Full wwPDB X-ray Structure Validation Report

May 13, 2020 – 11:50 am BST

PDB ID	:	1ULH
Title	:	A short peptide insertion crucial for angiostatic activity of human tryptophanyl-tRNA synthetase
Authors	:	Kise, Y.; Sengoku, T.; Ishii, R.; Yokoyama, S.; Park, S.G.; Lee, S.W.; Kim, S.; Nureki, O.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2003-09-12
Resolution	:	2.31 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 following versions of software and data (see references (1)) were used in the production of this report:

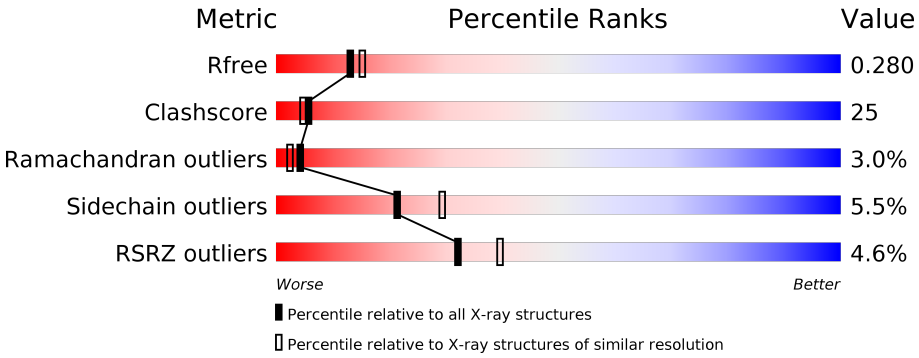
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.31 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 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	390	6% 47% 40% 6% • 7%
1	B	390	3% 53% 39% • •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6488 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 Tryptophanyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	0	0
			2958	1903	500	541	14			
1	B	379	Total	C	N	O	S	0	0	0
			3053	1960	513	565	15			

- Molecule 2 is water.

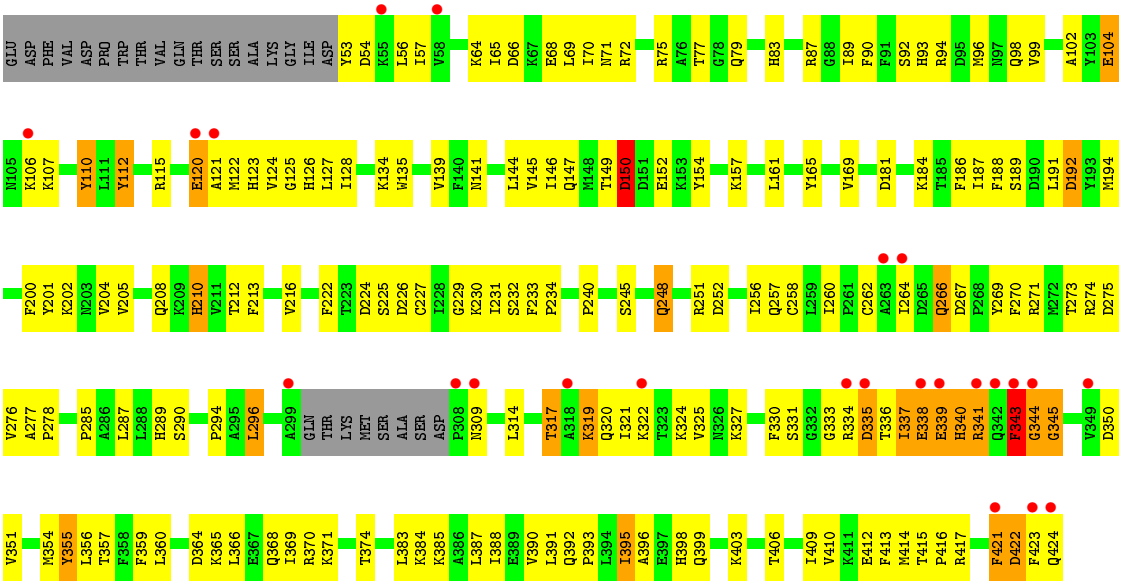
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	219	Total	O	0	0
			219	219		
2	B	258	Total	O	0	0
			258	258		

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.

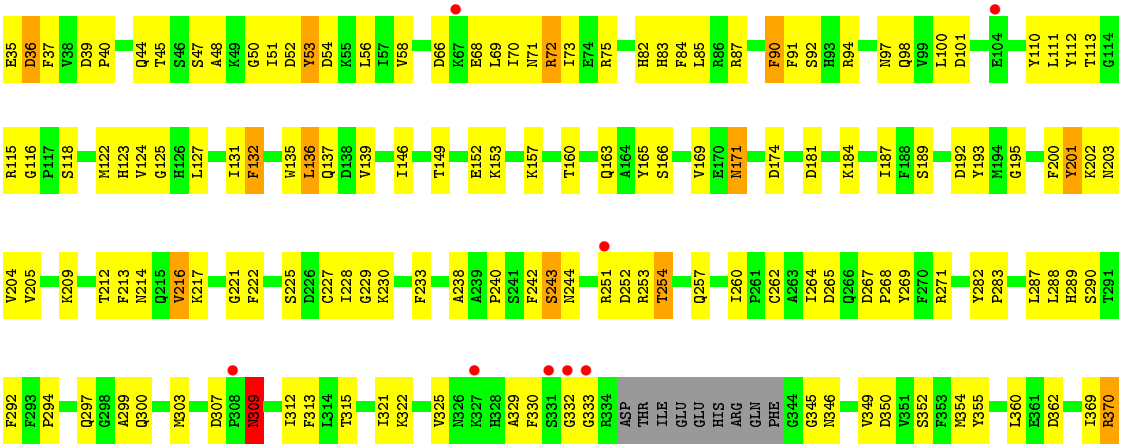
- Molecule 1: Tryptophanyl-tRNA synthetase

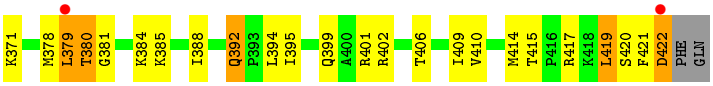
Chain A:



- Molecule 1: Tryptophanyl-tRNA synthetase

Chain B:




K371
M378
L379
T380
G381
K384
K385
I388
Q392
P393
L394
I395
Q399
A400
R401
R402
T406
I409
V410
M414
T415
P416
R417
K418
L419
S420
F421
D422
PHE
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	136.03Å 96.61Å 98.32Å 90.00° 130.26° 90.00°	Depositor
Resolution (Å)	42.89 – 2.31 42.89 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.7 (42.89-2.31) 90.6 (42.89-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.66 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.241 , 0.292 0.234 , 0.280	Depositor DCC
R_{free} test set	1939 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	42.8	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6488	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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	1.18	8/3031 (0.3%)	0.82	2/4086 (0.0%)
1	B	1.17	9/3127 (0.3%)	0.84	4/4221 (0.1%)
All	All	1.17	17/6158 (0.3%)	0.83	6/8307 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	TYR	CD2-CE2	5.88	1.48	1.39
1	A	135	TRP	CE3-CZ3	5.80	1.48	1.38
1	B	112	TYR	CD1-CE1	5.72	1.48	1.39
1	B	355	TYR	CD2-CE2	5.64	1.47	1.39
1	A	269	TYR	CD1-CE1	5.51	1.47	1.39
1	B	165	TYR	CD1-CE1	5.48	1.47	1.39
1	B	110	TYR	CD1-CE1	5.34	1.47	1.39
1	B	282	TYR	CD1-CE1	5.34	1.47	1.39
1	B	53	TYR	CD1-CE1	5.32	1.47	1.39
1	A	154	TYR	CD1-CE1	5.23	1.47	1.39
1	A	421	PHE	CE2-CZ	5.18	1.47	1.37
1	B	132	PHE	CE2-CZ	5.16	1.47	1.37
1	B	165	TYR	CD2-CE2	5.16	1.47	1.39
1	B	269	TYR	CD1-CE1	5.16	1.47	1.39
1	A	355	TYR	CD2-CE2	5.07	1.47	1.39
1	A	355	TYR	CD1-CE1	5.04	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	TYR	CD2-CE2	5.03	1.46	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	332	GLY	N-CA-C	-6.98	95.66	113.10
1	A	338	GLU	N-CA-C	-6.18	94.32	111.00
1	A	150	ASP	CB-CG-OD2	5.96	123.66	118.30
1	B	90	PHE	N-CA-C	-5.90	95.08	111.00
1	B	380	THR	N-CA-C	5.81	126.68	111.00
1	B	379	LEU	CA-CB-CG	5.53	128.01	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	TYR	Sidechain
1	B	201	TYR	Sidechain

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	2958	0	2917	163	0
1	B	3053	0	3010	144	0
2	A	219	0	0	64	0
2	B	258	0	0	67	0
All	All	6488	0	5927	303	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 25.

All (303) 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:356:LEU:HD22	1:A:360:LEU:HD22	1.48	0.95
1:B:72:ARG:HG2	1:B:100:LEU:HD13	1.53	0.91
1:B:184:LYS:HB3	2:B:573:HOH:O	1.76	0.85
1:A:345:GLY:HA3	1:A:374:THR:HA	1.57	0.85
1:B:329:ALA:HB1	2:B:645:HOH:O	1.77	0.85
1:B:82:HIS:HD2	1:B:84:PHE:H	1.34	0.75
1:B:92:SER:HB3	1:B:289:HIS:HB2	1.68	0.74
1:A:94:ARG:HD2	1:A:287:LEU:HD12	1.70	0.74
1:A:145:VAL:HG13	1:A:188:PHE:HE2	1.52	0.73
1:B:123:HIS:HD2	1:B:125:GLY:H	1.36	0.71
1:A:226:ASP:HB2	2:A:593:HOH:O	1.89	0.71
1:A:99:VAL:HG22	1:A:257:GLN:HG2	1.71	0.71
1:B:395:ILE:HG22	1:B:399:GLN:HE21	1.58	0.69
2:A:492:HOH:O	1:B:228:ILE:HG22	1.94	0.67
1:A:189:SER:HB3	1:A:192:ASP:HB2	1.77	0.67
1:A:66:ASP:HB2	1:A:68:GLU:H	1.59	0.67
1:A:415:THR:O	1:A:417:ARG:HG3	1.96	0.66
1:A:231:ILE:HG23	2:A:492:HOH:O	1.96	0.66
1:A:144:LEU:HD21	2:A:588:HOH:O	1.98	0.64
1:A:325:VAL:HG21	1:A:388:ILE:HG12	1.77	0.64
1:A:187:ILE:O	1:A:414:MET:HA	1.99	0.63
1:B:137:GLN:HE22	1:B:181:ASP:H	1.46	0.63
2:A:520:HOH:O	1:B:225:SER:HA	1.98	0.63
1:A:355:TYR:HB3	2:A:451:HOH:O	1.98	0.63
1:A:92:SER:HB3	1:A:289:HIS:HB2	1.81	0.62
1:B:349:VAL:HB	2:B:649:HOH:O	2.00	0.62
1:B:83:HIS:HB3	2:B:511:HOH:O	2.00	0.61
1:A:141:ASN:O	1:A:422:ASP:HB2	2.01	0.61
1:A:245:SER:HB2	2:A:497:HOH:O	2.01	0.61
1:A:233:PHE:HA	2:A:608:HOH:O	2.00	0.61
1:B:238:ALA:HA	2:B:660:HOH:O	2.00	0.59
1:A:224:ASP:HA	2:A:593:HOH:O	2.02	0.59
1:B:379:LEU:HB2	2:B:619:HOH:O	2.03	0.59
1:A:93:HIS:HD2	1:A:96:MET:H	1.49	0.59
1:B:360:LEU:HB3	2:B:446:HOH:O	2.02	0.59
1:A:77:THR:HG23	1:A:139:VAL:HB	1.85	0.59
1:A:68:GLU:HA	1:A:71:ASN:ND2	2.19	0.58
1:B:35:GLU:N	1:B:45:THR:HG23	2.19	0.58
1:B:87:ARG:HB2	2:B:502:HOH:O	2.02	0.58
1:B:73:ILE:HD13	1:B:100:LEU:HD11	1.86	0.58
1:A:204:VAL:O	1:A:208:GLN:HG3	2.05	0.57
1:A:260:ILE:HB	1:A:287:LEU:HD23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ILE:HD13	1:A:64:LYS:HB2	1.86	0.57
1:A:371:LYS:HE3	2:A:542:HOH:O	2.05	0.57
1:B:312:ILE:HG13	2:B:466:HOH:O	2.04	0.56
1:B:115:ARG:HD2	2:B:577:HOH:O	2.03	0.56
1:B:35:GLU:HB3	1:B:52:ASP:H	1.71	0.56
1:A:115:ARG:NH2	1:A:122:MET:HG2	2.21	0.56
1:B:394:LEU:HD23	2:B:570:HOH:O	2.04	0.56
1:B:300:GLN:HA	2:B:523:HOH:O	2.05	0.55
1:A:152:GLU:HB2	1:A:233:PHE:CZ	2.41	0.55
1:B:242:PHE:HA	2:B:433:HOH:O	2.06	0.55
1:B:370:ARG:HH12	1:B:371:LYS:HG3	1.72	0.55
1:A:187:ILE:HG13	2:A:436:HOH:O	2.06	0.55
1:B:209:LYS:HG3	2:B:560:HOH:O	2.05	0.55
1:B:267:ASP:HB3	2:B:545:HOH:O	2.05	0.55
1:A:324:LYS:HG3	2:A:641:HOH:O	2.07	0.55
1:A:320:GLN:HB2	2:A:438:HOH:O	2.07	0.55
1:A:396:ALA:N	2:A:496:HOH:O	2.39	0.55
1:A:213:PHE:HA	2:A:492:HOH:O	2.07	0.55
1:A:335:ASP:C	1:A:337:ILE:H	2.10	0.55
1:B:139:VAL:HB	2:B:486:HOH:O	2.06	0.54
1:A:392:GLN:HB2	1:A:393:PRO:HD3	1.88	0.54
1:B:136:LEU:HD11	2:B:534:HOH:O	2.07	0.54
1:B:136:LEU:HA	2:B:486:HOH:O	2.08	0.54
1:B:288:LEU:HD13	2:B:534:HOH:O	2.08	0.54
1:B:388:ILE:O	1:B:392:GLN:HB2	2.08	0.54
1:B:388:ILE:HG22	1:B:392:GLN:NE2	2.23	0.54
1:A:264:ILE:HA	1:A:289:HIS:CD2	2.42	0.53
1:A:364:ASP:O	1:A:368:GLN:HG3	2.08	0.53
1:B:394:LEU:HD12	2:B:552:HOH:O	2.09	0.53
1:A:248:GLN:HG2	2:A:589:HOH:O	2.06	0.53
1:B:124:VAL:HB	2:B:500:HOH:O	2.07	0.53
1:B:401:ARG:HD2	2:B:621:HOH:O	2.08	0.53
1:B:73:ILE:HG22	2:B:605:HOH:O	2.09	0.53
1:A:384:LYS:O	1:A:388:ILE:HG13	2.09	0.53
1:B:68:GLU:HA	2:B:483:HOH:O	2.08	0.53
1:A:231:ILE:HG13	2:A:628:HOH:O	2.08	0.53
1:B:85:LEU:HB3	2:B:659:HOH:O	2.08	0.53
1:A:271:ARG:HG3	2:A:469:HOH:O	2.09	0.53
1:A:383:LEU:HB3	2:A:452:HOH:O	2.09	0.53
1:B:253:ARG:HH11	1:B:253:ARG:HG2	1.73	0.53
1:B:309:ASN:HB2	2:B:565:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:PHE:CZ	1:B:290:SER:HB3	2.43	0.52
1:B:346:ASN:HD21	1:B:349:VAL:HG23	1.74	0.52
1:B:48:ALA:HA	1:B:300:GLN:NE2	2.25	0.52
1:A:275:ASP:O	1:A:278:PRO:HD2	2.09	0.52
1:A:77:THR:HG22	1:A:79:GLN:HB2	1.91	0.52
1:B:216:VAL:HG13	1:B:222:PHE:HD2	1.73	0.52
1:B:122:MET:HE1	1:B:171:ASN:HA	1.92	0.52
1:A:384:LYS:HG3	2:A:452:HOH:O	2.10	0.52
1:B:69:LEU:O	1:B:73:ILE:HG12	2.10	0.51
1:B:82:HIS:HB3	2:B:562:HOH:O	2.10	0.51
1:B:181:ASP:HB3	1:B:184:LYS:HB2	1.91	0.51
1:A:212:THR:HA	1:B:227:CYS:HA	1.91	0.51
1:A:365:LYS:O	1:A:369:ILE:HG13	2.11	0.51
1:A:334:ARG:O	1:A:336:THR:N	2.43	0.51
1:A:360:LEU:HD13	1:A:390:VAL:CG2	2.41	0.51
1:B:202:LYS:HG3	2:B:474:HOH:O	2.11	0.51
1:A:229:GLY:HA2	2:B:488:HOH:O	2.11	0.51
1:A:424:GLN:HG2	2:A:507:HOH:O	2.10	0.51
1:A:277:ALA:HB2	2:A:445:HOH:O	2.11	0.51
1:A:53:TYR:HA	1:A:56:LEU:HD12	1.93	0.51
1:A:393:PRO:C	2:A:496:HOH:O	2.50	0.50
1:B:203:ASN:HD21	1:B:244:ASN:HB2	1.75	0.50
1:A:285:PRO:HD3	2:A:445:HOH:O	2.10	0.50
1:A:327:LYS:HE3	2:A:609:HOH:O	2.11	0.50
1:A:338:GLU:O	1:A:339:GLU:HG3	2.10	0.50
1:B:137:GLN:NE2	1:B:181:ASP:H	2.09	0.50
1:B:243:SER:HB2	2:B:591:HOH:O	2.11	0.50
1:B:251:ARG:HG3	2:B:652:HOH:O	2.10	0.50
1:B:346:ASN:HB3	2:B:428:HOH:O	2.11	0.50
1:B:94:ARG:HD3	2:B:614:HOH:O	2.10	0.50
1:A:123:HIS:HB2	2:A:605:HOH:O	2.12	0.50
1:A:387:LEU:HD11	2:A:451:HOH:O	2.12	0.50
1:A:417:ARG:HD2	2:A:603:HOH:O	2.11	0.50
1:B:350:ASP:HB2	2:B:463:HOH:O	2.12	0.50
1:A:72:ARG:HB2	2:A:458:HOH:O	2.12	0.50
1:A:124:VAL:HG12	2:A:605:HOH:O	2.12	0.50
1:A:360:LEU:HD13	1:A:390:VAL:HG21	1.93	0.50
1:A:266:GLN:HG2	2:A:455:HOH:O	2.12	0.50
1:A:370:ARG:HA	2:A:484:HOH:O	2.12	0.49
1:B:283:PRO:HG2	2:B:599:HOH:O	2.12	0.49
1:B:303:MET:HA	2:B:643:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:THR:HG22	1:B:47:SER:H	1.77	0.49
1:B:321:ILE:O	1:B:325:VAL:HG23	2.12	0.49
1:B:66:ASP:HB3	2:B:633:HOH:O	2.12	0.49
1:A:224:ASP:HB3	2:B:503:HOH:O	2.13	0.49
1:B:100:LEU:HD21	2:B:631:HOH:O	2.12	0.49
1:B:415:THR:O	1:B:417:ARG:HG3	2.12	0.49
1:B:69:LEU:HD23	1:B:73:ILE:HD11	1.93	0.49
1:A:106:LYS:HD2	1:A:424:GLN:HG3	1.93	0.49
1:B:35:GLU:HG3	1:B:36:ASP:H	1.77	0.49
1:A:208:GLN:HB3	1:B:229:GLY:CA	2.43	0.49
1:B:240:PRO:HA	2:B:508:HOH:O	2.12	0.49
1:A:72:ARG:HD2	2:A:572:HOH:O	2.13	0.48
1:A:161:LEU:HD13	2:A:464:HOH:O	2.11	0.48
1:A:77:THR:CG2	1:A:79:GLN:HB2	2.43	0.48
1:B:406:THR:HG21	2:B:525:HOH:O	2.12	0.48
1:A:125:GLY:O	1:A:128:ILE:HG12	2.14	0.48
1:A:276:VAL:HG23	2:A:471:HOH:O	2.12	0.48
1:A:337:ILE:HD13	2:A:554:HOH:O	2.13	0.48
1:B:152:GLU:HB2	1:B:233:PHE:CZ	2.48	0.48
1:A:202:LYS:HG3	2:B:611:HOH:O	2.12	0.48
1:A:248:GLN:HG3	1:A:416:PRO:HB3	1.96	0.48
1:A:65:ILE:HG23	1:A:69:LEU:HD23	1.95	0.48
1:B:71:ASN:HB3	2:B:543:HOH:O	2.12	0.48
1:A:395:ILE:O	1:A:398:HIS:HB3	2.14	0.48
1:B:217:LYS:HA	1:B:222:PHE:H	1.78	0.48
1:B:85:LEU:N	2:B:562:HOH:O	2.47	0.48
1:A:354:MET:O	1:A:357:THR:HB	2.14	0.48
1:A:70:ILE:HG13	2:A:466:HOH:O	2.13	0.48
1:B:313:PHE:HB3	1:B:315:THR:HG22	1.96	0.48
1:B:253:ARG:O	1:B:254:THR:HG22	2.13	0.47
1:A:90:PHE:HA	1:A:290:SER:HA	1.96	0.47
1:A:240:PRO:HG2	2:A:544:HOH:O	2.15	0.47
1:B:174:ASP:CG	1:B:402:ARG:HE	2.18	0.47
1:B:200:PHE:O	1:B:204:VAL:HG23	2.14	0.47
1:B:260:ILE:HB	1:B:287:LEU:HD23	1.96	0.47
1:B:169:VAL:HG13	1:B:410:VAL:HG11	1.97	0.47
1:A:391:LEU:HD21	2:A:451:HOH:O	2.14	0.47
1:A:75:ARG:HB2	2:A:572:HOH:O	2.15	0.47
1:A:355:TYR:HB3	1:A:387:LEU:HD11	1.97	0.47
1:B:71:ASN:N	2:B:483:HOH:O	2.35	0.47
1:A:321:ILE:HG13	2:A:438:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ILE:HG12	2:B:659:HOH:O	2.15	0.47
1:B:187:ILE:O	1:B:414:MET:HA	2.15	0.47
1:A:331:SER:HA	1:A:350:ASP:OD2	2.15	0.46
1:A:413:PHE:HA	1:A:417:ARG:HH21	1.79	0.46
1:B:90:PHE:CE1	1:B:290:SER:HB3	2.51	0.46
1:B:75:ARG:HG3	2:B:543:HOH:O	2.14	0.46
1:A:134:LYS:HA	2:A:560:HOH:O	2.14	0.46
1:A:87:ARG:HB3	1:A:89:ILE:CD1	2.45	0.46
1:A:309:ASN:HA	1:A:324:LYS:HE2	1.98	0.46
1:A:317:THR:HG22	1:A:320:GLN:OE1	2.16	0.46
1:A:398:HIS:HA	2:A:634:HOH:O	2.16	0.46
1:B:45:THR:HB	2:B:523:HOH:O	2.16	0.46
1:A:120:GLU:HB2	2:A:531:HOH:O	2.16	0.46
1:A:406:THR:HG23	2:A:526:HOH:O	2.16	0.46
1:A:356:LEU:HD21	1:A:387:LEU:HA	1.98	0.46
1:B:53:TYR:HB3	1:B:91:PHE:CE2	2.51	0.46
1:A:112:TYR:HD1	1:A:260:ILE:HG12	1.81	0.46
1:A:200:PHE:N	2:A:561:HOH:O	2.48	0.46
1:A:314:LEU:HD13	1:A:398:HIS:NE2	2.30	0.46
1:A:98:GLN:HE21	1:A:257:GLN:HE22	1.64	0.46
1:A:181:ASP:OD2	1:A:184:LYS:HE3	2.15	0.45
1:A:296:LEU:O	1:A:351:VAL:HG21	2.16	0.45
1:A:200:PHE:HD1	1:A:245:SER:HB3	1.81	0.45
1:B:40:PRO:HD3	1:B:268:PRO:HG2	1.98	0.45
1:B:300:GLN:HG3	2:B:523:HOH:O	2.16	0.45
1:B:395:ILE:HG13	2:B:570:HOH:O	2.15	0.45
1:B:160:THR:HG23	1:B:163:GLN:NE2	2.32	0.45
1:A:201:TYR:O	1:A:205:VAL:HG23	2.16	0.45
1:A:341:ARG:HG2	2:A:472:HOH:O	2.17	0.45
1:B:193:TYR:HB3	2:B:439:HOH:O	2.16	0.45
1:B:50:GLY:HA2	1:B:299:ALA:O	2.16	0.45
1:A:231:ILE:HD12	2:B:541:HOH:O	2.15	0.45
1:A:194:MET:O	1:B:195:GLY:HA2	2.16	0.45
1:A:359:PHE:HD1	2:A:451:HOH:O	1.99	0.45
1:B:410:VAL:HG13	2:B:554:HOH:O	2.16	0.45
1:A:194:MET:SD	1:A:200:PHE:HD2	2.40	0.45
1:A:260:ILE:HG21	1:A:270:PHE:CE2	2.52	0.45
1:A:335:ASP:C	1:A:337:ILE:N	2.70	0.45
1:B:369:ILE:HG23	1:B:378:MET:SD	2.57	0.45
1:A:115:ARG:CZ	1:A:122:MET:HG2	2.46	0.45
1:A:146:ILE:HD12	1:A:187:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LEU:HD22	2:A:560:HOH:O	2.16	0.44
1:A:360:LEU:HG	2:A:636:HOH:O	2.17	0.44
1:B:222:PHE:HA	2:B:451:HOH:O	2.17	0.44
1:A:333:GLY:C	1:A:335:ASP:H	2.19	0.44
1:B:111:LEU:HD11	1:B:136:LEU:HB3	1.99	0.44
1:A:334:ARG:HG2	1:A:344:GLY:HA2	1.98	0.44
1:A:110:TYR:HD2	1:A:256:ILE:HG22	1.82	0.44
1:A:317:THR:HG23	1:A:320:GLN:H	1.82	0.44
1:A:333:GLY:C	1:A:335:ASP:N	2.70	0.44
1:B:113:THR:O	1:B:146:ILE:HA	2.17	0.44
1:B:313:PHE:C	1:B:315:THR:H	2.20	0.44
1:B:330:PHE:CE2	1:B:349:VAL:HG12	2.52	0.44
1:B:97:ASN:HB2	2:B:566:HOH:O	2.18	0.44
1:A:104:GLU:C	1:A:106:LYS:H	2.21	0.44
1:A:257:GLN:HG3	1:A:258:CYS:N	2.32	0.44
1:A:274:ARG:HG2	1:A:285:PRO:HD2	1.98	0.44
1:A:112:TYR:HD2	1:A:145:VAL:HG12	1.82	0.44
1:A:399:GLN:O	1:A:403:LYS:HG3	2.17	0.44
1:A:409:ILE:HG13	2:A:526:HOH:O	2.17	0.44
1:A:406:THR:O	1:A:410:VAL:HG23	2.18	0.44
1:B:217:LYS:O	1:B:221:GLY:HA2	2.18	0.44
1:B:98:GLN:HA	1:B:101:ASP:HB2	2.00	0.44
1:A:343:PHE:HB3	1:A:344:GLY:H	1.52	0.44
1:B:48:ALA:O	1:B:299:ALA:HB3	2.18	0.44
1:A:202:LYS:HE3	2:B:588:HOH:O	2.18	0.44
1:A:216:VAL:HG12	2:A:620:HOH:O	2.17	0.44
1:B:116:GLY:HA3	1:B:153:LYS:HE2	1.99	0.44
1:A:294:PRO:HG2	1:A:354:MET:HB3	2.00	0.43
1:B:333:GLY:HA2	2:B:661:HOH:O	2.17	0.43
1:B:406:THR:HG22	1:B:409:ILE:HD12	2.00	0.43
1:B:294:PRO:HG2	1:B:354:MET:SD	2.58	0.43
1:B:395:ILE:HG22	1:B:399:GLN:NE2	2.29	0.43
1:A:94:ARG:HE	1:A:267:ASP:CG	2.21	0.43
1:A:360:LEU:HG	2:A:450:HOH:O	2.18	0.43
1:B:51:ILE:HD12	1:B:51:ILE:H	1.81	0.43
1:A:127:LEU:HD11	1:A:314:LEU:HD21	2.01	0.43
1:B:118:SER:HB3	1:B:157:LYS:HE3	1.99	0.43
1:B:227:CYS:SG	1:B:230:LYS:HG3	2.59	0.43
1:B:257:GLN:HA	2:B:599:HOH:O	2.18	0.43
1:B:352:SER:N	2:B:645:HOH:O	2.52	0.43
1:A:216:VAL:HG23	1:A:222:PHE:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:VAL:HG22	1:A:359:PHE:CZ	2.53	0.43
1:A:150:ASP:N	1:A:150:ASP:OD2	2.51	0.43
1:A:104:GLU:HG3	2:A:480:HOH:O	2.19	0.43
1:A:147:GLN:NE2	2:A:544:HOH:O	2.52	0.42
1:A:317:THR:C	2:A:438:HOH:O	2.57	0.42
1:B:66:ASP:O	1:B:70:ILE:HG13	2.19	0.42
1:A:273:THR:HG22	2:A:445:HOH:O	2.18	0.42
1:A:69:LEU:O	1:A:72:ARG:HB3	2.19	0.42
1:A:210:HIS:N	1:A:210:HIS:ND1	2.67	0.42
1:A:186:PHE:CZ	1:A:188:PHE:HB3	2.55	0.42
1:A:385:LYS:HA	1:A:388:ILE:HD12	2.01	0.42
1:B:381:GLY:O	1:B:385:LYS:HB2	2.19	0.42
1:A:340:HIS:CD2	1:A:344:GLY:HA3	2.55	0.42
1:B:82:HIS:HB2	1:B:135:TRP:CD2	2.55	0.42
1:A:319:LYS:HD3	1:A:322:LYS:HD2	2.01	0.42
1:A:83:HIS:O	1:A:87:ARG:HB2	2.20	0.42
1:A:322:LYS:HG3	2:A:518:HOH:O	2.19	0.42
1:A:169:VAL:HG13	1:A:410:VAL:HG11	2.02	0.42
1:B:201:TYR:O	1:B:205:VAL:HG23	2.20	0.42
1:B:54:ASP:O	1:B:58:VAL:HG23	2.19	0.42
1:A:330:PHE:HB3	1:A:351:VAL:HG23	2.02	0.41
1:B:166:SER:HB3	2:B:638:HOH:O	2.19	0.41
1:B:378:MET:HG2	2:B:447:HOH:O	2.19	0.41
1:B:419:LEU:HD22	2:B:526:HOH:O	2.19	0.41
1:A:264:ILE:HA	1:A:289:HIS:HD2	1.85	0.41
1:B:322:LYS:HG3	1:B:388:ILE:HD13	2.01	0.41
1:A:122:MET:HA	1:A:126:HIS:ND1	2.36	0.41
1:B:213:PHE:CE2	1:B:217:LYS:HD3	2.56	0.41
1:B:271:ARG:HB3	2:B:465:HOH:O	2.20	0.41
1:B:44:GLN:HB2	1:B:44:GLN:HE21	1.72	0.41
1:A:149:THR:HG21	2:A:494:HOH:O	2.20	0.41
1:A:337:ILE:HG21	2:A:554:HOH:O	2.21	0.41
1:B:132:PHE:O	1:B:136:LEU:HD22	2.21	0.41
1:B:420:SER:C	1:B:422:ASP:H	2.24	0.41
1:A:102:ALA:HB1	1:A:107:LYS:HB2	2.03	0.41
1:A:227:CYS:HA	1:B:212:THR:HA	2.03	0.41
1:B:262:CYS:O	1:B:289:HIS:HA	2.21	0.41
1:B:409:ILE:HG23	2:B:572:HOH:O	2.21	0.41
1:B:84:PHE:CZ	1:B:131:ILE:HD11	2.56	0.41
1:A:96:MET:N	2:A:598:HOH:O	2.53	0.41
1:B:35:GLU:O	1:B:37:PHE:N	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:LYS:O	1:B:388:ILE:HG13	2.21	0.41
1:B:253:ARG:HH11	1:B:253:ARG:CG	2.34	0.40
1:B:333:GLY:N	2:B:428:HOH:O	2.54	0.40
1:A:413:PHE:HD2	2:A:436:HOH:O	2.05	0.40
1:B:116:GLY:HA2	1:B:149:THR:OG1	2.21	0.40
1:B:127:LEU:HB3	2:B:485:HOH:O	2.19	0.40
1:A:191:LEU:HD22	2:A:464:HOH:O	2.21	0.40
1:A:230:LYS:HB2	2:A:628:HOH:O	2.20	0.40
1:A:262:CYS:O	1:A:289:HIS:HA	2.21	0.40
1:B:330:PHE:HE2	1:B:349:VAL:HG12	1.86	0.40
1:B:123:HIS:CD2	1:B:125:GLY:H	2.25	0.40
1:B:214:ASN:HA	1:B:217:LYS:HE2	2.04	0.40
1:B:265:ASP:HB3	1:B:292:PHE:CE2	2.56	0.40
1:A:145:VAL:HG13	1:A:188:PHE:CE2	2.43	0.40
1:B:87:ARG:NE	2:B:550:HOH:O	2.55	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	360/390 (92%)	318 (88%)	29 (8%)	13 (4%)	3	2
1	B	375/390 (96%)	343 (92%)	23 (6%)	9 (2%)	6	4
All	All	735/780 (94%)	661 (90%)	52 (7%)	22 (3%)	4	2

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	ALA
1	A	251	ARG
1	A	317	THR

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Mol	Chain	Res	Type
1	A	335	ASP
1	A	337	ILE
1	A	343	PHE
1	B	36	ASP
1	B	309	ASN
1	B	345	GLY
1	B	380	THR
1	A	340	HIS
1	A	344	GLY
1	A	345	GLY
1	B	362	ASP
1	B	419	LEU
1	A	296	LEU
1	B	254	THR
1	A	339	GLU
1	A	341	ARG
1	B	307	ASP
1	B	264	ILE
1	A	395	ILE

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	323/346 (93%)	303 (94%)	20 (6%)	18	24
1	B	335/346 (97%)	319 (95%)	16 (5%)	25	35
All	All	658/692 (95%)	622 (94%)	36 (6%)	21	29

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ASP
1	A	104	GLU
1	A	120	GLU
1	A	150	ASP

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Mol	Chain	Res	Type
1	A	157	LYS
1	A	192	ASP
1	A	210	HIS
1	A	225	SER
1	A	232	SER
1	A	234	PRO
1	A	248	GLN
1	A	252	ASP
1	A	266	GLN
1	A	319	LYS
1	A	343	PHE
1	A	366	LEU
1	A	412	GLU
1	A	421	PHE
1	A	422	ASP
1	A	423	PHE
1	B	39	ASP
1	B	56	LEU
1	B	72	ARG
1	B	136	LEU
1	B	171	ASN
1	B	189	SER
1	B	192	ASP
1	B	216	VAL
1	B	243	SER
1	B	252	ASP
1	B	297	GLN
1	B	309	ASN
1	B	370	ARG
1	B	392	GLN
1	B	421	PHE
1	B	422	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	93	HIS
1	A	98	GLN
1	A	141	ASN
1	A	171	ASN
1	A	208	GLN

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Mol	Chain	Res	Type
1	A	266	GLN
1	A	297	GLN
1	A	309	ASN
1	B	44	GLN
1	B	71	ASN
1	B	82	HIS
1	B	98	GLN
1	B	105	ASN
1	B	123	HIS
1	B	137	GLN
1	B	203	ASN
1	B	208	GLN
1	B	210	HIS
1	B	237	GLN
1	B	244	ASN
1	B	309	ASN
1	B	346	ASN
1	B	392	GLN
1	B	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

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	364/390 (93%)	0.38	24 (6%)	18	24	21, 54, 84, 106	0
1	B	379/390 (97%)	0.14	10 (2%)	56	63	27, 48, 68, 90	0
All	All	743/780 (95%)	0.25	34 (4%)	32	40	21, 51, 79, 106	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	121	ALA	6.4
1	B	422	ASP	5.8
1	A	349	VAL	5.2
1	A	423	PHE	5.1
1	A	338	GLU	5.1
1	A	424	GLN	5.0
1	A	342	GLN	5.0
1	A	299	ALA	4.6
1	A	344	GLY	4.4
1	A	335	ASP	4.1
1	B	331	SER	3.7
1	A	343	PHE	3.6
1	B	251	ARG	3.3
1	A	120	GLU	3.1
1	A	309	ASN	3.1
1	B	333	GLY	3.0
1	B	104	GLU	3.0
1	A	264	ILE	2.7
1	A	308	PRO	2.7
1	B	67	LYS	2.6
1	A	263	ALA	2.6
1	A	421	PHE	2.4
1	B	332	GLY	2.4
1	A	106	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	341	ARG	2.3
1	B	327	LYS	2.3
1	A	322	LYS	2.3
1	B	379	LEU	2.2
1	A	334	ARG	2.2
1	B	308	PRO	2.2
1	A	318	ALA	2.2
1	A	55	LYS	2.2
1	A	58	VAL	2.1
1	A	339	GLU	2.1

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.