



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:13 PM UTC

PDB ID : 5MGV / pdb_00005mgv
Title : Kinetic and Structural Changes in HsmtPheRS, Induced by Pathogenic Mutations in Human FARS2
Authors : Kartvelishvili, E.; Tworowski, D.; Vernon, H.; Chrzanowska-Lightowlers, Z.; Moor, N.; Wang, J.; Wong, L.-J.; Safro, M.
Deposited on : 2016-11-22
Resolution : 2.05 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

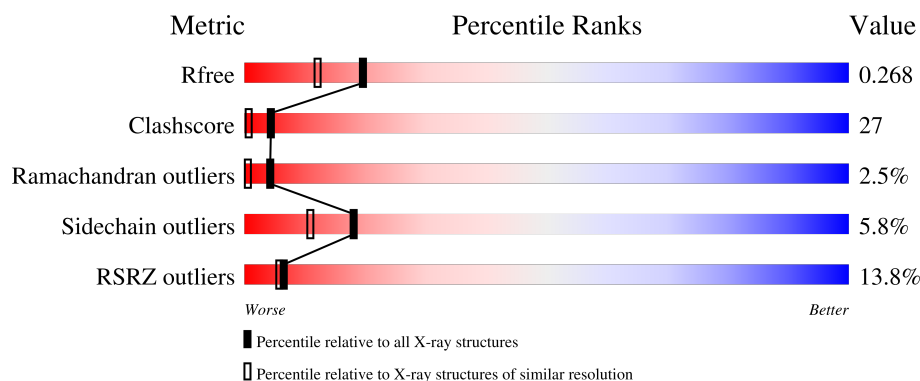
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	405	14% 60% 31% 6% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3607 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 Phenylalanine-tRNA ligase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3358	2153	593	600	12			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	289	TYR	ASP	engineered mutation	UNP O95363

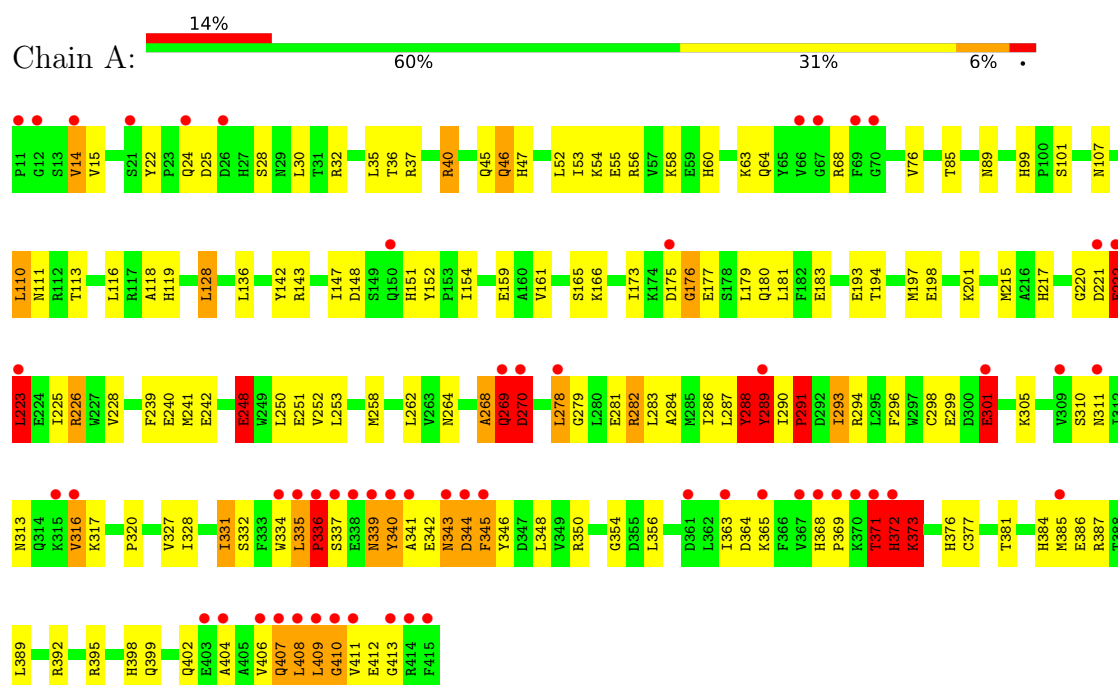
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	249	Total	O	0	0
			249	249		

3 Residue-property plots

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: Phenylalanine-tRNA ligase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.77Å 90.37Å 95.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.05 50.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	93.2 (50.00-2.05) 93.2 (50.00-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.05Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.271 0.227 , 0.268	Depositor DCC
R_{free} test set	1373 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3607	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.11% 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	1.40	26/3450 (0.8%)	1.58	41/4667 (0.9%)

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	12

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	268	ALA	C-N	33.30	1.80	1.33
1	A	408	LEU	C-N	28.84	1.78	1.33
1	A	289	TYR	C-N	-27.55	1.04	1.33
1	A	269	GLN	C-N	-22.79	1.01	1.33
1	A	372	HIS	C-N	-18.80	1.07	1.33
1	A	365	LYS	C-N	16.56	1.53	1.33
1	A	335	LEU	C-N	15.60	1.70	1.33
1	A	278	LEU	C-N	14.57	1.54	1.33
1	A	46	GLN	C-N	14.22	1.53	1.33
1	A	180	GLN	C-N	13.56	1.53	1.33
1	A	248	GLU	C-N	-12.42	1.16	1.33
1	A	222	GLU	C-N	10.62	1.47	1.33
1	A	299	GLU	C-N	10.47	1.48	1.33
1	A	336	PRO	C-N	-10.09	1.19	1.33
1	A	339	ASN	C-N	9.89	1.45	1.33
1	A	221	ASP	C-N	-8.96	1.20	1.33
1	A	340	TYR	C-N	-8.35	1.21	1.33
1	A	223	LEU	C-N	7.86	1.44	1.33
1	A	175	ASP	C-N	7.81	1.44	1.33
1	A	270	ASP	C-N	7.58	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	344	ASP	C-N	7.13	1.43	1.34
1	A	63	LYS	C-N	6.99	1.43	1.34
1	A	183	GLU	C-N	-6.65	1.21	1.34
1	A	373	LYS	C-N	6.46	1.42	1.33
1	A	288	TYR	C-N	6.44	1.42	1.33
1	A	40	ARG	C-N	-5.11	1.26	1.33

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	TYR	O-C-N	-38.15	71.84	122.59
1	A	269	GLN	O-C-N	-29.17	83.79	122.59
1	A	372	HIS	CA-C-N	22.68	164.85	121.54
1	A	372	HIS	C-N-CA	22.68	164.85	121.54
1	A	372	HIS	O-C-N	-21.83	93.56	122.59
1	A	270	ASP	O-C-N	-19.74	96.34	122.59
1	A	336	PRO	O-C-N	-17.10	99.56	122.64
1	A	335	LEU	CA-C-N	-17.03	98.56	119.84
1	A	335	LEU	C-N-CA	-17.03	98.56	119.84
1	A	289	TYR	CA-C-N	13.38	146.06	120.11
1	A	289	TYR	C-N-CA	13.38	146.06	120.11
1	A	268	ALA	CA-C-N	-13.28	96.17	121.54
1	A	268	ALA	C-N-CA	-13.28	96.17	121.54
1	A	269	GLN	CA-C-N	12.09	144.62	121.54
1	A	269	GLN	C-N-CA	12.09	144.62	121.54
1	A	248	GLU	O-C-N	-11.85	107.11	123.34
1	A	373	LYS	O-C-N	-11.47	107.33	122.59
1	A	340	TYR	O-C-N	-9.08	113.93	123.56
1	A	301	GLU	O-C-N	-8.87	110.79	122.59
1	A	278	LEU	O-C-N	8.31	134.03	123.23
1	A	288	TYR	O-C-N	-8.08	111.76	122.19
1	A	365	LYS	O-C-N	8.05	132.38	123.52
1	A	299	GLU	O-C-N	7.89	132.00	122.21
1	A	289	TYR	CB-CA-C	-7.62	95.26	110.42
1	A	110	LEU	N-CA-C	-7.39	102.61	111.69
1	A	46	GLN	O-C-N	7.13	131.62	123.06
1	A	180	GLN	O-C-N	7.10	132.83	122.97
1	A	408	LEU	O-C-N	6.51	130.00	122.25
1	A	371	THR	N-CA-C	6.24	118.08	111.28
1	A	165	SER	N-CA-C	-6.07	101.53	110.52
1	A	63	LYS	O-C-N	5.88	128.20	122.09
1	A	290	ILE	CB-CA-C	5.86	117.42	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ASP	O-C-N	5.80	129.40	122.26
1	A	291	PRO	CA-N-CD	-5.64	104.11	112.00
1	A	220	GLY	O-C-N	5.40	129.16	122.78
1	A	348	LEU	N-CA-C	-5.39	105.40	111.28
1	A	220	GLY	N-CA-C	-5.28	106.03	112.68
1	A	345	PHE	N-CA-C	-5.26	105.66	111.71
1	A	76	VAL	N-CA-C	5.26	115.47	108.11
1	A	240	GLU	N-CA-C	-5.14	100.66	109.24
1	A	116	LEU	N-CA-C	-5.04	101.09	109.46

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	222	GLU	Mainchain
1	A	248	GLU	Mainchain
1	A	269	GLN	Mainchain
1	A	270	ASP	Mainchain
1	A	288	TYR	Mainchain,Peptide
1	A	289	TYR	Mainchain
1	A	301	GLU	Mainchain
1	A	336	PRO	Mainchain
1	A	372	HIS	Mainchain,Peptide
1	A	373	LYS	Mainchain

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	3358	0	3259	177	0
2	A	249	0	0	28	0
All	All	3607	0	3259	177	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 27.

All (177) 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:335:LEU:C	1:A:336:PRO:N	1.70	1.46
1:A:408:LEU:C	1:A:409:LEU:N	1.78	1.39
1:A:268:ALA:C	1:A:269:GLN:N	1.80	1.39
1:A:223:LEU:HD12	1:A:223:LEU:O	1.24	1.27
1:A:406:VAL:C	1:A:407:GLN:N	2.02	1.18
1:A:371:THR:OG1	1:A:373:LYS:HB2	1.43	1.17
1:A:223:LEU:O	1:A:223:LEU:CD1	1.98	1.11
1:A:223:LEU:HD13	1:A:225:ILE:HG23	1.41	1.02
1:A:377:CYS:HB3	2:A:503:HOH:O	1.65	0.96
1:A:40:ARG:NH2	1:A:45:GLN:OE1	2.01	0.93
1:A:335:LEU:C	1:A:336:PRO:CA	2.41	0.93
1:A:406:VAL:C	1:A:407:GLN:CA	2.42	0.92
1:A:268:ALA:C	1:A:269:GLN:CA	2.43	0.91
1:A:406:VAL:C	1:A:407:GLN:HA	1.96	0.89
1:A:289:TYR:HB3	2:A:504:HOH:O	1.72	0.89
1:A:58:LYS:HD3	2:A:501:HOH:O	1.72	0.88
1:A:223:LEU:HD12	1:A:223:LEU:C	1.98	0.87
1:A:223:LEU:CD1	1:A:223:LEU:C	2.43	0.87
1:A:407:GLN:N	1:A:408:LEU:N	2.23	0.86
1:A:368:HIS:HB3	1:A:371:THR:HG23	1.58	0.86
1:A:239:PHE:HB3	2:A:505:HOH:O	1.75	0.85
1:A:342:GLU:HG2	1:A:346:TYR:CE2	2.13	0.83
1:A:320:PRO:HG3	2:A:504:HOH:O	1.77	0.83
1:A:223:LEU:CD1	1:A:225:ILE:HG23	2.08	0.82
1:A:269:GLN:N	1:A:269:GLN:CD	2.36	0.81
1:A:371:THR:OG1	1:A:373:LYS:CB	2.27	0.81
1:A:363:ILE:HG13	2:A:503:HOH:O	1.78	0.80
1:A:408:LEU:CA	1:A:409:LEU:N	2.44	0.80
1:A:336:PRO:HD2	1:A:339:ASN:O	1.83	0.78
1:A:343:ASN:HA	1:A:346:TYR:CD2	2.19	0.77
1:A:409:LEU:O	1:A:411:VAL:HG13	1.83	0.77
1:A:270:ASP:N	1:A:270:ASP:OD1	2.16	0.76
1:A:268:ALA:C	1:A:269:GLN:C	2.55	0.75
1:A:225:ILE:C	1:A:225:ILE:HD12	2.13	0.73
1:A:343:ASN:HA	1:A:346:TYR:HD2	1.53	0.73
1:A:250:LEU:HD12	1:A:286:ILE:HD11	1.70	0.72
1:A:301:GLU:OE1	1:A:305:LYS:HB3	1.89	0.72
1:A:311:ASN:HD22	1:A:313:ASN:HB2	1.57	0.70
1:A:147:ILE:HD12	1:A:350:ARG:NE	2.07	0.69
1:A:408:LEU:N	1:A:409:LEU:N	2.39	0.69
1:A:404:ALA:O	1:A:408:LEU:N	2.26	0.69
1:A:46:GLN:HG2	1:A:47:HIS:CD2	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:HIS:HD2	1:A:101:SER:OG	1.79	0.66
1:A:248:GLU:HG2	1:A:250:LEU:HD21	1.76	0.66
1:A:25:ASP:OD2	1:A:111:ASN:HB2	1.96	0.66
1:A:288:TYR:CE1	1:A:316:VAL:HG11	2.31	0.65
1:A:147:ILE:HD12	1:A:350:ARG:HE	1.62	0.65
1:A:24:GLN:OE1	1:A:28:SER:HB3	1.97	0.65
1:A:54:LYS:HG2	2:A:501:HOH:O	1.97	0.64
1:A:327:VAL:C	1:A:328:ILE:HD13	2.22	0.64
1:A:410:GLY:N	2:A:502:HOH:O	2.31	0.63
1:A:225:ILE:HD12	1:A:225:ILE:O	1.98	0.63
1:A:252:VAL:HG12	1:A:282:ARG:HG3	1.80	0.62
1:A:384:HIS:HB3	1:A:387:ARG:O	1.99	0.62
1:A:223:LEU:HD13	1:A:223:LEU:C	2.25	0.61
1:A:368:HIS:HB3	2:A:506:HOH:O	1.98	0.61
1:A:268:ALA:O	1:A:269:GLN:C	2.44	0.60
1:A:335:LEU:HG	1:A:340:TYR:CG	2.36	0.60
1:A:334:TRP:O	1:A:411:VAL:HA	2.00	0.60
1:A:226:ARG:HD3	1:A:242:GLU:OE1	2.01	0.59
1:A:406:VAL:O	1:A:407:GLN:HA	2.03	0.58
1:A:371:THR:O	1:A:372:HIS:HB2	2.02	0.58
1:A:15:VAL:HG23	1:A:24:GLN:CD	2.29	0.58
1:A:253:LEU:C	1:A:253:LEU:HD12	2.29	0.58
1:A:364:ASP:N	2:A:503:HOH:O	2.35	0.58
1:A:35:LEU:O	1:A:35:LEU:HD23	2.03	0.58
1:A:248:GLU:HG2	1:A:250:LEU:CD2	2.34	0.57
1:A:408:LEU:C	1:A:409:LEU:CA	2.75	0.57
1:A:55:GLU:OE2	2:A:501:HOH:O	2.17	0.57
1:A:281:GLU:HG2	1:A:293:ILE:HD11	1.86	0.57
1:A:341:ALA:HB3	1:A:344:ASP:CG	2.31	0.56
1:A:364:ASP:HB3	2:A:503:HOH:O	2.05	0.56
1:A:407:GLN:C	1:A:408:LEU:N	2.64	0.56
1:A:328:ILE:CD1	1:A:381:THR:HG23	2.36	0.55
1:A:409:LEU:O	1:A:411:VAL:N	2.39	0.55
1:A:288:TYR:CE1	1:A:316:VAL:CG1	2.89	0.55
1:A:14:VAL:HG12	1:A:14:VAL:O	2.05	0.55
1:A:197:MET:O	1:A:201:LYS:HG2	2.07	0.54
1:A:392:ARG:HA	1:A:395:ARG:HH12	1.72	0.54
1:A:328:ILE:HD12	1:A:381:THR:HA	1.89	0.54
1:A:89:ASN:ND2	1:A:118:ALA:H	2.06	0.53
1:A:128:LEU:HD21	1:A:258:MET:HE1	1.91	0.52
1:A:392:ARG:HA	1:A:395:ARG:NH1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLU:N	2:A:501:HOH:O	2.43	0.52
1:A:262:LEU:C	1:A:262:LEU:HD23	2.34	0.52
1:A:293:ILE:HD13	1:A:293:ILE:O	2.09	0.52
1:A:342:GLU:HG2	1:A:346:TYR:CZ	2.43	0.52
1:A:89:ASN:HD21	1:A:118:ALA:H	1.57	0.52
1:A:369:PRO:O	1:A:372:HIS:CE1	2.63	0.51
1:A:279:GLY:O	1:A:283:LEU:HD13	2.11	0.51
1:A:278:LEU:HD12	1:A:278:LEU:O	2.11	0.51
1:A:53:ILE:HD11	1:A:284:ALA:HA	1.93	0.51
1:A:404:ALA:O	1:A:407:GLN:N	2.43	0.51
1:A:341:ALA:HB3	1:A:344:ASP:OD1	2.12	0.50
1:A:177:GLU:HA	2:A:583:HOH:O	2.11	0.50
1:A:225:ILE:C	1:A:225:ILE:CD1	2.83	0.50
1:A:334:TRP:HB2	1:A:412:GLU:HB3	1.94	0.50
1:A:291:PRO:HD3	2:A:504:HOH:O	2.12	0.50
1:A:407:GLN:CB	1:A:408:LEU:HD23	2.42	0.49
1:A:35:LEU:HD23	1:A:35:LEU:C	2.36	0.49
1:A:147:ILE:HD12	1:A:350:ARG:CZ	2.42	0.49
1:A:128:LEU:HD11	1:A:161:VAL:HG11	1.95	0.49
1:A:334:TRP:CH2	1:A:368:HIS:HB2	2.46	0.49
1:A:253:LEU:HB3	1:A:278:LEU:HB3	1.95	0.49
1:A:384:HIS:HB2	1:A:389:LEU:HG	1.95	0.49
1:A:287:LEU:HD23	1:A:288:TYR:CZ	2.47	0.49
1:A:107:ASN:HA	2:A:534:HOH:O	2.13	0.48
1:A:331:ILE:HD12	1:A:332:SER:N	2.28	0.48
1:A:179:LEU:HD22	1:A:198:GLU:HG2	1.94	0.48
1:A:336:PRO:HG3	1:A:410:GLY:O	2.12	0.48
1:A:142:TYR:CD1	1:A:154:ILE:HG12	2.48	0.48
1:A:395:ARG:O	1:A:399:GLN:HG3	2.14	0.48
1:A:407:GLN:C	1:A:408:LEU:HA	2.39	0.47
1:A:409:LEU:O	1:A:410:GLY:C	2.57	0.47
1:A:407:GLN:HB3	1:A:408:LEU:HD23	1.97	0.47
1:A:64:GLN:HE22	1:A:68:ARG:HE	1.63	0.47
1:A:369:PRO:O	1:A:372:HIS:ND1	2.48	0.47
1:A:32:ARG:O	1:A:36:THR:HG23	2.15	0.47
1:A:356:LEU:HD11	1:A:389:LEU:HD21	1.97	0.47
1:A:166:LYS:HB2	1:A:181:LEU:HG	1.97	0.47
1:A:264:ASN:OD1	1:A:269:GLN:HA	2.16	0.46
1:A:345:PHE:HA	1:A:409:LEU:HD21	1.98	0.46
1:A:364:ASP:CB	2:A:503:HOH:O	2.62	0.46
1:A:22:TYR:CG	1:A:110:LEU:HD23	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:PRO:O	1:A:337:SER:C	2.58	0.46
1:A:148:ASP:OD2	1:A:151:HIS:HD2	1.98	0.46
1:A:54:LYS:C	2:A:501:HOH:O	2.59	0.46
1:A:228:VAL:N	2:A:505:HOH:O	2.49	0.45
1:A:294:ARG:NH2	1:A:385:MET:HE3	2.31	0.45
1:A:328:ILE:HD11	1:A:381:THR:HG23	1.98	0.45
1:A:335:LEU:O	1:A:336:PRO:CA	2.61	0.45
1:A:336:PRO:HG3	1:A:410:GLY:C	2.42	0.45
1:A:409:LEU:C	1:A:411:VAL:N	2.73	0.45
1:A:311:ASN:ND2	1:A:313:ASN:HB2	2.27	0.45
1:A:399:GLN:HG2	2:A:582:HOH:O	2.16	0.44
1:A:294:ARG:HH21	1:A:385:MET:HE3	1.83	0.44
1:A:373:LYS:N	2:A:506:HOH:O	2.49	0.44
1:A:215:MET:HB3	1:A:223:LEU:HD21	2.00	0.44
1:A:340:TYR:OH	1:A:345:PHE:HB2	2.18	0.44
1:A:250:LEU:HB3	1:A:282:ARG:HE	1.82	0.44
1:A:215:MET:HG3	1:A:241:MET:HE1	1.99	0.43
1:A:193:GLU:HG2	1:A:194:THR:HG23	1.99	0.43
1:A:371:THR:O	1:A:372:HIS:CB	2.66	0.43
1:A:298:CYS:HB2	1:A:386:GLU:OE2	2.19	0.43
1:A:269:GLN:N	1:A:269:GLN:NE2	2.67	0.43
1:A:293:ILE:HD13	1:A:296:PHE:HD2	1.83	0.43
1:A:46:GLN:O	1:A:47:HIS:HB2	2.19	0.42
1:A:223:LEU:O	1:A:223:LEU:HD13	2.04	0.42
1:A:250:LEU:HD12	1:A:286:ILE:CD1	2.45	0.42
1:A:328:ILE:HD13	1:A:328:ILE:N	2.33	0.42
1:A:24:GLN:OE1	1:A:28:SER:CB	2.67	0.42
1:A:282:ARG:O	1:A:286:ILE:HG12	2.19	0.42
1:A:371:THR:HG23	2:A:506:HOH:O	2.19	0.42
1:A:52:LEU:O	1:A:56:ARG:HG3	2.19	0.42
1:A:60:HIS:HB2	1:A:217:HIS:CD2	2.55	0.42
1:A:54:LYS:HE2	2:A:501:HOH:O	2.19	0.42
1:A:173:ILE:HG22	1:A:176:GLY:N	2.34	0.42
1:A:372:HIS:N	2:A:506:HOH:O	2.52	0.42
1:A:85:THR:HA	1:A:113:THR:O	2.20	0.42
1:A:340:TYR:CD2	1:A:340:TYR:C	2.98	0.42
1:A:342:GLU:O	1:A:344:ASP:N	2.53	0.42
1:A:143:ARG:HA	2:A:534:HOH:O	2.20	0.41
1:A:335:LEU:C	1:A:336:PRO:HA	2.40	0.41
1:A:289:TYR:O	1:A:291:PRO:HD3	2.20	0.41
1:A:310:SER:HB2	2:A:547:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ILE:HD11	1:A:284:ALA:CA	2.51	0.41
1:A:136:LEU:HA	1:A:159:GLU:O	2.21	0.41
1:A:223:LEU:CD1	1:A:225:ILE:CG2	2.90	0.41
1:A:268:ALA:C	1:A:270:ASP:OD1	2.64	0.41
1:A:350:ARG:O	1:A:354:GLY:HA2	2.21	0.41
1:A:407:GLN:C	2:A:502:HOH:O	2.62	0.41
1:A:332:SER:HA	1:A:376:HIS:O	2.21	0.41
1:A:342:GLU:C	1:A:344:ASP:H	2.29	0.41
1:A:53:ILE:HD12	1:A:284:ALA:HB2	2.03	0.40
1:A:37:ARG:NH1	1:A:152:TYR:OH	2.46	0.40
1:A:398:HIS:O	1:A:402:GLN:HG3	2.21	0.40
1:A:409:LEU:N	2:A:502:HOH:O	2.54	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	400/405 (99%)	366 (92%)	24 (6%)	10 (2%)	4 0

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	343	ASN
1	A	410	GLY
1	A	413	GLY
1	A	301	GLU
1	A	336	PRO
1	A	270	ASP
1	A	289	TYR
1	A	372	HIS
1	A	373	LYS

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Mol	Chain	Res	Type
1	A	176	GLY

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	364/364 (100%)	343 (94%)	21 (6%)	18	11

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	30	LEU
1	A	119	HIS
1	A	128	LEU
1	A	222	GLU
1	A	223	LEU
1	A	226	ARG
1	A	251	GLU
1	A	269	GLN
1	A	270	ASP
1	A	282	ARG
1	A	291	PRO
1	A	293	ILE
1	A	301	GLU
1	A	316	VAL
1	A	317	LYS
1	A	331	ILE
1	A	371	THR
1	A	373	LYS
1	A	407	GLN
1	A	409	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	64	GLN
1	A	89	ASN
1	A	99	HIS
1	A	146	GLN
1	A	151	HIS
1	A	217	HIS
1	A	269	GLN
1	A	311	ASN
1	A	339	ASN
1	A	368	HIS
1	A	376	HIS
1	A	399	GLN

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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	10

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	407:GLN	C	408:LEU	N	2.64
1	A	406:VAL	C	407:GLN	N	2.02
1	A	268:ALA	C	269:GLN	N	1.80
1	A	408:LEU	C	409:LEU	N	1.78
1	A	335:LEU	C	336:PRO	N	1.70
1	A	336:PRO	C	337:SER	N	1.19
1	A	248:GLU	C	249:TRP	N	1.16
1	A	372:HIS	C	373:LYS	N	1.07
1	A	289:TYR	C	290:ILE	N	1.04
1	A	269:GLN	C	270:ASP	N	1.01

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	405/405 (100%)	0.67	56 (13%) 6 6	12, 27, 55, 83	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	411	VAL	6.9
1	A	415	PHE	6.8
1	A	409	LEU	5.8
1	A	11	PRO	5.7
1	A	336	PRO	5.3
1	A	289	TYR	4.3
1	A	221	ASP	4.1
1	A	340	TYR	4.0
1	A	408	LEU	3.9
1	A	344	ASP	3.8
1	A	341	ALA	3.7
1	A	335	LEU	3.3
1	A	69	PHE	3.3
1	A	406	VAL	3.2
1	A	407	GLN	3.2
1	A	66	VAL	3.0
1	A	12	GLY	3.0
1	A	339	ASN	2.9
1	A	369	PRO	2.9
1	A	70	GLY	2.7
1	A	410	GLY	2.7
1	A	269	GLN	2.6
1	A	414	ARG	2.6
1	A	403	GLU	2.6
1	A	315	LYS	2.6
1	A	372	HIS	2.6
1	A	223	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	278	LEU	2.6
1	A	338	GLU	2.5
1	A	385	MET	2.5
1	A	222	GLU	2.5
1	A	337	SER	2.4
1	A	365	LYS	2.4
1	A	404	ALA	2.4
1	A	14	VAL	2.4
1	A	334	TRP	2.4
1	A	24	GLN	2.3
1	A	368	HIS	2.3
1	A	343	ASN	2.3
1	A	361	ASP	2.2
1	A	26	ASP	2.2
1	A	301	GLU	2.2
1	A	270	ASP	2.2
1	A	363	ILE	2.2
1	A	309	VAL	2.2
1	A	21	SER	2.2
1	A	370	LYS	2.2
1	A	413	GLY	2.1
1	A	345	PHE	2.1
1	A	150	GLN	2.1
1	A	316	VAL	2.1
1	A	367	VAL	2.1
1	A	311	ASN	2.0
1	A	175	ASP	2.0
1	A	67	GLY	2.0
1	A	371	THR	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.