Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 11:08 PM EDT

PDB ID	:	3PNV
Title	:	V369M mutant of Glutamyl-tRNA synthetase from Mycobacterium tuberculosis
Authors	:	Kachalova, G.S.; Laurinavichiute, D.; Bartunik, H.D.
Deposited on	:	2010-11-19
Resolution	:	1.95 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:

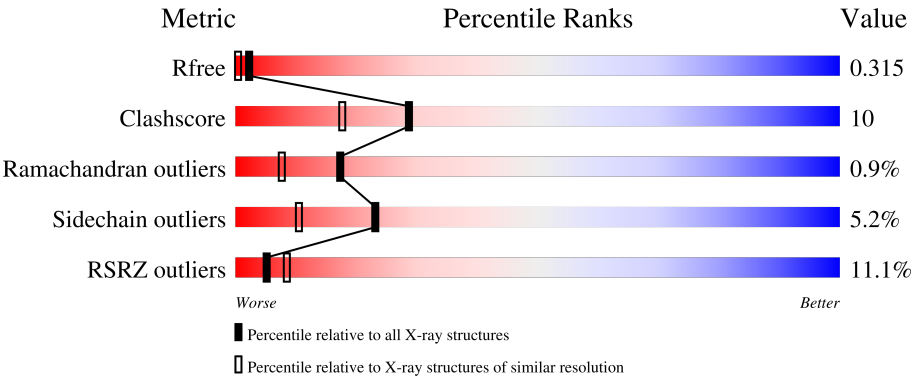
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 <=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	505	10% 73% 20% · 5%
1	B	505	11% 77% 16% · ·

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7687 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 Glutamyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3745	2369	672	696	8			
1	B	485	Total	C	N	O	S	0	0	0
			3772	2385	676	702	9			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	expression tag	UNP P0A636
A	-13	HIS	-	expression tag	UNP P0A636
A	-12	HIS	-	expression tag	UNP P0A636
A	-11	HIS	-	expression tag	UNP P0A636
A	-10	HIS	-	expression tag	UNP P0A636
A	-9	HIS	-	expression tag	UNP P0A636
A	-8	SER	-	expression tag	UNP P0A636
A	-7	SER	-	expression tag	UNP P0A636
A	-6	GLY	-	expression tag	UNP P0A636
A	-5	LEU	-	expression tag	UNP P0A636
A	-4	VAL	-	expression tag	UNP P0A636
A	-3	PRO	-	expression tag	UNP P0A636
A	-2	ARG	-	expression tag	UNP P0A636
A	-1	GLY	-	expression tag	UNP P0A636
A	0	SER	-	expression tag	UNP P0A636
A	369	MET	VAL	engineered mutation	UNP P0A636
B	-14	HIS	-	expression tag	UNP P0A636
B	-13	HIS	-	expression tag	UNP P0A636
B	-12	HIS	-	expression tag	UNP P0A636
B	-11	HIS	-	expression tag	UNP P0A636
B	-10	HIS	-	expression tag	UNP P0A636
B	-9	HIS	-	expression tag	UNP P0A636
B	-8	SER	-	expression tag	UNP P0A636
B	-7	SER	-	expression tag	UNP P0A636
B	-6	GLY	-	expression tag	UNP P0A636

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	LEU	-	expression tag	UNP P0A636
B	-4	VAL	-	expression tag	UNP P0A636
B	-3	PRO	-	expression tag	UNP P0A636
B	-2	ARG	-	expression tag	UNP P0A636
B	-1	GLY	-	expression tag	UNP P0A636
B	0	SER	-	expression tag	UNP P0A636
B	369	MET	VAL	engineered mutation	UNP P0A636

- Molecule 2 is water.

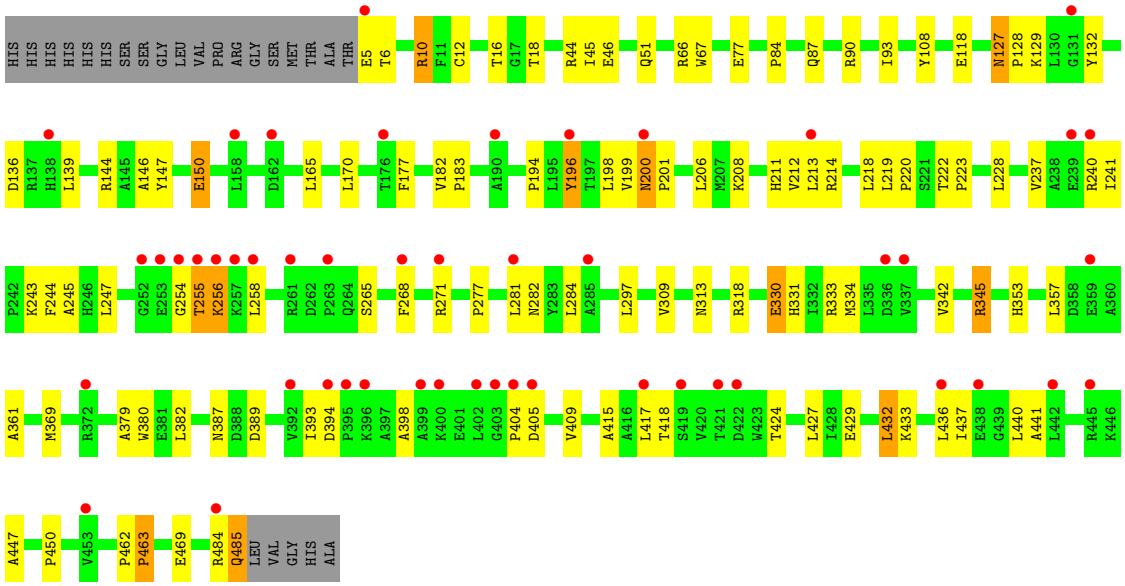
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	73	Total O 73 73	0	11
2	B	97	Total O 97 97	0	7

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.

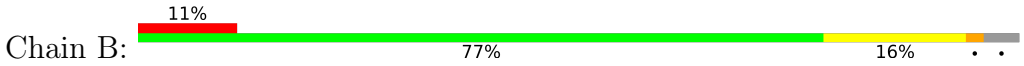
• Molecule 1: Glutamyl-tRNA synthetase

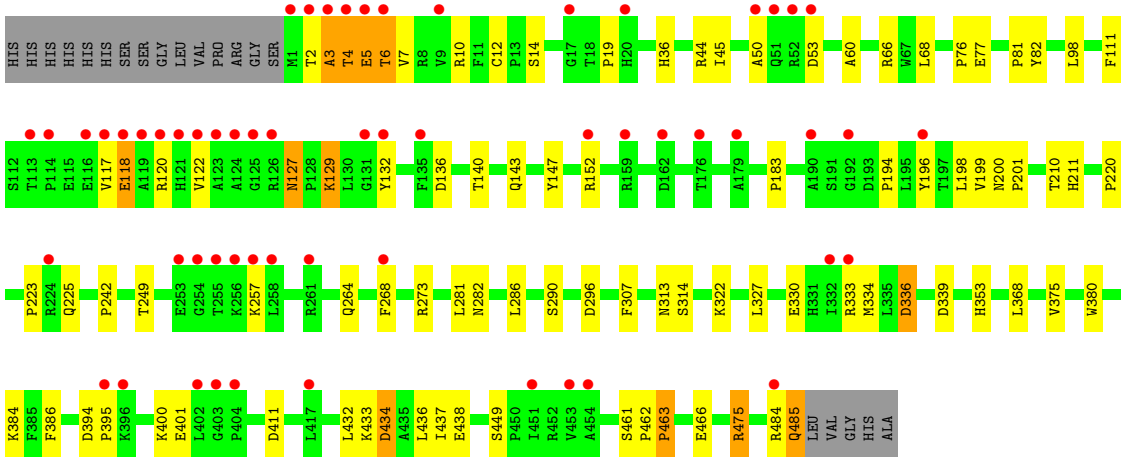
Chain A:



• Molecule 1: Glutamyl-tRNA synthetase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	43.43Å 210.35Å 57.98Å 90.00° 99.35° 90.00°	Depositor
Resolution (Å)	10.41 – 1.95 19.84 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.9 (10.41-1.95) 96.9 (19.84-1.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.80 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.272 , 0.316 0.273 , 0.315	Depositor DCC
R_{free} test set	3620 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	27.3	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 54.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7687	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.46	0/3832	0.61	0/5216
1	B	0.51	0/3859	0.65	0/5253
All	All	0.48	0/7691	0.63	0/10469

There are no bond length outliers.

There are no bond angle outliers.

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	3745	0	3691	88	0
1	B	3772	0	3722	57	0
2	A	73	0	0	2	0
2	B	97	0	0	5	0
All	All	7687	0	7413	145	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 10.

All (145) 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:268:PHE:CE1	1:A:271:ARG:NH1	2.28	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ARG:NH2	1:A:77:GLU:OE1	1.99	0.95
1:B:200:ASN:HB3	1:B:201:PRO:HD3	1.51	0.93
1:B:4:THR:HG22	1:B:7:VAL:HG22	1.55	0.88
1:B:242:PRO:HG3	2:B:511:HOH:O	1.74	0.88
1:A:222:THR:N	1:A:223:PRO:HD2	1.92	0.83
1:A:268:PHE:CZ	1:A:271:ARG:NH1	2.49	0.81
1:A:194:PRO:HB3	1:A:198:LEU:HD23	1.66	0.78
1:A:127:ASN:HD22	1:A:129:LYS:H	1.34	0.76
1:A:206:LEU:HD21	1:A:237:VAL:HG13	1.68	0.76
1:A:213:LEU:HG	1:A:245:ALA:HB3	1.67	0.75
1:B:386:PHE:O	1:B:475:ARG:NH2	2.20	0.74
1:A:170:LEU:HD12	1:A:244:PHE:O	1.89	0.72
1:A:146:ALA:O	1:A:150:GLU:HG2	1.90	0.72
1:A:201:PRO:HG2	1:A:228:LEU:HD23	1.71	0.72
1:A:132:TYR:OH	1:A:136:ASP:HB2	1.88	0.72
1:A:409:VAL:HG11	1:A:450:PRO:HG2	1.73	0.71
1:A:222:THR:N	1:A:223:PRO:CD	2.52	0.71
1:B:4:THR:HG22	1:B:7:VAL:CG2	2.20	0.71
1:A:437:ILE:O	1:A:441:ALA:HA	1.93	0.69
1:A:196:TYR:CZ	2:A:509[B]:HOH:O	2.45	0.68
1:B:4:THR:HB	1:B:211:HIS:HE1	1.58	0.68
1:B:336:ASP:OD1	1:B:339:ASP:HB2	1.92	0.68
1:A:330:GLU:HG2	1:A:333:ARG:HH21	1.60	0.68
1:A:5:GLU:HG2	1:A:6:THR:HA	1.75	0.67
1:B:485:GLN:HE21	1:B:485:GLN:HA	1.60	0.66
1:B:461:SER:HB2	1:B:462:PRO:HD2	1.79	0.65
1:A:297:LEU:HD11	1:A:334:MET:HE1	1.79	0.64
1:B:2:THR:HG22	1:B:3:ALA:H	1.62	0.63
1:B:200:ASN:HB3	1:B:201:PRO:CD	2.27	0.63
1:B:273:ARG:HG2	1:B:375:VAL:HG21	1.80	0.63
1:A:353:HIS:HB3	1:A:380:TRP:CE3	2.34	0.62
1:A:369:MET:HE1	1:A:382:LEU:HB2	1.80	0.62
1:A:220:PRO:O	1:A:223:PRO:HD2	2.00	0.62
1:A:213:LEU:CG	1:A:245:ALA:HB3	2.30	0.61
1:A:342:VAL:HG22	1:A:345:ARG:NH2	2.16	0.61
1:A:436:LEU:HB3	1:A:447:ALA:HB1	1.82	0.61
1:B:66:ARG:NH2	1:B:77:GLU:OE1	2.33	0.60
1:B:140:THR:OG1	1:B:143:GLN:HG3	2.01	0.59
1:A:84:PRO:HG2	1:A:90:ARG:HG3	1.85	0.59
1:A:369:MET:HE1	1:A:379:ALA:HA	1.84	0.59
1:A:409:VAL:HG11	1:A:450:PRO:CG	2.34	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:LEU:O	1:B:436:LEU:HG	2.03	0.57
1:B:111:PHE:N	1:B:136:ASP:OD1	2.29	0.57
1:A:219:LEU:N	1:A:220:PRO:CD	2.67	0.57
1:A:417:LEU:HG	1:A:432:LEU:HD21	1.85	0.57
1:A:213:LEU:CD1	1:A:245:ALA:HB3	2.35	0.57
1:B:225:GLN:NE2	2:B:518:HOH:O	2.38	0.56
1:A:212:VAL:C	1:A:213:LEU:HD12	2.26	0.56
1:A:206:LEU:CD2	1:A:237:VAL:HG13	2.35	0.56
1:B:433:LYS:HA	1:B:437:ILE:HD12	1.88	0.56
1:A:462:PRO:O	1:A:463:PRO:C	2.44	0.56
1:A:132:TYR:HH	1:A:136:ASP:HB2	1.71	0.55
1:B:353:HIS:HB3	1:B:380:TRP:CE3	2.42	0.55
1:A:424:THR:HA	1:A:469:GLU:HG3	1.89	0.55
1:A:90:ARG:HG2	1:A:93:ILE:HD12	1.89	0.54
1:A:219:LEU:HB3	1:A:220:PRO:HD3	1.91	0.53
1:B:330:GLU:OE2	1:B:333:ARG:NH1	2.41	0.53
1:B:132:TYR:CG	1:B:183:PRO:HB3	2.45	0.52
1:B:127:ASN:HD22	1:B:127:ASN:N	2.08	0.52
1:A:484:ARG:HB2	1:A:485:GLN:OE1	2.11	0.51
1:B:60:ALA:HB1	1:B:268:PHE:HE2	1.76	0.51
1:A:213:LEU:HG	1:A:245:ALA:CB	2.36	0.50
1:A:170:LEU:HD11	1:A:243:LYS:HB3	1.92	0.50
1:A:212:VAL:O	1:A:213:LEU:HD12	2.13	0.49
1:A:331:HIS:HA	1:A:334:MET:HE3	1.93	0.49
1:B:12:CYS:HA	1:B:44:ARG:O	2.13	0.49
1:A:297:LEU:HD11	1:A:334:MET:CE	2.42	0.48
1:A:211:HIS:NE2	1:A:243:LYS:HD2	2.28	0.48
1:B:81:PRO:HG2	1:B:82:TYR:CE2	2.48	0.48
1:B:286:LEU:HD12	1:B:327:LEU:HD11	1.95	0.48
1:B:220:PRO:O	1:B:223:PRO:HD2	2.13	0.48
1:A:147:TYR:HA	1:A:150:GLU:HG3	1.95	0.48
1:A:433:LYS:HG2	1:A:437:ILE:HD12	1.95	0.48
1:A:369:MET:CE	1:A:379:ALA:HA	2.44	0.48
1:A:342:VAL:HG22	1:A:345:ARG:HH21	1.78	0.48
1:B:273:ARG:NH1	2:B:572[A]:HOH:O	1.68	0.47
1:A:118:GLU:HG3	1:A:128:PRO:HB3	1.97	0.47
1:B:2:THR:HG22	1:B:3:ALA:N	2.30	0.47
1:A:12:CYS:HA	1:A:44:ARG:O	2.14	0.47
1:A:309:VAL:HG22	1:A:309:VAL:O	2.15	0.47
1:B:249:THR:HG21	1:B:257:LYS:HG2	1.97	0.47
1:A:139:LEU:O	1:A:144:ARG:NH1	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:LYS:HB3	1:B:129:LYS:HE3	1.77	0.46
1:A:255:THR:HA	1:A:318:ARG:HH22	1.79	0.46
1:B:45:ILE:HD11	1:B:76:PRO:HG2	1.97	0.46
1:B:6:THR:O	1:B:210:THR:HG21	2.15	0.46
1:A:393:ILE:CG2	1:A:398:ALA:HB2	2.46	0.46
1:B:36:HIS:CG	1:B:307:PHE:O	2.68	0.46
1:B:81:PRO:HG2	1:B:82:TYR:CD2	2.51	0.45
1:A:46:GLU:HA	1:A:87:GLN:HG3	1.97	0.45
1:A:254:GLY:O	1:A:256:LYS:N	2.50	0.45
1:A:436:LEU:HD23	1:A:440:LEU:HD12	1.98	0.45
1:A:196:TYR:CE1	2:A:509[B]:HOH:O	2.68	0.45
1:B:485:GLN:OE1	2:B:568[A]:HOH:O	2.21	0.45
1:A:415:ALA:O	1:A:418:THR:HG22	2.16	0.45
1:B:434:ASP:HA	1:B:438:GLU:HB2	1.99	0.45
1:A:417:LEU:CG	1:A:432:LEU:HD21	2.47	0.45
1:B:68:LEU:O	1:B:281:LEU:HD11	2.16	0.45
1:B:485:GLN:HE21	1:B:485:GLN:CA	2.26	0.45
1:A:196:TYR:HA	1:A:199:VAL:HG22	1.99	0.45
1:B:194:PRO:HB3	1:B:198:LEU:HD23	1.99	0.44
1:B:400:LYS:HB2	1:B:400:LYS:HE3	1.58	0.44
1:B:368:LEU:HD21	1:B:466:GLU:HG3	1.99	0.44
1:B:484:ARG:NE	2:B:568[A]:HOH:O	2.51	0.44
1:A:211:HIS:HE2	1:A:243:LYS:HD2	1.83	0.44
1:B:196:TYR:HA	1:B:199:VAL:HG22	1.99	0.44
1:A:212:VAL:O	1:A:245:ALA:N	2.50	0.44
1:A:213:LEU:HD12	1:A:245:ALA:HB3	2.00	0.44
1:B:394:ASP:HA	1:B:395:PRO:HD2	1.83	0.44
1:A:136:ASP:HA	1:A:139:LEU:HD13	1.99	0.43
1:A:254:GLY:C	1:A:256:LYS:H	2.21	0.43
1:A:196:TYR:O	1:A:200:ASN:HB2	2.18	0.43
1:B:98:LEU:HG	1:B:198:LEU:HD21	1.99	0.43
1:B:117:VAL:O	1:B:118:GLU:C	2.57	0.43
1:A:196:TYR:C	1:A:196:TYR:CD2	2.91	0.43
1:A:219:LEU:N	1:A:220:PRO:HD2	2.33	0.43
1:A:432:LEU:O	1:A:436:LEU:HB2	2.18	0.43
1:B:147:TYR:O	1:B:152:ARG:HG3	2.19	0.43
1:A:214:ARG:HD2	1:A:218:LEU:HD12	1.99	0.42
1:B:286:LEU:HD21	1:B:296:ASP:HB2	2.01	0.42
1:A:108:TYR:OH	1:A:132:TYR:HE2	2.02	0.42
1:A:200:ASN:CB	1:A:201:PRO:HD3	2.50	0.42
1:B:401:GLU:CD	1:B:449:SER:HB2	2.38	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:GLN:CA	1:B:485:GLN:NE2	2.83	0.42
1:A:51:GLN:HE21	1:A:51:GLN:HA	1.85	0.42
1:A:258:LEU:HG	1:A:265:SER:HB3	2.01	0.42
1:B:484:ARG:CZ	1:B:485:GLN:HE22	2.32	0.42
1:A:10:ARG:O	1:A:10:ARG:HG2	2.20	0.42
1:A:208:LYS:HA	1:A:208:LYS:HD3	1.93	0.42
1:A:45:ILE:O	1:A:87:GLN:HG3	2.20	0.41
1:A:213:LEU:CD2	1:A:309:VAL:HG21	2.49	0.41
1:B:50:ALA:O	1:B:53:ASP:N	2.53	0.41
1:A:67:TRP:CE2	1:A:277:PRO:HG3	2.56	0.41
1:A:182:VAL:HA	1:A:183:PRO:HD3	1.87	0.41
1:A:387:ASN:HB3	1:A:389:ASP:OD1	2.20	0.41
1:A:424:THR:CG2	1:A:427:LEU:HD12	2.50	0.41
1:B:330:GLU:O	1:B:334:MET:HG3	2.21	0.41
1:A:165:LEU:HB2	1:A:177:PHE:HB2	2.01	0.41
1:A:241:ILE:HD12	1:A:241:ILE:N	2.36	0.41
1:A:357:LEU:HD22	1:A:361:ALA:HB1	2.03	0.41
1:B:132:TYR:CD2	1:B:183:PRO:HB3	2.56	0.41
1:B:286:LEU:CD1	1:B:327:LEU:HD11	2.50	0.41
1:B:264:GLN:HE21	1:B:264:GLN:HB2	1.66	0.40
1:A:429:GLU:HG2	1:A:433:LYS:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	479/505 (95%)	459 (96%)	16 (3%)	4 (1%)	19 9
1	B	483/505 (96%)	462 (96%)	16 (3%)	5 (1%)	15 6
All	All	962/1010 (95%)	921 (96%)	32 (3%)	9 (1%)	17 8

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	5	GLU
1	B	118	GLU
1	A	255	THR
1	B	3	ALA
1	A	284	LEU
1	A	404	PRO
1	A	463	PRO
1	B	463	PRO
1	B	19	PRO

5.3.2 Protein sidechains (i)

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	383/402 (95%)	364 (95%)	19 (5%)	24	11
1	B	386/402 (96%)	365 (95%)	21 (5%)	22	10
All	All	769/804 (96%)	729 (95%)	40 (5%)	23	10

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	16	THR
1	A	18	THR
1	A	127	ASN
1	A	150	GLU
1	A	196	TYR
1	A	200	ASN
1	A	240	ARG
1	A	247	LEU
1	A	256	LYS
1	A	281	LEU
1	A	282	ASN
1	A	313	ASN
1	A	330	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	345	ARG
1	A	394	ASP
1	A	405	ASP
1	A	432	LEU
1	A	485	GLN
1	B	4	THR
1	B	5	GLU
1	B	6	THR
1	B	10	ARG
1	B	14	SER
1	B	120	ARG
1	B	122	VAL
1	B	127	ASN
1	B	129	LYS
1	B	282	ASN
1	B	290	SER
1	B	313	ASN
1	B	314	SER
1	B	322	LYS
1	B	336	ASP
1	B	384	LYS
1	B	411	ASP
1	B	434	ASP
1	B	463	PRO
1	B	475	ARG
1	B	485	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	127	ASN
1	A	313	ASN
1	B	127	ASN
1	B	225	GLN
1	B	264	GLN
1	B	313	ASN
1	B	485	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 monosaccharides 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, 95^{th} 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	481/505 (95%)	0.73	49 (10%) 6 11	10, 31, 50, 61	19 (3%)
1	B	485/505 (96%)	0.82	58 (11%) 4 7	10, 30, 55, 70	10 (2%)
All	All	966/1010 (95%)	0.78	107 (11%) 5 8	10, 31, 53, 70	29 (3%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	281	LEU	9.8
1	B	3	ALA	9.5
1	B	119	ALA	7.6
1	B	4	THR	7.3
1	B	117	VAL	7.2
1	A	200	ASN	6.6
1	B	2	THR	6.3
1	B	124	ALA	5.6
1	A	403	GLY	5.2
1	B	159	ARG	5.2
1	B	51	GLN	5.1
1	B	118	GLU	5.1
1	B	114	PRO	5.0
1	B	5	GLU	4.9
1	B	162	ASP	4.7
1	A	404	PRO	4.5
1	B	1	MET	4.1
1	B	484	ARG	4.1
1	A	162	ASP	4.0
1	A	176	THR	3.9
1	A	419	SER	3.8
1	B	52	ARG	3.8
1	B	224	ARG	3.7
1	B	50	ALA	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	176	THR	3.6
1	A	257	LYS	3.6
1	B	403	GLY	3.6
1	B	6	THR	3.6
1	A	395	PRO	3.5
1	A	271	ARG	3.4
1	A	436	LEU	3.4
1	A	337	VAL	3.4
1	B	404	PRO	3.4
1	B	120	ARG	3.4
1	A	421	THR	3.4
1	B	253	GLU	3.3
1	B	113	THR	3.2
1	B	261	ARG	3.2
1	A	422	ASP	3.2
1	B	121	HIS	3.2
1	B	126	ARG	3.2
1	B	402	LEU	3.1
1	A	256	LYS	3.1
1	B	135	PHE	3.1
1	B	268	PHE	3.1
1	A	5	GLU	3.1
1	A	402	LEU	3.1
1	A	484	ARG	3.0
1	A	285	ALA	3.0
1	B	125	GLY	3.0
1	B	254	GLY	3.0
1	A	359	GLU	3.0
1	A	445	ARG	2.9
1	B	333	ARG	2.9
1	A	396	LYS	2.9
1	B	190	ALA	2.9
1	B	255	THR	2.8
1	B	454	ALA	2.8
1	B	116	GLU	2.8
1	A	261	ARG	2.8
1	B	258	LEU	2.8
1	B	131	GLY	2.7
1	B	9	VAL	2.7
1	A	254	GLY	2.7
1	A	336	ASP	2.7
1	A	190	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	392	VAL	2.7
1	A	394	ASP	2.6
1	B	122	VAL	2.6
1	B	453	VAL	2.6
1	A	240	ARG	2.6
1	B	17	GLY	2.6
1	A	213	LEU	2.5
1	B	256	LYS	2.4
1	A	268	PHE	2.4
1	A	252	GLY	2.4
1	B	53	ASP	2.4
1	A	131	GLY	2.4
1	A	400	LYS	2.4
1	A	417	LEU	2.4
1	A	442	LEU	2.3
1	A	438	GLU	2.3
1	B	20	HIS	2.3
1	B	395	PRO	2.3
1	A	258	LEU	2.2
1	A	196	TYR	2.2
1	B	132	TYR	2.2
1	B	192	GLY	2.2
1	A	405	ASP	2.2
1	B	332	ILE	2.2
1	A	453	VAL	2.2
1	B	123	ALA	2.1
1	B	396	LYS	2.1
1	A	239	GLU	2.1
1	A	138	HIS	2.1
1	B	257	LYS	2.1
1	A	158	LEU	2.1
1	A	399	ALA	2.1
1	B	152	ARG	2.1
1	A	255	THR	2.1
1	A	253	GLU	2.1
1	B	451	ILE	2.1
1	B	196	TYR	2.0
1	A	263	PRO	2.0
1	B	179	ALA	2.0
1	B	417	LEU	2.0
1	A	372	ARG	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 monosaccharides 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.