A	138	HIS	2.2
1	1-A	187	ALA	2.2
1	1-A	232	GLN	2.2
1	1-A	167	LYS	2.2
1	1-A	363	LEU	2.2
1	1-A	283	ARG	2.2
1	1-A	326	LYS	2.2
1	1-A	248	THR	2.2
1	1-A	196	GLY	2.1
1	1-A	186	ALA	2.1
1	1-A	123	THR	2.1
1	1-A	43	LEU	2.1
1	1-A	407	SER	2.1
1	1-A	276	GLY	2.1
1	1-A	183	PHE	2.1
1	1-A	154	LEU	2.1
1	1-A	118	HIS	2.1
1	1-A	384	GLU	2.0

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

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.