



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:29 PM UTC

PDB ID : 8EWW / pdb_00008eww
Title : Structure of Arabidopsis fatty acid amide hydrolase mutant S305A
Authors : Aziz, M.; Wang, X.; Gaguancela, O.A.; Chapman, K.D.
Deposited on : 2022-10-24
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

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

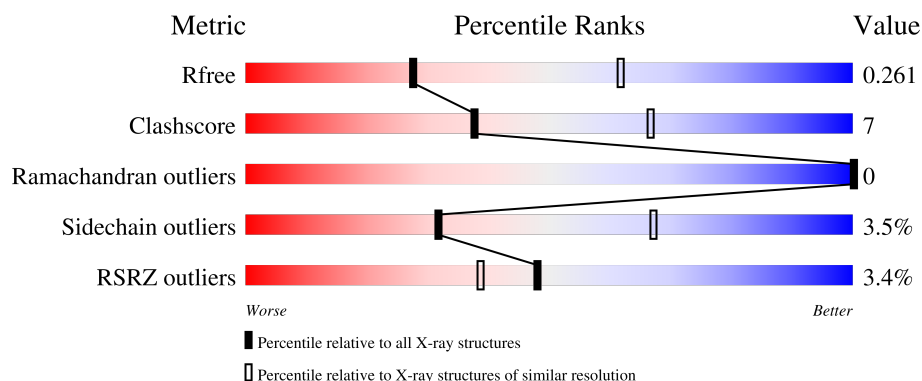
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 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	636	 4% 79% 13% • 7%
1	B	636	 3% 78% 14% • 6%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 9228 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 Fatty acid amide hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	593	Total	C	N	O	S	0	0	0
			4537	2881	764	869	23			
1	B	596	Total	C	N	O	S	0	0	0
			4558	2894	768	872	24			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	305	ALA	SER	engineered mutation	UNP Q7XJJ7
A	608	LYS	-	expression tag	UNP Q7XJJ7
A	609	GLY	-	expression tag	UNP Q7XJJ7
A	610	GLU	-	expression tag	UNP Q7XJJ7
A	611	PHE	-	expression tag	UNP Q7XJJ7
A	612	GLU	-	expression tag	UNP Q7XJJ7
A	613	ALA	-	expression tag	UNP Q7XJJ7
A	614	TYR	-	expression tag	UNP Q7XJJ7
A	615	VAL	-	expression tag	UNP Q7XJJ7
A	616	GLU	-	expression tag	UNP Q7XJJ7
A	617	GLN	-	expression tag	UNP Q7XJJ7
A	618	LYS	-	expression tag	UNP Q7XJJ7
A	619	LEU	-	expression tag	UNP Q7XJJ7
A	620	ILE	-	expression tag	UNP Q7XJJ7
A	621	SER	-	expression tag	UNP Q7XJJ7
A	622	GLU	-	expression tag	UNP Q7XJJ7
A	623	GLU	-	expression tag	UNP Q7XJJ7
A	624	ASP	-	expression tag	UNP Q7XJJ7
A	625	LEU	-	expression tag	UNP Q7XJJ7
A	626	ASN	-	expression tag	UNP Q7XJJ7
A	627	SER	-	expression tag	UNP Q7XJJ7
A	628	ALA	-	expression tag	UNP Q7XJJ7
A	629	VAL	-	expression tag	UNP Q7XJJ7
A	630	ASP	-	expression tag	UNP Q7XJJ7
A	631	HIS	-	expression tag	UNP Q7XJJ7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	632	HIS	-	expression tag	UNP Q7XJJ7
A	633	HIS	-	expression tag	UNP Q7XJJ7
A	634	HIS	-	expression tag	UNP Q7XJJ7
A	635	HIS	-	expression tag	UNP Q7XJJ7
A	636	HIS	-	expression tag	UNP Q7XJJ7
B	305	ALA	SER	engineered mutation	UNP Q7XJJ7
B	608	LYS	-	expression tag	UNP Q7XJJ7
B	609	GLY	-	expression tag	UNP Q7XJJ7
B	610	GLU	-	expression tag	UNP Q7XJJ7
B	611	PHE	-	expression tag	UNP Q7XJJ7
B	612	GLU	-	expression tag	UNP Q7XJJ7
B	613	ALA	-	expression tag	UNP Q7XJJ7
B	614	TYR	-	expression tag	UNP Q7XJJ7
B	615	VAL	-	expression tag	UNP Q7XJJ7
B	616	GLU	-	expression tag	UNP Q7XJJ7
B	617	GLN	-	expression tag	UNP Q7XJJ7
B	618	LYS	-	expression tag	UNP Q7XJJ7
B	619	LEU	-	expression tag	UNP Q7XJJ7
B	620	ILE	-	expression tag	UNP Q7XJJ7
B	621	SER	-	expression tag	UNP Q7XJJ7
B	622	GLU	-	expression tag	UNP Q7XJJ7
B	623	GLU	-	expression tag	UNP Q7XJJ7
B	624	ASP	-	expression tag	UNP Q7XJJ7
B	625	LEU	-	expression tag	UNP Q7XJJ7
B	626	ASN	-	expression tag	UNP Q7XJJ7
B	627	SER	-	expression tag	UNP Q7XJJ7
B	628	ALA	-	expression tag	UNP Q7XJJ7
B	629	VAL	-	expression tag	UNP Q7XJJ7
B	630	ASP	-	expression tag	UNP Q7XJJ7
B	631	HIS	-	expression tag	UNP Q7XJJ7
B	632	HIS	-	expression tag	UNP Q7XJJ7
B	633	HIS	-	expression tag	UNP Q7XJJ7
B	634	HIS	-	expression tag	UNP Q7XJJ7
B	635	HIS	-	expression tag	UNP Q7XJJ7
B	636	HIS	-	expression tag	UNP Q7XJJ7

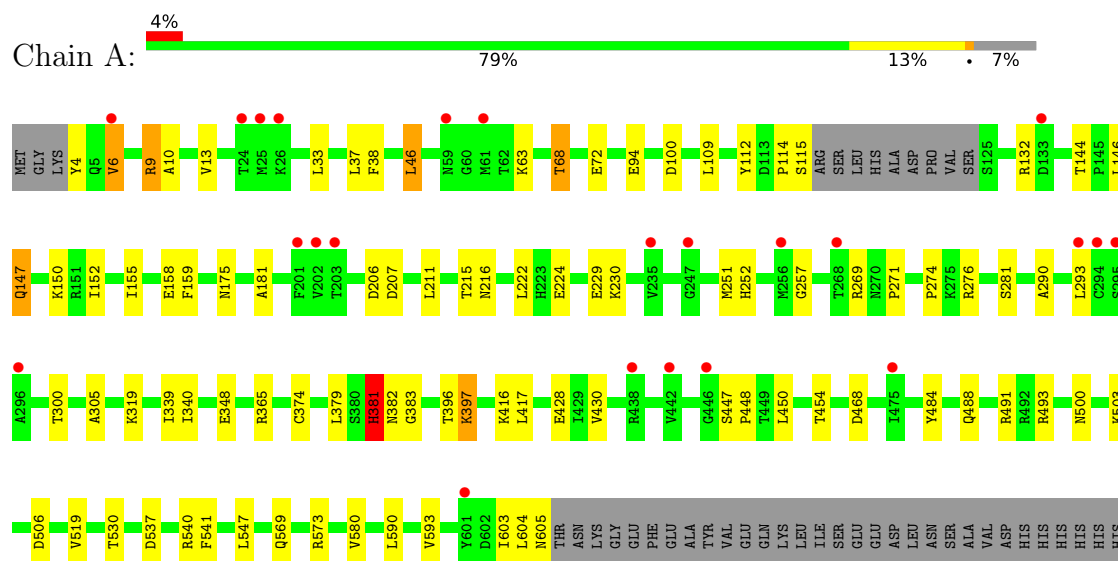
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	66	Total O 66 66	0	0
2	B	67	Total O 67 67	0	0

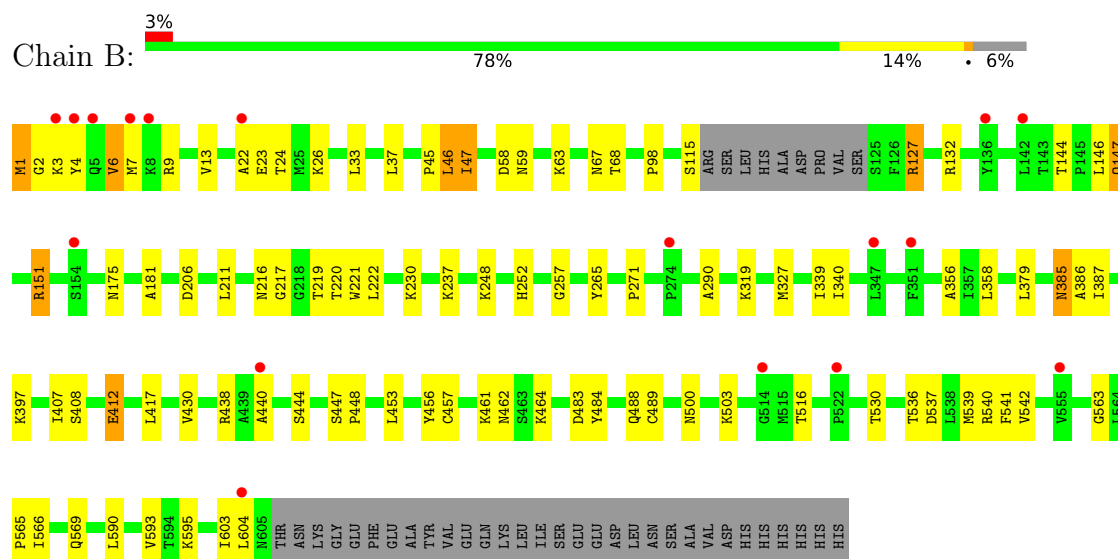
3 Residue-property plots [i](#)

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: Fatty acid amide hydrolase



• Molecule 1: Fatty acid amide hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.45Å 81.32Å 133.18Å 90.00° 104.51° 90.00°	Depositor
Resolution (Å)	38.78 – 2.80 38.78 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (38.78-2.80) 98.6 (38.78-2.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.234 , 0.260 0.237 , 0.261	Depositor DCC
R_{free} test set	1883 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	82.6	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9228	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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	A	0.14	0/4633	0.34	2/6292 (0.0%)
1	B	0.12	0/4654	0.33	2/6318 (0.0%)
All	All	0.13	0/9287	0.33	4/12610 (0.0%)

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	22	ALA	N-CA-C	-9.71	97.71	110.43
1	B	22	ALA	CB-CA-C	6.25	122.60	109.65
1	A	381	HIS	N-CA-C	5.59	122.70	110.80
1	A	10	ALA	N-CA-C	-5.11	105.89	112.68

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	381	HIS	Peptide

5.2 Too-close contacts [i](#)

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	4537	0	4560	62	0
1	B	4558	0	4588	66	0
2	A	66	0	0	17	0
2	B	67	0	0	20	0
All	All	9228	0	9148	127	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 7.

All (127) 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:221:TRP:CD1	1:B:464:LYS:HB3	2.00	0.97
1:B:489:CYS:SG	2:B:720:HOH:O	2.29	0.91
1:A:224:GLU:O	2:A:701:HOH:O	1.93	0.86
1:B:386:ALA:N	2:B:706:HOH:O	2.22	0.73
1:B:221:TRP:CD1	2:B:703:HOH:O	2.41	0.72
1:B:221:TRP:CD1	1:B:464:LYS:CB	2.73	0.71
1:A:63:LYS:O	1:A:68:THR:OG1	2.09	0.69
1:A:540:ARG:NH2	2:A:711:HOH:O	2.27	0.68
1:B:221:TRP:HD1	2:B:703:HOH:O	1.75	0.68
1:A:397:LYS:NZ	1:A:428:GLU:OE2	2.25	0.68
1:A:381:HIS:H	1:A:383:GLY:H	1.40	0.67
1:A:319:LYS:HE2	1:A:339:ILE:HG12	1.79	0.65
1:B:221:TRP:HD1	1:B:464:LYS:HB3	1.57	0.65
1:B:6:VAL:HB	1:B:68:THR:HG23	1.81	0.63
1:B:319:LYS:HE2	1:B:339:ILE:HG12	1.81	0.62
1:B:397:LYS:NZ	2:B:717:HOH:O	2.32	0.61
1:B:385:ASN:ND2	2:B:715:HOH:O	2.32	0.61
1:A:603:ILE:HG22	1:A:604:LEU:H	1.66	0.61
1:B:603:ILE:HG22	1:B:604:LEU:H	1.67	0.60
1:A:365:ARG:NH1	2:A:708:HOH:O	2.24	0.59
1:A:381:HIS:H	1:A:383:GLY:N	2.01	0.59
1:B:23:GLU:OE2	1:B:438:ARG:NH1	2.36	0.58
1:A:216:ASN:HA	1:A:222:LEU:HB3	1.86	0.58
1:A:229:GLU:OE1	2:A:702:HOH:O	2.17	0.58
1:B:151:ARG:HG2	1:B:603:ILE:HG23	1.85	0.58
1:B:211:LEU:HD11	1:B:230:LYS:HA	1.86	0.58
1:A:271:PRO:HG2	1:A:290:ALA:HB3	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:THR:HB	1:A:397:LYS:HZ1	1.69	0.57
1:B:563:GLY:O	1:B:595:LYS:NZ	2.37	0.57
1:B:327:MET:HG2	1:B:340:ILE:HG13	1.88	0.56
1:A:9:ARG:O	1:A:13:VAL:HG23	2.06	0.56
1:B:500:ASN:HA	1:B:503:LYS:HD3	1.88	0.55
1:A:381:HIS:N	1:A:383:GLY:H	2.05	0.55
1:B:1:MET:HB3	1:B:7:MET:HG2	1.87	0.55
1:A:605:ASN:ND2	2:A:724:HOH:O	2.39	0.54
1:B:387:ILE:HG12	2:B:706:HOH:O	2.07	0.54
1:A:155:ILE:O	2:A:703:HOH:O	2.18	0.53
1:A:46:LEU:HD21	1:B:46:LEU:HD21	1.91	0.53
1:B:541:PHE:O	1:B:569:GLN:NE2	2.36	0.53
1:B:216:ASN:HA	1:B:222:LEU:HB3	1.91	0.53
1:A:381:HIS:HA	1:A:383:GLY:H	1.74	0.52
1:A:132:ARG:NH2	1:A:348:GLU:OE2	2.42	0.52
1:A:379:LEU:H	1:A:379:LEU:HD23	1.74	0.52
1:B:63:LYS:HA	1:B:67:ASN:HB2	1.91	0.52
1:A:146:LEU:HG	1:A:150:LYS:HE2	1.91	0.52
1:B:417:LEU:HD23	1:B:590:LEU:HB3	1.92	0.52
1:B:536:THR:O	2:B:701:HOH:O	2.19	0.51
1:A:374:CYS:HB2	2:A:719:HOH:O	2.10	0.51
1:A:215:THR:HA	2:A:723:HOH:O	2.11	0.51
1:B:417:LEU:HB3	1:B:590:LEU:HD13	1.93	0.50
1:B:565:PRO:HD2	2:B:732:HOH:O	2.11	0.50
1:A:152:ILE:HG23	1:A:293:LEU:HD22	1.93	0.49
1:A:305:ALA:HB2	2:A:761:HOH:O	2.12	0.49
1:A:417:LEU:HD23	1:A:590:LEU:HB3	1.94	0.49
1:B:356:ALA:HB3	2:B:714:HOH:O	2.12	0.49
1:A:38:PHE:HB3	2:A:718:HOH:O	2.12	0.49
1:B:221:TRP:O	1:B:221:TRP:HE3	1.96	0.49
1:A:300:THR:HG22	1:A:340:ILE:HG12	1.94	0.48
1:A:491:ARG:HG3	1:A:547:LEU:HG	1.96	0.48
1:A:500:ASN:HA	1:A:503:LYS:HD3	1.95	0.48
1:A:276:ARG:HA	1:A:519:VAL:HA	1.96	0.48
1:B:144:THR:HG23	1:B:147:GLN:H	1.78	0.47
1:B:206:ASP:OD2	1:B:217:GLY:N	2.47	0.47
1:A:506:ASP:OD1	1:A:573:ARG:NH2	2.40	0.47
1:B:483:ASP:OD2	2:B:702:HOH:O	2.20	0.47
1:B:219:THR:O	1:B:265:TYR:OH	2.33	0.47
1:A:541:PHE:O	1:A:569:GLN:NE2	2.39	0.46
1:A:159:PHE:N	2:A:703:HOH:O	2.20	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ASP:OD2	1:A:300:THR:OG1	2.33	0.46
1:B:115:SER:N	2:B:727:HOH:O	2.46	0.46
1:B:271:PRO:HG2	1:B:290:ALA:HB3	1.98	0.46
1:B:457:CYS:HB3	1:B:462:ASN:HB2	1.97	0.46
1:A:109:LEU:HD22	1:A:348:GLU:HG3	1.98	0.45
1:B:9:ARG:O	1:B:13:VAL:HG23	2.16	0.45
1:B:2:GLY:O	1:B:3:LYS:HD2	2.16	0.45
1:A:252:HIS:CE1	1:A:257:GLY:HA3	2.51	0.45
1:B:98:PRO:HB3	1:B:356:ALA:HB1	1.99	0.45
1:B:407:ILE:HA	1:B:566:ILE:HD13	1.99	0.45
1:A:94:GLU:O	2:A:704:HOH:O	2.21	0.44
1:A:252:HIS:NE2	1:A:468:ASP:OD2	2.46	0.44
1:A:484:TYR:O	1:A:488:GLN:HG2	2.17	0.44
1:B:221:TRP:NE1	1:B:464:LYS:CB	2.80	0.44
1:B:444:SER:N	2:B:709:HOH:O	2.28	0.44
1:A:381:HIS:N	1:A:383:GLY:N	2.64	0.44
1:B:461:LYS:HD3	1:B:464:LYS:HD2	2.00	0.44
1:A:158:GLU:HB3	2:A:703:HOH:O	2.17	0.44
1:B:146:LEU:HA	1:B:181:ALA:HB1	2.00	0.44
1:B:206:ASP:HA	1:B:248:LYS:HE2	1.98	0.44
1:B:252:HIS:CE1	1:B:257:GLY:HA3	2.53	0.44
1:A:112:TYR:CE2	1:A:114:PRO:HG3	2.53	0.44
1:A:146:LEU:HA	1:A:181:ALA:HB1	2.00	0.44
1:B:603:ILE:HG22	1:B:604:LEU:N	2.32	0.44
1:A:100:ASP:OD2	2:A:705:HOH:O	2.21	0.43
1:B:537:ASP:OD1	1:B:540:ARG:NH1	2.41	0.43
1:A:450:LEU:O	1:A:454:THR:OG1	2.32	0.43
1:B:1:MET:O	1:B:6:VAL:HA	2.18	0.43
1:B:453:LEU:HD23	1:B:456:TYR:HD2	1.83	0.43
1:A:144:THR:HG23	1:A:147:GLN:H	1.84	0.42
1:B:132:ARG:NH1	2:B:724:HOH:O	2.41	0.42
1:B:63:LYS:HE2	1:B:63:LYS:HB3	1.81	0.42
1:B:220:THR:OG1	2:B:703:HOH:O	2.21	0.42
1:B:408:SER:O	1:B:412:GLU:HB2	2.20	0.42
1:A:537:ASP:HA	1:A:540:ARG:HH12	1.85	0.42
1:B:537:ASP:N	2:B:711:HOH:O	2.52	0.42
1:B:539:MET:HA	1:B:542:VAL:HG22	2.00	0.42
1:A:281:SER:H	1:A:305:ALA:CB	2.33	0.42
1:B:484:TYR:O	1:B:488:GLN:HG2	2.20	0.42
1:B:447:SER:HB2	1:B:448:PRO:HD3	2.01	0.42
1:A:6:VAL:HB	1:A:68:THR:HG23	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:GLU:HB2	2:A:707:HOH:O	2.20	0.41
1:A:6:VAL:CG2	1:A:68:THR:HG23	2.51	0.41
1:A:211:LEU:HD11	1:A:230:LYS:HA	2.03	0.41
1:B:26:LYS:NZ	2:B:704:HOH:O	2.34	0.41
1:B:58:ASP:OD2	2:B:704:HOH:O	2.21	0.41
1:A:115:SER:N	2:A:727:HOH:O	2.42	0.41
1:B:47:ILE:H	1:B:47:ILE:HG13	1.51	0.41
1:B:237:LYS:NZ	1:B:358:LEU:O	2.49	0.41
1:A:72:GLU:OE1	1:A:493:ARG:NH1	2.52	0.41
1:A:281:SER:H	1:A:305:ALA:HB1	1.85	0.41
1:A:381:HIS:HA	1:A:382:ASN:HA	1.71	0.41
1:B:127:ARG:HH11	1:B:127:ARG:H	1.68	0.41
1:A:416:LYS:HA	2:A:749:HOH:O	2.20	0.41
1:A:269:ARG:HB3	1:A:274:PRO:HA	2.03	0.40
1:A:447:SER:HB2	1:A:448:PRO:HD3	2.02	0.40
1:B:45:PRO:O	2:B:707:HOH:O	2.22	0.40
1:A:206:ASP:HB3	1:A:251:MET:SD	2.62	0.40
1:B:440:ALA:C	2:B:709:HOH:O	2.64	0.40

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	589/636 (93%)	569 (97%)	20 (3%)	0	100	100
1	B	592/636 (93%)	566 (96%)	26 (4%)	0	100	100
All	All	1181/1272 (93%)	1135 (96%)	46 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	501/539 (93%)	486 (97%)	15 (3%)	36	72
1	B	503/539 (93%)	483 (96%)	20 (4%)	28	63
All	All	1004/1078 (93%)	969 (96%)	35 (4%)	32	67

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	TYR
1	A	6	VAL
1	A	9	ARG
1	A	33	LEU
1	A	37	LEU
1	A	46	LEU
1	A	68	THR
1	A	147	GLN
1	A	175	ASN
1	A	381	HIS
1	A	397	LYS
1	A	430	VAL
1	A	530	THR
1	A	580	VAL
1	A	593	VAL
1	B	1	MET
1	B	4	TYR
1	B	6	VAL
1	B	24	THR
1	B	33	LEU
1	B	37	LEU
1	B	46	LEU
1	B	47	ILE
1	B	59	ASN
1	B	127	ARG
1	B	147	GLN
1	B	151	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	175	ASN
1	B	379	LEU
1	B	385	ASN
1	B	412	GLU
1	B	430	VAL
1	B	516	THR
1	B	530	THR
1	B	593	VAL

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

Mol	Chain	Res	Type
1	A	67	ASN
1	A	192	ASN
1	A	213	HIS
1	B	147	GLN
1	B	272	HIS
1	B	527	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	A	593/636 (93%)	0.34	23 (3%) 43 34	67, 92, 124, 141	0
1	B	596/636 (93%)	0.36	17 (2%) 53 43	67, 103, 143, 170	0
All	All	1189/1272 (93%)	0.35	40 (3%) 48 39	67, 97, 136, 170	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	442	VAL	5.2
1	A	201	PHE	4.6
1	A	203	THR	4.4
1	A	296	ALA	3.7
1	A	247	GLY	3.6
1	A	446	GLY	3.5
1	B	22	ALA	3.5
1	B	604	LEU	3.2
1	A	25	MET	3.2
1	A	59	ASN	3.1
1	A	61	MET	3.1
1	A	293	LEU	2.9
1	B	7	MET	2.7
1	A	202	VAL	2.7
1	B	154	SER	2.7
1	B	555	VAL	2.7
1	B	351	PHE	2.6
1	A	268	THR	2.6
1	A	294	CYS	2.5
1	A	6	VAL	2.5
1	B	514	GLY	2.4
1	A	133	ASP	2.4
1	B	5	GLN	2.3
1	A	24	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	4	TYR	2.3
1	B	522	PRO	2.2
1	B	347	LEU	2.2
1	A	475	ILE	2.2
1	B	8	LYS	2.2
1	A	295	SER	2.2
1	A	438	ARG	2.1
1	A	235	VAL	2.1
1	B	440	ALA	2.1
1	B	142	LEU	2.1
1	A	601	TYR	2.1
1	A	26	LYS	2.1
1	B	136	TYR	2.1
1	A	256	MET	2.0
1	B	274	PRO	2.0
1	B	3	LYS	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 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.