



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 23, 2017 – 08:22 AM EDT

PDB ID : 5MGV
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.; Safo, M.
Deposited on : unknown
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

<http://wwpdb.org/validation/2016/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)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

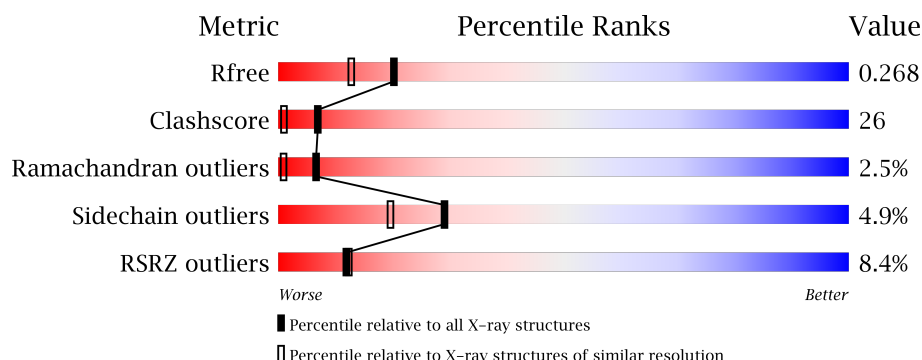
1 Overall quality at a glance

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}	100719	1316 (2.04-2.04)
Clashscore	112137	1394 (2.04-2.04)
Ramachandran outliers	110173	1383 (2.04-2.04)
Sidechain outliers	110143	1383 (2.04-2.04)
RSRZ outliers	101464	1319 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	405	<div> <div>8%</div> <div>63%</div> <div>30%</div> <div>5%</div> </div>

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

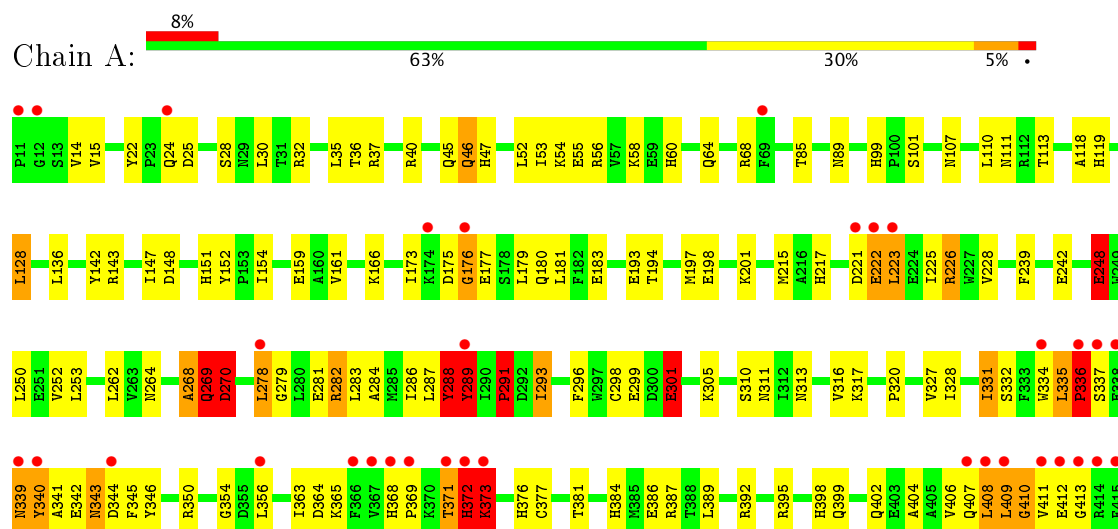
- Molecule 2 is water.

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

3 Residue-property plots [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: 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 47.59 – 2.05	Depositor EDS
% Data completeness (in resolution range)	93.2 (50.00-2.05) 93.2 (47.59-2.05)	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%)	DCC
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 , 48.2	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	0.94	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	0.96	19/3450 (0.6%)	1.22	33/4667 (0.7%)

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 (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	268	ALA	C-N	20.11	1.80	1.34
1	A	408	LEU	C-N	19.43	1.78	1.34
1	A	335	LEU	C-N	19.00	1.70	1.34
1	A	269	GLN	C-N	-14.03	1.01	1.34
1	A	289	TYR	C-N	-13.00	1.04	1.34
1	A	278	LEU	C-N	12.07	1.54	1.33
1	A	372	HIS	C-N	-11.60	1.07	1.34
1	A	365	LYS	C-N	8.62	1.53	1.34
1	A	46	GLN	C-N	8.50	1.53	1.34
1	A	180	GLN	C-N	8.41	1.53	1.34
1	A	248	GLU	C-N	-7.67	1.16	1.34
1	A	175	ASP	C-N	6.58	1.44	1.33
1	A	299	GLU	C-N	6.25	1.48	1.34
1	A	336	PRO	C-N	-6.24	1.19	1.34
1	A	222	GLU	C-N	6.00	1.47	1.34
1	A	221	ASP	C-N	-5.82	1.20	1.34
1	A	340	TYR	C-N	-5.70	1.21	1.34
1	A	183	GLU	C-N	-5.40	1.21	1.34
1	A	339	ASN	C-N	5.04	1.45	1.34

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	TYR	O-C-N	-31.78	71.84	122.70
1	A	269	GLN	O-C-N	-24.32	83.79	122.70
1	A	289	TYR	CA-C-N	20.10	161.42	117.20
1	A	372	HIS	O-C-N	-18.21	93.56	122.70
1	A	372	HIS	C-N-CA	17.26	164.85	121.70
1	A	270	ASP	O-C-N	-16.48	96.34	122.70
1	A	336	PRO	O-C-N	-14.46	99.56	122.70
1	A	372	HIS	CA-C-N	11.24	141.94	117.20
1	A	289	TYR	CB-CG-CD1	-10.29	114.83	121.00
1	A	408	LEU	CA-C-N	-10.27	94.61	117.20
1	A	268	ALA	C-N-CA	-10.21	96.17	121.70
1	A	248	GLU	O-C-N	-9.75	107.11	122.70
1	A	289	TYR	C-N-CA	9.74	146.06	121.70
1	A	269	GLN	CA-C-N	9.69	138.51	117.20
1	A	373	LYS	O-C-N	-9.60	107.33	122.70
1	A	269	GLN	C-N-CA	9.17	144.62	121.70
1	A	289	TYR	CB-CA-C	-7.57	95.26	110.40
1	A	301	GLU	O-C-N	-7.44	110.79	122.70
1	A	335	LEU	C-N-CD	7.38	143.90	128.40
1	A	288	TYR	O-C-N	-6.83	111.76	122.70
1	A	278	LEU	O-C-N	6.37	134.03	123.20
1	A	278	LEU	CA-C-N	-6.36	103.47	116.20
1	A	180	GLN	O-C-N	6.33	132.83	122.70
1	A	365	LYS	O-C-N	6.05	132.38	122.70
1	A	289	TYR	CB-CG-CD2	5.81	124.49	121.00
1	A	299	GLU	O-C-N	5.81	132.00	122.70
1	A	335	LEU	C-N-CA	-5.58	98.56	122.00
1	A	46	GLN	O-C-N	5.58	131.62	122.70
1	A	248	GLU	CA-C-N	5.52	129.34	117.20
1	A	340	TYR	O-C-N	-5.48	113.93	122.70
1	A	180	GLN	CA-C-N	-5.46	105.18	117.20
1	A	291	PRO	CA-N-CD	-5.28	104.11	111.50
1	A	365	LYS	CA-C-N	-5.28	105.59	117.20

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

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Mol	Chain	Res	Type	Group
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	3256	169	0
2	A	249	0	0	27	0
All	All	3607	0	3256	169	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 26.

All (169) 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	1.43
1:A:408:LEU:C	1:A:409:LEU:N	1.78	1.34
1:A:268:ALA:C	1:A:269:GLN:N	1.80	1.34
1:A:223:LEU:O	1:A:223:LEU:HD12	1.24	1.27
1:A:371:THR:OG1	1:A:373:LYS:HB2	1.43	1.17
1:A:406:VAL:C	1:A:407:GLN:N	2.02	1.13
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:289:TYR:HB3	2:A:504:HOH:O	1.72	0.89
1:A:335:LEU:C	1:A:336:PRO:CA	2.41	0.88
1:A:58:LYS:HD3	2:A:501:HOH:O	1.72	0.88
1:A:406:VAL:C	1:A:407:GLN:CA	2.42	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ALA:C	1:A:269:GLN:CA	2.43	0.86
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:406:VAL:C	1:A:407:GLN:HA	1.96	0.84
1:A:342:GLU:HG2	1:A:346:TYR:CE2	2.13	0.83
1:A:223:LEU:C	1:A:223:LEU:HD12	1.98	0.83
1:A:320:PRO:HG3	2:A:504:HOH:O	1.77	0.83
1:A:223:LEU:C	1:A:223:LEU:CD1	2.43	0.82
1:A:223:LEU:CD1	1:A:225:ILE:HG23	2.08	0.82
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:269:GLN:CD	1:A:269:GLN:N	2.36	0.79
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:OD1	1:A:270:ASP:N	2.16	0.76
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:408:LEU:N	1:A:409:LEU:N	2.39	0.70
1:A:147:ILE:HD12	1:A:350:ARG:NE	2.07	0.69
1:A:225:ILE:HD12	1:A:225:ILE:C	2.13	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
1:A:248:GLU:HG2	1:A:250:LEU:HD21	1.76	0.66
1:A:99:HIS:HD2	1:A:101:SER:OG	1.79	0.66
1:A:268:ALA:C	1:A:269:GLN:C	2.55	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: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:368:HIS:HB3	2:A:506:HOH:O	1.98	0.61
1:A:335:LEU:HG	1:A:340:TYR:CG	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:TRP:O	1:A:411:VAL:HA	2.00	0.60
1:A:327:VAL:C	1:A:328:ILE:HD13	2.22	0.59
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: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: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:223:LEU:HD13	1:A:223:LEU:C	2.25	0.56
1:A:364:ASP:HB3	2:A:503:HOH:O	2.05	0.56
1:A:268:ALA:O	1:A:269:GLN:C	2.44	0.55
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:O	1:A:14:VAL:HG12	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:253:LEU:HD12	1:A:253:LEU:C	2.29	0.53
1:A:408:LEU:C	1:A:409:LEU:CA	2.75	0.53
1:A:15:VAL:HG23	1:A:24:GLN:CD	2.29	0.53
1:A:392:ARG:HA	1:A:395:ARG:NH1	2.24	0.52
1:A:55:GLU:N	2:A:501:HOH:O	2.43	0.52
1:A:293:ILE:O	1:A:293:ILE:HD13	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:341:ALA:HB3	1:A:344:ASP:CG	2.31	0.51
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:O	1:A:278:LEU:HD12	2.11	0.51
1:A:53:ILE:HD11	1:A:284:ALA:HA	1.93	0.51
1:A:407:GLN:C	1:A:408:LEU:N	2.64	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:335:LEU:O	1:A:336:PRO:CA	2.61	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:HB3	1:A:408:LEU:HD23	1.97	0.47
1:A:369:PRO:O	1:A:372:HIS:ND1	2.48	0.47
1:A:64:GLN:HE22	1:A:68:ARG:HE	1.63	0.47
1:A:262:LEU:C	1:A:262:LEU:HD23	2.34	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:268:ALA:CA	1:A:269:GLN:N	2.75	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:225:ILE:C	1:A:225:ILE:CD1	2.83	0.46
1:A:22:TYR:CG	1:A:110:LEU:HD23	2.49	0.46
1:A:148:ASP:OD2	1:A:151:HIS:HD2	1.98	0.46
1:A:228:VAL:N	2:A:505:HOH:O	2.49	0.45
1:A:328:ILE:HD11	1:A:381:THR:HG23	1.98	0.45
1:A:35:LEU:C	1:A:35:LEU:HD23	2.36	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:409:LEU:O	1:A:410:GLY:C	2.57	0.42
1:A:46:GLN:O	1:A:47:HIS:HB2	2.19	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:407:GLN:C	1:A:408:LEU:HA	2.39	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: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:54:LYS:HE2	2:A:501:HOH:O	2.19	0.42
1:A:85:THR:HA	1:A:113:THR:O	2.20	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:336:PRO:O	1:A:337:SER:C	2.58	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
1:A:54:LYS:C	2:A:501:HOH:O	2.59	0.41
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:350:ARG:O	1:A:354:GLY:HA2	2.21	0.41
1:A:332:SER:HA	1:A:376:HIS:O	2.21	0.41
1:A:53:ILE:HD12	1:A:284:ALA:HB2	2.03	0.40
1:A:409:LEU:C	1:A:411:VAL:N	2.73	0.40
1:A:37:ARG:NH1	1:A:152:TYR:OH	2.46	0.40
1:A:336:PRO:HG3	1:A:410:GLY:C	2.42	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%)	6 1

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
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%)	346 (95%)	18 (5%)	29 20

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	119	HIS
1	A	128	LEU
1	A	223	LEU
1	A	226	ARG
1	A	269	GLN
1	A	270	ASP

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Mol	Chain	Res	Type
1	A	282	ARG
1	A	289	TYR
1	A	291	PRO
1	A	293	ILE
1	A	301	GLU
1	A	317	LYS
1	A	331	ILE
1	A	371	THR
1	A	372	HIS
1	A	373	LYS
1	A	409	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) 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	311	ASN
1	A	376	HIS
1	A	399	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 ⓘ

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](#)

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%)	0.65	34 (8%)	12 12	12, 27, 55, 83	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	415	PHE	8.9
1	A	336	PRO	8.0
1	A	411	VAL	7.5
1	A	339	ASN	6.2
1	A	340	TYR	5.9
1	A	11	PRO	5.0
1	A	409	LEU	5.0
1	A	338	GLU	5.0
1	A	413	GLY	4.5
1	A	408	LEU	4.0
1	A	221	ASP	3.8
1	A	12	GLY	3.4
1	A	337	SER	3.2
1	A	414	ARG	3.0
1	A	412	GLU	3.0
1	A	407	GLN	3.0
1	A	344	ASP	2.8
1	A	372	HIS	2.8
1	A	174	LYS	2.8
1	A	368	HIS	2.7
1	A	289	TYR	2.6
1	A	223	LEU	2.6
1	A	366	PHE	2.5
1	A	371	THR	2.5
1	A	278	LEU	2.4
1	A	367	VAL	2.3
1	A	369	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	69	PHE	2.3
1	A	373	LYS	2.3
1	A	222	GLU	2.2
1	A	334	TRP	2.1
1	A	356	LEU	2.1
1	A	176	GLY	2.1
1	A	24	GLN	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.