Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 07:09 PM EDT

PDB ID	:	4Q2Y
Title	:	Crystal structure of Arginyl-tRNA synthetase
Authors	:	Kim, H.S.; Jo, C.H.; Cha, S.Y.; Han, A.R.; Hwang, K.Y.
Deposited on	:	2014-04-10
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 (i) 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 (1)) were used in the production of this report:

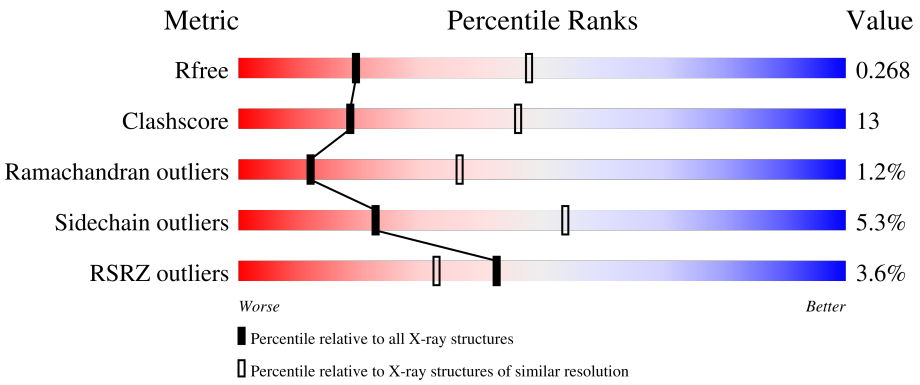
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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	607	3% 61% 30% • 7%
1	B	607	3% 67% 26% • 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9333 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 Arginine–tRNA ligase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	565	4533	2901	768	836	28	0	0	0
1	B	577	4629	2960	786	856	27	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	HIS	-	expression tag	UNP P54136
A	-17	HIS	-	expression tag	UNP P54136
A	-16	HIS	-	expression tag	UNP P54136
A	-15	HIS	-	expression tag	UNP P54136
A	-14	HIS	-	expression tag	UNP P54136
A	-13	HIS	-	expression tag	UNP P54136
A	-12	SER	-	expression tag	UNP P54136
A	-11	SER	-	expression tag	UNP P54136
A	-10	GLY	-	expression tag	UNP P54136
A	-9	LEU	-	expression tag	UNP P54136
A	-8	VAL	-	expression tag	UNP P54136
A	-7	PRO	-	expression tag	UNP P54136
A	-6	ARG	-	expression tag	UNP P54136
A	-5	GLY	-	expression tag	UNP P54136
A	-4	SER	-	expression tag	UNP P54136
A	-3	HIS	-	expression tag	UNP P54136
A	-2	MET	-	expression tag	UNP P54136
A	-1	ALA	-	expression tag	UNP P54136
A	0	SER	-	expression tag	UNP P54136
A	438	ARG	HIS	engineered mutation	UNP P54136
B	-18	HIS	-	expression tag	UNP P54136
B	-17	HIS	-	expression tag	UNP P54136
B	-16	HIS	-	expression tag	UNP P54136
B	-15	HIS	-	expression tag	UNP P54136
B	-14	HIS	-	expression tag	UNP P54136

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	HIS	-	expression tag	UNP P54136
B	-12	SER	-	expression tag	UNP P54136
B	-11	SER	-	expression tag	UNP P54136
B	-10	GLY	-	expression tag	UNP P54136
B	-9	LEU	-	expression tag	UNP P54136
B	-8	VAL	-	expression tag	UNP P54136
B	-7	PRO	-	expression tag	UNP P54136
B	-6	ARG	-	expression tag	UNP P54136
B	-5	GLY	-	expression tag	UNP P54136
B	-4	SER	-	expression tag	UNP P54136
B	-3	HIS	-	expression tag	UNP P54136
B	-2	MET	-	expression tag	UNP P54136
B	-1	ALA	-	expression tag	UNP P54136
B	0	SER	-	expression tag	UNP P54136
B	438	ARG	HIS	engineered mutation	UNP P54136

- Molecule 2 is water.

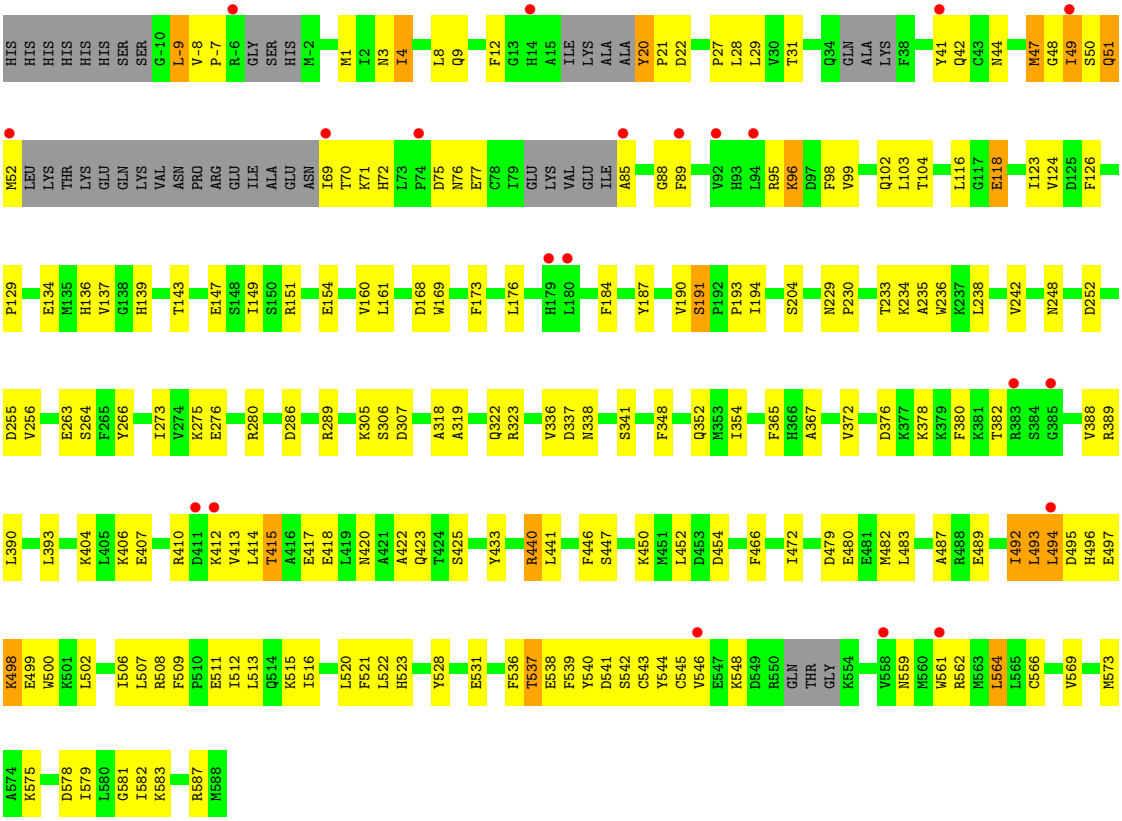
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	84	84	84	0	0
			Total	O		
2	B	87	87	87	0	0

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.

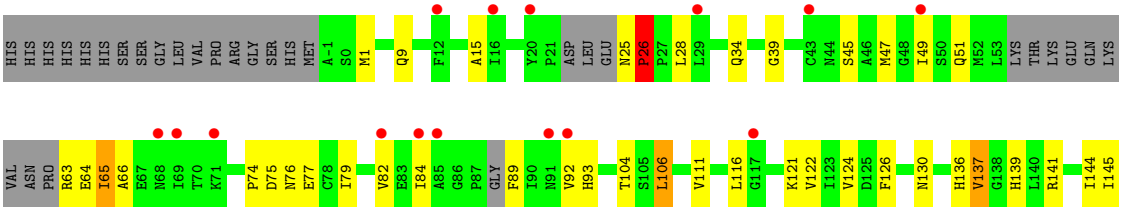
• Molecule 1: Arginine–tRNA ligase, cytoplasmic

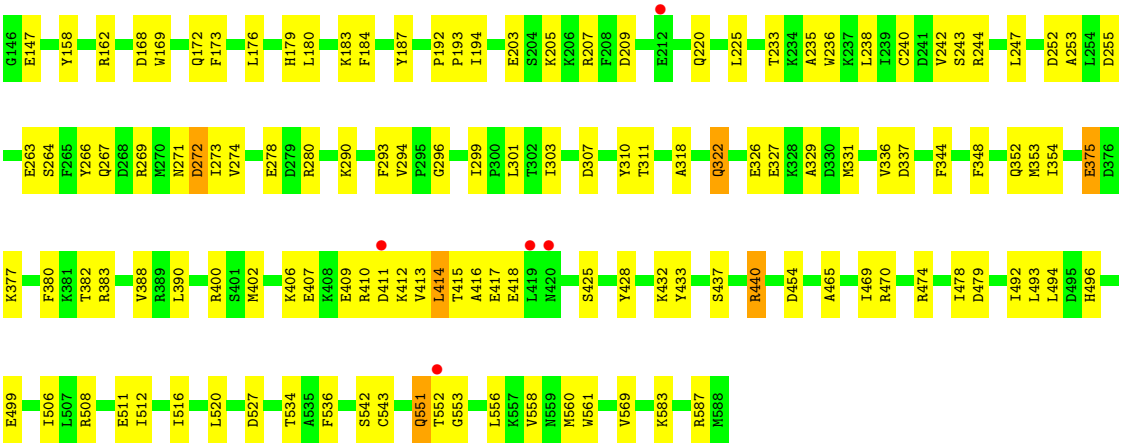
Chain A:



• Molecule 1: Arginine–tRNA ligase, cytoplasmic

Chain B:




G146 E147 Y158 R162 D168 W169 Q172 F173 L176 H179 L180 K183 F184 Y187 P192 P193 I194 E203 S204 K205 K206 R207 F208 D209 E212 Q220 L225 T233 K234 A235 W236 K237 L238 I239 C240 D241 V242 S243 R244 L247 D252 A253 L254 D255
E263 S264 F265 Y266 Q267 D268 R269 M270 N271 D272 I273 V274 E278 D279 R280 K290 F293 V294 P295 G296 I299 P300 L301 T302 I303 D307 Y310 T311 A318 Q322 E326 E327 K328 A329 D330 M331 V336 D337 F344 F348 Q352 M353 I354 E375 D376
K377 F380 K381 T382 R383 V388 R389 L390 R400 S401 M402 K406 E407 K408 E409 R410 D411 K412 V413 L414 T415 A416 E417 E418 L419 N420 S425 Y428 K432 Y433 S437 R440 D454 A465 I469 R470 R474 I478 D479 I492 L493 L494 D495 H496
E499 I506 L507 R508 E511 I512 I516 L520 D527 T534 A535 F536 S542 C543 Q551 T552 G553 L556 K557 V558 N559 M560 W561 V569 K583 R587 M588

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.62Å 105.23Å 172.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.90 – 2.80 44.90 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.5 (44.90-2.80) 95.5 (44.90-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.00 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.208 , 0.268 0.208 , 0.268	Depositor DCC
R_{free} test set	1712 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	44.8	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 64.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9333	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.96 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1991e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (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	0.48	0/4616	0.67	1/6214 (0.0%)
1	B	0.52	0/4714	0.68	2/6349 (0.0%)
All	All	0.50	0/9330	0.68	3/12563 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	26	PRO	C-N-CD	-5.43	108.64	120.60
1	A	440	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	B	440	ARG	NE-CZ-NH1	-5.07	117.76	120.30

There are no chirality outliers.

There are no planarity outliers.

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	4533	0	4561	137	0
1	B	4629	0	4666	109	0
2	A	84	0	0	11	0
2	B	87	0	0	14	0
All	All	9333	0	9227	244	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 13.

All (244) 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:578:ASP:OD1	2:A:604:HOH:O	1.91	0.89
1:A:502:LEU:HD12	1:A:536:PHE:HA	1.61	0.83
1:B:440:ARG:NH1	1:B:520:LEU:O	2.11	0.83
1:A:137:VAL:HG12	1:A:372:VAL:HG21	1.58	0.83
1:B:75:ASP:OD2	2:B:623:HOH:O	1.95	0.82
1:A:406:LYS:HD2	1:A:410:ARG:HD3	1.61	0.80
1:B:496:HIS:ND1	1:B:543:CYS:SG	2.54	0.79
1:B:406:LYS:HD2	1:B:410:ARG:HD3	1.66	0.77
1:B:474:ARG:NH1	2:B:685:HOH:O	2.12	0.77
1:B:130:ASN:HD21	1:B:172:GLN:HE22	1.35	0.75
1:A:20:TYR:OH	1:A:69:ILE:O	2.04	0.75
1:B:179:HIS:ND1	2:B:683:HOH:O	2.21	0.73
1:B:207:ARG:NH1	2:B:683:HOH:O	2.19	0.72
1:A:495:ASP:N	1:A:499:GLU:OE2	2.23	0.71
1:B:205:LYS:NZ	1:B:209:ASP:OD2	2.25	0.70
1:A:508:ARG:NE	2:A:621:HOH:O	2.25	0.70
1:A:499:GLU:HB3	2:A:601:HOH:O	1.92	0.70
1:A:508:ARG:NH2	1:A:531:GLU:OE2	2.23	0.70
1:B:527:ASP:OD2	2:B:620:HOH:O	2.09	0.70
1:B:194:ILE:HD12	1:B:242:VAL:HG21	1.72	0.69
1:A:450:LYS:NZ	2:A:663:HOH:O	2.25	0.69
1:A:27:PRO:HG3	1:A:48:GLY:HA3	1.75	0.69
1:A:496:HIS:ND1	1:A:543:CYS:SG	2.66	0.68
1:A:413:VAL:HG12	1:A:418:GLU:HB2	1.76	0.68
1:A:338:ASN:O	1:A:341:SER:OG	2.11	0.67
1:B:496:HIS:HB3	1:B:499:GLU:HG2	1.75	0.67
1:A:29:LEU:HD23	1:A:44:ASN:HB2	1.75	0.67
1:B:122:VAL:HG22	1:B:331:MET:HB3	1.75	0.67
1:B:272:ASP:OD1	1:B:272:ASP:N	2.29	0.66
1:A:266:TYR:HE1	1:A:322:GLN:HG2	1.60	0.65
1:A:96:LYS:HE3	1:A:96:LYS:O	1.95	0.65
1:B:496:HIS:HD1	1:B:543:CYS:HG	1.44	0.65
1:B:9:GLN:HG2	1:B:28:LEU:HB3	1.80	0.64
1:B:433:TYR:O	1:B:437:SER:OG	2.08	0.64
1:A:506:ILE:HD11	1:A:569:VAL:HG23	1.79	0.64
1:A:149:ILE:HD13	1:A:520:LEU:HD13	1.79	0.64
1:A:42:GLN:NE2	2:A:627:HOH:O	2.30	0.64
1:A:480:GLU:HA	1:A:483:LEU:HD12	1.80	0.64
1:B:414:LEU:HD22	1:B:417:GLU:H	1.64	0.63
1:B:252:ASP:O	2:B:650:HOH:O	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:587:ARG:O	2:B:686:HOH:O	2.15	0.62
1:B:380:PHE:CE2	1:B:388:VAL:HG21	2.34	0.62
1:B:508:ARG:O	1:B:511:GLU:HG2	1.99	0.62
1:B:409:GLU:O	1:B:413:VAL:HG22	1.99	0.62
1:A:194:ILE:HD12	1:A:242:VAL:HG21	1.83	0.60
1:A:404:LYS:HE2	1:A:452:LEU:O	2.02	0.60
1:B:173:PHE:HD1	1:B:176:LEU:HD12	1.67	0.60
1:A:51:GLN:HG2	1:A:52:MET:N	2.17	0.59
1:B:124:VAL:HG12	1:B:126:PHE:HD1	1.66	0.59
1:A:96:LYS:HD2	1:A:500:TRP:HZ3	1.68	0.59
1:B:269:ARG:NH1	1:B:326:GLU:OE2	2.35	0.59
1:B:47:MET:SD	1:B:47:MET:N	2.76	0.58
1:B:512:ILE:O	1:B:516:ILE:HG13	2.03	0.58
1:A:77:GLU:O	1:A:95:ARG:NH2	2.38	0.57
1:A:96:LYS:HD2	1:A:500:TRP:CZ3	2.39	0.57
1:A:20:TYR:HB2	1:A:21:PRO:HD3	1.87	0.57
1:A:124:VAL:HG12	1:A:126:PHE:HD1	1.68	0.57
1:A:234:LYS:HE2	1:A:238:LEU:HD21	1.87	0.57
1:A:498:LYS:HG2	1:A:538:GLU:O	2.05	0.57
1:B:269:ARG:O	1:B:273:ILE:HG12	2.05	0.57
1:B:382:THR:HG22	1:B:383:ARG:H	1.70	0.56
1:B:411:ASP:OD2	2:B:622:HOH:O	2.18	0.56
1:A:420:ASN:O	1:A:423:GLN:N	2.39	0.56
1:B:428:TYR:O	1:B:432:LYS:HG3	2.07	0.55
1:B:63:ARG:NH2	2:B:672:HOH:O	2.40	0.54
1:A:69:ILE:O	1:A:71:LYS:N	2.39	0.54
1:B:506:ILE:HD11	1:B:569:VAL:HG23	1.90	0.54
1:A:506:ILE:HG22	1:A:507:LEU:HD12	1.90	0.54
1:B:121:LYS:NZ	1:B:327:GLU:OE1	2.36	0.54
1:B:273:ILE:HG13	1:B:318:ALA:HA	1.90	0.54
1:A:173:PHE:HD1	1:A:176:LEU:HD12	1.74	0.53
1:A:184:PHE:CE1	1:A:193:PRO:HD2	2.42	0.53
1:B:15:ALA:HB2	1:B:74:PRO:HD3	1.90	0.53
1:A:414:LEU:HG	1:A:417:GLU:HB2	1.91	0.53
1:A:169:TRP:CE3	1:A:264:SER:HB3	2.43	0.53
1:A:447:SER:HB3	1:A:450:LYS:HB2	1.90	0.53
1:A:508:ARG:O	1:A:511:GLU:HG2	2.09	0.53
1:A:187:TYR:CE2	1:A:235:ALA:HB2	2.44	0.53
1:B:407:GLU:OE1	1:B:407:GLU:N	2.42	0.53
1:A:124:VAL:HG12	1:A:126:PHE:CD1	2.43	0.53
1:A:425:SER:OG	1:A:583:LYS:O	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:ARG:HD3	2:B:630:HOH:O	2.09	0.52
1:A:47:MET:SD	1:A:47:MET:N	2.82	0.52
1:A:417:GLU:OE2	1:A:587:ARG:HD3	2.09	0.52
1:A:487:ALA:HA	1:A:564:LEU:HD21	1.91	0.52
1:A:561:TRP:CE2	1:A:562:ARG:HG3	2.45	0.52
1:A:234:LYS:O	1:A:238:LEU:HG	2.09	0.52
1:A:561:TRP:NE1	1:A:562:ARG:HG3	2.25	0.52
1:A:27:PRO:HD2	1:A:49:ILE:HG23	1.91	0.52
1:B:136:HIS:HD1	1:B:136:HIS:H	1.58	0.52
1:A:496:HIS:HB3	1:A:499:GLU:HG2	1.92	0.52
1:A:540:TYR:HE1	1:A:545:CYS:HB3	1.75	0.52
1:A:543:CYS:O	1:A:562:ARG:NH1	2.42	0.52
1:A:447:SER:CB	1:A:450:LYS:HB2	2.41	0.51
1:A:143:THR:HG22	1:A:256:VAL:HG21	1.92	0.51
1:A:441:LEU:HD12	1:B:293:PHE:HE1	1.75	0.51
1:A:380:PHE:CE2	1:A:388:VAL:HG21	2.45	0.51
1:A:559:ASN:HB3	1:A:562:ARG:HB2	1.92	0.51
1:B:465:ALA:O	1:B:469:ILE:HG13	2.11	0.51
1:B:348:PHE:O	1:B:352:GLN:HG3	2.11	0.51
1:A:413:VAL:HG13	1:A:417:GLU:HB3	1.92	0.50
1:B:233:THR:O	1:B:236:TRP:HB3	2.11	0.50
1:A:129:PRO:HA	1:A:139:HIS:CE1	2.46	0.50
1:A:393:LEU:HD11	1:A:446:PHE:CE1	2.47	0.50
1:A:440:ARG:NH1	1:A:520:LEU:O	2.44	0.50
1:A:20:TYR:OH	1:A:69:ILE:HG13	2.12	0.50
1:A:76:ASN:OD1	1:A:77:GLU:N	2.43	0.50
1:A:516:ILE:HD13	1:A:522:LEU:HA	1.93	0.50
1:A:404:LYS:NZ	1:A:454:ASP:OD1	2.39	0.49
1:A:508:ARG:HD2	2:A:621:HOH:O	2.13	0.49
1:A:48:GLY:O	1:A:50:SER:N	2.45	0.49
1:A:184:PHE:O	1:A:187:TYR:HB3	2.13	0.49
1:A:116:LEU:HB2	1:A:118:GLU:O	2.12	0.49
1:A:348:PHE:O	1:A:352:GLN:HG3	2.13	0.49
1:A:489:GLU:OE1	2:A:649:HOH:O	2.19	0.49
1:B:413:VAL:HG23	1:B:418:GLU:HB2	1.95	0.49
1:A:380:PHE:CE1	1:A:446:PHE:HB3	2.49	0.48
1:A:275:LYS:NZ	2:A:660:HOH:O	2.26	0.48
1:B:173:PHE:CD1	1:B:176:LEU:HD12	2.47	0.48
1:B:280:ARG:HH11	1:B:354:ILE:HG12	1.78	0.48
1:B:187:TYR:CE2	1:B:235:ALA:HB2	2.48	0.48
1:B:474:ARG:NH2	2:B:626:HOH:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:TYR:CD1	1:A:20:TYR:N	2.81	0.48
1:A:492:ILE:HA	1:A:561:TRP:HB2	1.95	0.47
1:B:469:ILE:HD13	1:B:569:VAL:HG11	1.95	0.47
1:B:169:TRP:HB2	1:B:263:GLU:HG3	1.96	0.47
1:B:238:LEU:O	1:B:242:VAL:HG23	2.14	0.47
1:A:168:ASP:H	1:A:263:GLU:HG2	1.80	0.47
1:A:498:LYS:NZ	1:A:538:GLU:OE1	2.47	0.47
1:B:34:GLN:H	1:B:34:GLN:CD	2.14	0.47
1:A:407:GLU:N	1:A:407:GLU:OE1	2.47	0.47
1:A:508:ARG:CD	2:A:621:HOH:O	2.61	0.47
1:B:322:GLN:OE1	1:B:327:GLU:HG2	2.15	0.47
1:A:20:TYR:N	1:A:20:TYR:HD1	2.12	0.47
1:A:420:ASN:O	1:A:422:ALA:N	2.48	0.47
1:A:545:CYS:SG	1:A:546:VAL:N	2.87	0.47
1:A:9:GLN:HG2	1:A:28:LEU:HB3	1.97	0.47
1:A:376:ASP:OD1	1:A:378:LYS:HG2	2.14	0.47
1:B:240:CYS:HB3	1:B:244:ARG:HH21	1.80	0.47
1:A:440:ARG:HH12	1:A:520:LEU:HB2	1.79	0.46
1:A:286:ASP:OD2	1:A:289:ARG:NH2	2.36	0.46
1:A:509:PHE:CE2	1:A:513:LEU:HD11	2.51	0.46
1:B:64:GLU:O	1:B:66:ALA:N	2.48	0.46
1:A:493:LEU:HG	1:A:561:TRP:CE2	2.50	0.46
1:A:447:SER:OG	1:A:450:LYS:HB2	2.16	0.46
1:B:266:TYR:HE1	1:B:322:GLN:HG2	1.79	0.46
1:A:77:GLU:O	1:A:98:PHE:HB2	2.16	0.46
1:A:512:ILE:HG13	1:A:528:TYR:CD1	2.51	0.46
1:B:294:VAL:HG13	1:B:353:MET:SD	2.56	0.46
1:B:168:ASP:OD2	1:B:264:SER:OG	2.26	0.46
1:B:169:TRP:NE1	1:B:267:GLN:OE1	2.45	0.46
1:B:296:GLY:O	2:B:656:HOH:O	2.21	0.46
1:B:144:ILE:HD13	1:B:432:LYS:HA	1.97	0.45
1:B:130:ASN:ND2	1:B:172:GLN:HE22	2.10	0.45
1:B:414:LEU:H	1:B:414:LEU:HD13	1.81	0.45
1:B:253:ALA:HB1	1:B:428:TYR:CZ	2.52	0.45
1:B:425:SER:OG	1:B:583:LYS:O	2.19	0.45
1:A:8:LEU:O	1:A:12:PHE:HD1	1.99	0.45
1:A:123:ILE:HG12	1:A:161:LEU:HB3	1.97	0.45
1:A:307:ASP:OD1	1:A:307:ASP:N	2.48	0.45
1:A:276:GLU:OE2	1:A:280:ARG:NH2	2.50	0.45
1:A:433:TYR:HB2	1:A:582:ILE:HD11	1.98	0.45
1:B:274:VAL:HG22	1:B:303:ILE:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:556:LEU:HD23	1:B:556:LEU:HA	1.75	0.45
1:B:220:GLN:HG2	2:B:602:HOH:O	2.18	0.44
1:A:136:HIS:HD1	1:A:136:HIS:H	1.64	0.44
1:A:273:ILE:HD13	1:A:273:ILE:HA	1.77	0.44
1:A:521:PHE:HB3	1:A:523:HIS:CE1	2.52	0.44
1:A:136:HIS:HE1	1:A:139:HIS:CD2	2.35	0.44
1:A:548:LYS:HB2	1:A:548:LYS:HE3	1.76	0.44
1:A:99:VAL:O	1:A:103:LEU:HD12	2.18	0.44
1:A:496:HIS:CD2	1:A:497:GLU:H	2.35	0.44
1:A:515:LYS:HA	1:A:515:LYS:HD2	1.74	0.44
1:B:82:VAL:HG12	1:B:92:VAL:HG22	1.99	0.44
1:B:116:LEU:HD11	1:B:158:TYR:CD1	2.53	0.44
1:B:414:LEU:HB2	1:B:415:THR:H	1.61	0.44
1:A:85:ALA:O	1:A:89:PHE:HB2	2.18	0.44
1:A:229:ASN:HB2	2:A:632:HOH:O	2.18	0.44
1:B:106:LEU:HD13	1:B:111:VAL:HG22	2.00	0.44
1:B:271:ASN:OD1	1:B:310:TYR:OH	2.10	0.43
1:B:247:LEU:HD23	1:B:247:LEU:HA	1.67	0.43
1:A:187:TYR:HA	1:A:191:SER:HB2	2.00	0.43
1:B:147:GLU:OE2	1:B:162:ARG:NH1	2.48	0.43
1:A:147:GLU:HB2	1:A:256:VAL:HG22	2.00	0.43
1:A:273:ILE:HG13	1:A:318:ALA:HA	1.99	0.43
1:A:537:THR:O	1:A:541:ASP:HB2	2.19	0.43
1:B:375:GLU:C	1:B:377:LYS:H	2.22	0.43
1:A:319:ALA:O	1:A:323:ARG:HG3	2.18	0.43
1:A:154:GLU:HG3	1:A:160:VAL:HG21	2.00	0.43
1:A:233:THR:O	1:A:236:TRP:HB3	2.19	0.43
1:B:136:HIS:O	1:B:139:HIS:HB2	2.18	0.42
1:A:472:ILE:HD12	1:A:566:CYS:SG	2.60	0.42
1:A:134:GLU:OE2	1:A:389:ARG:HG3	2.19	0.42
1:A:414:LEU:HB2	1:A:415:THR:H	1.51	0.42
1:B:307:ASP:N	1:B:307:ASP:OD1	2.53	0.42
1:B:551:GLN:O	1:B:553:GLY:N	2.52	0.42
1:B:244:ARG:HE	1:B:244:ARG:HB2	1.64	0.42
1:A:280:ARG:HH21	1:A:354:ILE:HG12	1.85	0.42
1:A:479:ASP:OD1	1:A:482:MET:HG3	2.20	0.42
1:A:540:TYR:C	1:A:542:SER:HA	2.40	0.42
1:B:77:GLU:H	1:B:77:GLU:CD	2.22	0.42
1:B:415:THR:OG1	1:B:416:ALA:N	2.53	0.42
1:A:4:ILE:HD11	1:A:41:TYR:CE2	2.55	0.41
1:A:49:ILE:O	1:A:51:GLN:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:GLN:HB2	1:A:507:LEU:HD21	2.02	0.41
1:A:493:LEU:HG	1:A:561:TRP:NE1	2.35	0.41
1:B:84:ILE:HA	1:B:89:PHE:O	2.20	0.41
1:B:411:ASP:OD1	1:B:412:LYS:N	2.52	0.41
1:A:248:ASN:O	1:A:252:ASP:N	2.51	0.41
1:A:578:ASP:HA	2:A:604:HOH:O	2.21	0.41
1:B:45:SER:O	1:B:49:ILE:HG13	2.20	0.41
1:B:278:GLU:OE2	1:B:290:LYS:NZ	2.27	0.41
1:A:98:PHE:O	1:A:102:GLN:HG2	2.21	0.41
1:A:365:PHE:HE1	1:A:367:ALA:HA	1.84	0.41
1:B:180:LEU:HD23	1:B:235:ALA:HB1	2.03	0.41
1:B:382:THR:HG22	1:B:383:ARG:N	2.33	0.41
1:A:151:ARG:NH1	1:A:581:GLY:HA2	2.34	0.41
1:B:137:VAL:HA	1:B:390:LEU:HD21	2.01	0.41
1:B:470:ARG:NH1	2:B:654:HOH:O	2.53	0.41
1:A:390:LEU:HD23	1:A:390:LEU:HA	1.90	0.41
1:B:39:GLY:HA2	1:B:93:HIS:CD2	2.56	0.41
1:B:336:VAL:HG11	1:B:344:PHE:CE2	2.56	0.41
1:A:136:HIS:CE1	1:A:139:HIS:CG	3.09	0.41
1:B:192:PRO:HA	1:B:193:PRO:HD3	1.90	0.41
1:B:25:ASN:HA	1:B:26:PRO:HD2	1.62	0.41
1:B:124:VAL:HG12	1:B:126:PHE:CD1	2.52	0.41
1:B:402:MET:SD	1:B:418:GLU:OE2	2.80	0.41
1:B:413:VAL:CG2	1:B:418:GLU:HB2	2.50	0.41
1:A:494:LEU:HA	1:A:494:LEU:HD22	1.85	0.40
1:B:121:LYS:HB3	1:B:329:ALA:HA	2.03	0.40
1:B:469:ILE:HG12	1:B:536:PHE:CE2	2.57	0.40
1:B:492:ILE:HA	1:B:561:TRP:HB2	2.02	0.40
1:A:-8:VAL:HG13	1:A:-7:PRO:HD2	2.02	0.40
1:B:76:ASN:OD1	1:B:79:ILE:HB	2.21	0.40
1:B:141:ARG:O	1:B:145:ILE:HG13	2.21	0.40
1:A:441:LEU:HD12	1:B:293:PHE:CE1	2.55	0.40
1:A:575:LYS:O	1:A:579:ILE:HG13	2.22	0.40
1:B:116:LEU:HD21	1:B:158:TYR:CE1	2.56	0.40
1:B:183:LYS:NZ	1:B:203:GLU:OE1	2.52	0.40
1:A:137:VAL:HG11	1:A:372:VAL:HG11	2.03	0.40
1:B:169:TRP:CH2	1:B:225:LEU:HG	2.56	0.40
1:B:180:LEU:HD12	1:B:184:PHE:HD2	1.86	0.40
1:A:466:PHE:HD1	1:A:573:MET:HE2	1.87	0.40
1:B:169:TRP:CB	1:B:263:GLU:HG3	2.52	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	551/607 (91%)	490 (89%)	51 (9%)	10 (2%)	8 28
1	B	569/607 (94%)	520 (91%)	45 (8%)	4 (1%)	22 53
All	All	1120/1214 (92%)	1010 (90%)	96 (9%)	14 (1%)	12 36

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	ILE
1	A	70	THR
1	B	26	PRO
1	B	65	ILE
1	A	-9	LEU
1	B	552	THR
1	A	22	ASP
1	A	191	SER
1	A	544	TYR
1	B	542	SER
1	A	88	GLY
1	A	190	VAL
1	A	415	THR
1	A	230	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	494/530 (93%)	466 (94%)	28 (6%)	20	50
1	B	503/530 (95%)	478 (95%)	25 (5%)	24	56
All	All	997/1060 (94%)	944 (95%)	53 (5%)	22	54

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-9	LEU
1	A	1	MET
1	A	3	ASN
1	A	4	ILE
1	A	20	TYR
1	A	31	THR
1	A	47	MET
1	A	51	GLN
1	A	72	HIS
1	A	75	ASP
1	A	96	LYS
1	A	104	THR
1	A	118	GLU
1	A	204	SER
1	A	255	ASP
1	A	305	LYS
1	A	306	SER
1	A	336	VAL
1	A	337	ASP
1	A	382	THR
1	A	412	LYS
1	A	492	ILE
1	A	493	LEU
1	A	494	LEU
1	A	498	LYS
1	A	537	THR
1	A	539	PHE
1	A	564	LEU
1	B	1	MET
1	B	51	GLN
1	B	65	ILE
1	B	104	THR
1	B	106	LEU
1	B	137	VAL
1	B	243	SER

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Mol	Chain	Res	Type
1	B	255	ASP
1	B	272	ASP
1	B	299	ILE
1	B	301	LEU
1	B	311	THR
1	B	322	GLN
1	B	337	ASP
1	B	375	GLU
1	B	414	LEU
1	B	454	ASP
1	B	478	ILE
1	B	479	ASP
1	B	493	LEU
1	B	494	LEU
1	B	534	THR
1	B	551	GLN
1	B	558	VAL
1	B	560	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
1	B	172	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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	565/607 (93%)	0.19	21 (3%)	41	31	18, 52, 86, 113	0
1	B	577/607 (95%)	0.05	20 (3%)	44	34	15, 39, 74, 89	0
All	All	1142/1214 (94%)	0.12	41 (3%)	42	32	15, 44, 81, 113	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	419	LEU	4.4
1	B	117	GLY	3.9
1	A	89	PHE	3.9
1	A	94	LEU	3.8
1	A	385	GLY	3.8
1	B	49	ILE	3.7
1	B	69	ILE	3.7
1	B	82	VAL	3.5
1	A	494	LEU	3.4
1	B	20	TYR	3.4
1	A	92	VAL	3.4
1	B	29	LEU	3.3
1	A	558	VAL	3.2
1	B	12	PHE	3.1
1	B	71	LYS	3.1
1	A	49	ILE	2.9
1	A	85	ALA	2.9
1	A	52	MET	2.8
1	A	546	VAL	2.7
1	A	-6	ARG	2.7
1	B	85	ALA	2.6
1	A	69	ILE	2.6
1	B	411	ASP	2.5
1	B	212	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	561	TRP	2.4
1	B	16	ILE	2.4
1	A	180	LEU	2.3
1	B	43	CYS	2.2
1	B	92	VAL	2.2
1	B	552	THR	2.2
1	A	412	LYS	2.1
1	A	14	HIS	2.1
1	B	420	ASN	2.1
1	A	383	ARG	2.1
1	B	68	ASN	2.1
1	A	41	TYR	2.1
1	B	91	ASN	2.1
1	A	179	HIS	2.0
1	A	74	PRO	2.0
1	A	411	ASP	2.0
1	B	84	ILE	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.