Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:47 PM GMT

PDB ID	:	4G85
Title	:	Crystal structure of human HisRS
Authors	:	Wei, Z.; Wu, J.; Zhou, J.J.; Yang, X.-L.; Zhang, M.; Schimmel, P.
Deposited on	:	2012-07-21
Resolution	:	3.11 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

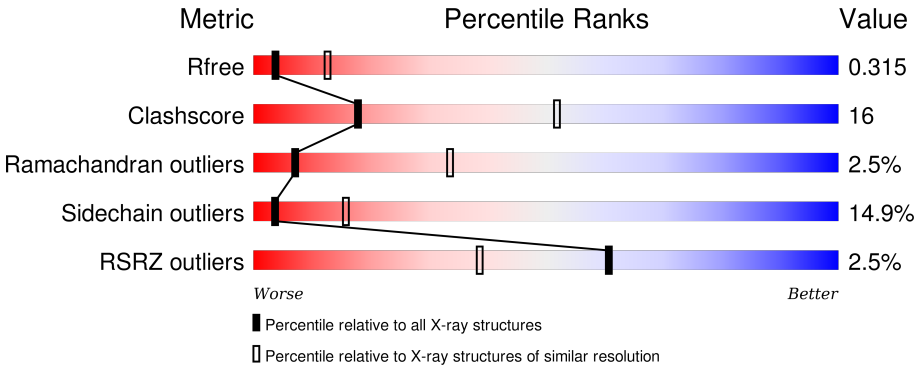
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.11 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}	91344	1112 (3.16-3.08)
Clashscore	102246	1218 (3.16-3.08)
Ramachandran outliers	100387	1175 (3.16-3.08)
Sidechain outliers	100360	1175 (3.16-3.08)
RSRZ outliers	91569	1114 (3.16-3.08)

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 <=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	517	56% 20% 6% 17%
1	B	517	4% 53% 23% 6% • 18%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6432 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 Histidine-tRNA ligase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3209	2051	536	608	14			
1	B	426	Total	C	N	O	S	0	0	0
			3223	2055	545	609	14			

There are 22 discrepancies between the modelled and reference sequences:

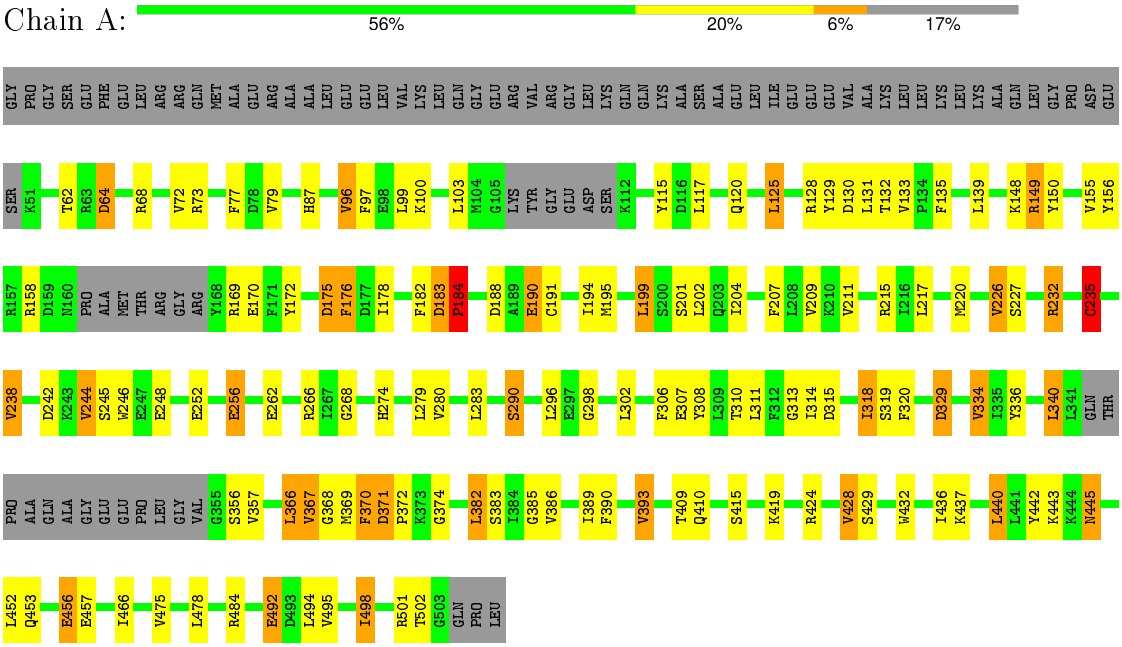
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLY	-	EXPRESSION TAG	UNP P12081
A	-9	PRO	-	EXPRESSION TAG	UNP P12081
A	-8	GLY	-	EXPRESSION TAG	UNP P12081
A	-7	SER	-	EXPRESSION TAG	UNP P12081
A	-6	GLU	-	EXPRESSION TAG	UNP P12081
A	-5	PHE	-	EXPRESSION TAG	UNP P12081
A	-4	GLU	-	EXPRESSION TAG	UNP P12081
A	-3	LEU	-	EXPRESSION TAG	UNP P12081
A	-2	ARG	-	EXPRESSION TAG	UNP P12081
A	-1	ARG	-	EXPRESSION TAG	UNP P12081
A	0	GLN	-	EXPRESSION TAG	UNP P12081
B	-10	GLY	-	EXPRESSION TAG	UNP P12081
B	-9	PRO	-	EXPRESSION TAG	UNP P12081
B	-8	GLY	-	EXPRESSION TAG	UNP P12081
B	-7	SER	-	EXPRESSION TAG	UNP P12081
B	-6	GLU	-	EXPRESSION TAG	UNP P12081
B	-5	PHE	-	EXPRESSION TAG	UNP P12081
B	-4	GLU	-	EXPRESSION TAG	UNP P12081
B	-3	LEU	-	EXPRESSION TAG	UNP P12081
B	-2	ARG	-	EXPRESSION TAG	UNP P12081
B	-1	ARG	-	EXPRESSION TAG	UNP P12081
B	0	GLN	-	EXPRESSION TAG	UNP P12081

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 errors 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.

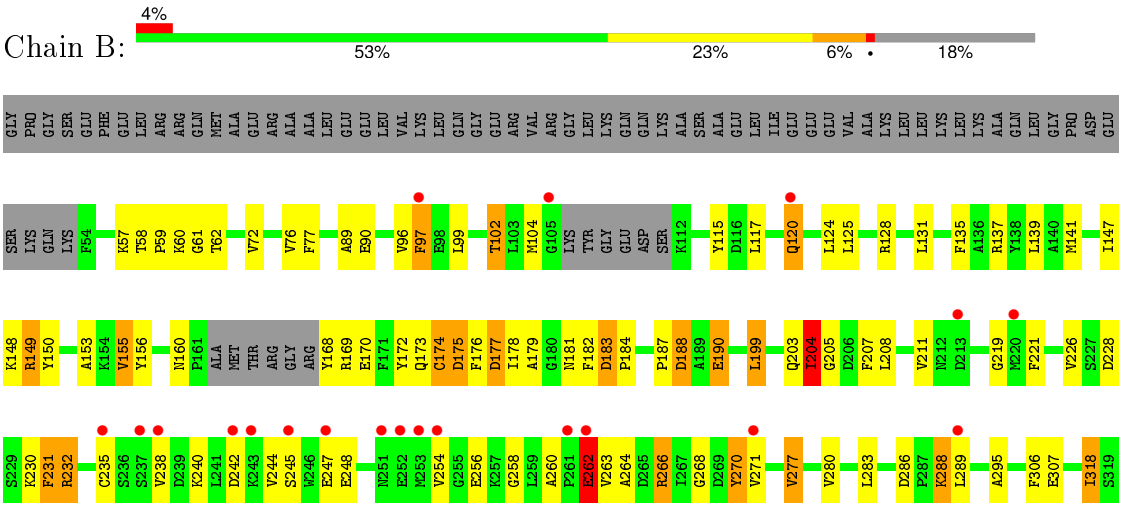
- Molecule 1: Histidine-tRNA ligase, cytoplasmic

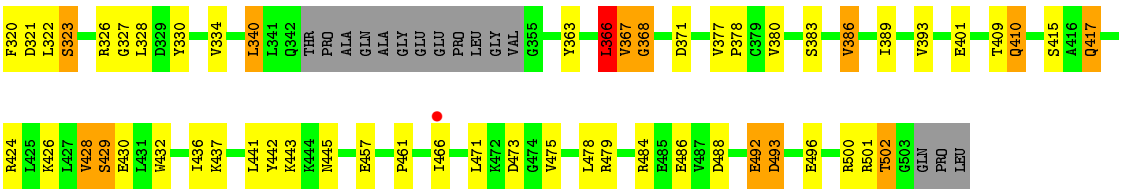
Chain A:



- Molecule 1: Histidine-tRNA ligase, cytoplasmic

Chain B:




F320 D321 L322 S323 R326 G327 L328 D329 Y330 V334 L340 L341 Q342 THR PRO ALA GLN ALA GLY GLU GLU PRO LEU GLY VAL G355 Y363 I366 V367 G368 D371 V377 P378 C379 V380 S383 V386 I389 V393 E401 T409 Q410 S415 A416 Q417
R424 L425 K426 L427 V428 S429 E430 L431 W432 I436 K437 L441 Y442 K443 K444 N445 E457 P461 I466 L471 K472 D473 G474 V475 L478 R479 R484 E485 E486 V487 D488 E492 D493 E496 R500 R501 T502 G503 GLN PRO LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	100.45Å 100.45Å 257.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.11 50.22 – 3.11	Depositor EDS
% Data completeness (in resolution range)	97.0 (50.00-3.11) 97.0 (50.22-3.11)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.39 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.271 , 0.327 0.259 , 0.315	Depositor DCC
R_{free} test set	1212 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	94.9	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 49.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.54$, $< L^2 > = 0.38$	Xtriage
Outliers	0 of 23872 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6432	wwPDB-VP
Average B, all atoms (Å^2)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.84	4/3255 (0.1%)	0.82	5/4412 (0.1%)
1	B	1.02	14/3269 (0.4%)	1.12	14/4427 (0.3%)
All	All	0.94	18/6524 (0.3%)	0.98	19/8839 (0.2%)

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	B	0	1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	367	VAL	CA-C	29.73	2.30	1.52
1	A	367	VAL	N-CA	21.76	1.89	1.46
1	A	367	VAL	CA-CB	21.22	1.99	1.54
1	B	288	LYS	CD-CE	12.26	1.81	1.51
1	B	367	VAL	N-CA	12.06	1.70	1.46
1	B	262	GLU	CD-OE1	-11.13	1.13	1.25
1	B	262	GLU	CD-OE2	11.05	1.37	1.25
1	A	367	VAL	CA-C	-8.82	1.30	1.52
1	B	367	VAL	CA-CB	8.28	1.72	1.54
1	B	248	GLU	CG-CD	7.29	1.62	1.51
1	A	235	CYS	CB-SG	-7.07	1.70	1.82
1	B	270	TYR	CB-CG	6.73	1.61	1.51
1	B	262	GLU	CG-CD	6.66	1.61	1.51
1	B	248	GLU	CD-OE2	-6.65	1.18	1.25
1	B	268	GLY	C-O	6.54	1.34	1.23
1	B	270	TYR	CE1-CZ	-6.09	1.30	1.38
1	B	266	ARG	CZ-NH2	5.35	1.40	1.33
1	B	264	ALA	CA-CB	5.33	1.63	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	367	VAL	CA-CB-CG2	29.00	154.39	110.90
1	B	367	VAL	CA-C-N	-25.52	65.15	116.20
1	B	367	VAL	CA-CB-CG1	-21.09	79.27	110.90
1	B	367	VAL	CA-C-O	19.23	160.48	120.10
1	A	367	VAL	CA-CB-CG1	-18.52	83.12	110.90
1	B	366	LEU	C-N-CA	-13.46	88.05	121.70
1	B	266	ARG	NE-CZ-NH2	-11.61	114.49	120.30
1	B	367	VAL	CB-CA-C	10.05	130.50	111.40
1	A	366	LEU	C-N-CA	-8.93	99.38	121.70
1	B	266	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	B	367	VAL	N-CA-C	7.59	131.51	111.00
1	B	270	TYR	CB-CG-CD1	7.41	125.45	121.00
1	A	367	VAL	N-CA-CB	-7.18	95.69	111.50
1	B	248	GLU	OE1-CD-OE2	-6.43	115.58	123.30
1	B	367	VAL	N-CA-CB	-6.41	97.39	111.50
1	B	262	GLU	CG-CD-OE2	-5.84	106.62	118.30
1	A	367	VAL	N-CA-C	5.62	126.18	111.00
1	A	334	VAL	CB-CA-C	-5.54	100.88	111.40
1	B	262	GLU	CG-CD-OE1	5.40	129.09	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	270	TYR	Sidechain

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	3209	0	3112	103	0
1	B	3223	0	3147	108	0
All	All	6432	0	6259	200	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 16.

All (200) 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:B:288:LYS:CE	1:B:288:LYS:CD	1.81	1.55
1:B:367:VAL:CA	1:B:367:VAL:N	1.70	1.52
1:A:367:VAL:CB	1:A:367:VAL:CA	1.99	1.39
1:A:367:VAL:CA	1:A:367:VAL:N	1.89	1.35
1:B:367:VAL:HA	1:B:367:VAL:C	1.48	1.30
1:B:366:LEU:C	1:B:367:VAL:CA	2.12	1.15
1:B:367:VAL:CA	1:B:368:GLY:N	2.12	1.12
1:A:367:VAL:CG1	1:A:367:VAL:CA	2.34	1.04
1:B:366:LEU:O	1:B:367:VAL:CA	2.08	1.00
1:B:367:VAL:CA	1:B:367:VAL:C	2.30	0.98
1:B:367:VAL:CA	1:B:368:GLY:H	1.71	0.96
1:A:183:ASP:OD1	1:B:443:LYS:HA	1.72	0.90
1:B:367:VAL:HA	1:B:368:GLY:N	1.77	0.90
1:B:244:VAL:HG12	1:B:245:SER:H	1.37	0.88
1:B:366:LEU:O	1:B:367:VAL:HA	1.78	0.81
1:A:366:LEU:C	1:A:367:VAL:CA	2.48	0.81
1:B:155:VAL:HG21	1:B:173:GLN:HB2	1.62	0.80
1:B:204:ILE:HG12	1:B:340:LEU:HD11	1.62	0.80
1:A:370:PHE:CD2	1:A:370:PHE:N	2.51	0.77
1:A:77:PHE:HE1	1:A:386:VAL:HG21	1.48	0.76
1:A:148:LYS:HG3	1:A:178:ILE:HG12	1.68	0.75
1:A:443:LYS:HA	1:B:183:ASP:OD1	1.85	0.75
1:A:370:PHE:HD2	1:A:370:PHE:N	1.84	0.73
1:B:288:LYS:CG	1:B:288:LYS:CE	2.67	0.73
1:A:445:ASN:N	1:A:445:ASN:HD22	1.87	0.73
1:A:195:MET:HG3	1:A:382:LEU:CD2	2.18	0.73
1:B:77:PHE:HE1	1:B:386:VAL:HG21	1.54	0.72
1:A:156:TYR:CE1	1:A:170:GLU:HG3	2.25	0.72
1:A:195:MET:HE1	1:A:209:VAL:HG13	1.71	0.72
1:B:244:VAL:HG12	1:B:245:SER:N	2.06	0.70
1:B:72:VAL:O	1:B:76:VAL:HG23	1.93	0.69
1:A:139:LEU:HD12	1:A:367:VAL:HG11	1.75	0.69
1:B:177:ASP:OD2	1:B:363:TYR:OH	2.10	0.68
1:B:367:VAL:CB	1:B:367:VAL:N	2.57	0.67
1:B:204:ILE:O	1:B:340:LEU:HD21	1.95	0.67
1:A:389:ILE:O	1:A:393:VAL:HG23	1.94	0.66
1:B:426:LYS:O	1:B:430:GLU:HG3	1.96	0.65
1:B:306:PHE:CZ	1:B:318:ILE:HD11	2.32	0.65
1:A:340:LEU:HD12	1:A:357:VAL:HG21	1.78	0.65
1:B:262:GLU:HB2	1:B:266:ARG:NH1	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ASP:CB	1:A:184:PRO:HD2	2.28	0.64
1:A:366:LEU:O	1:A:367:VAL:CA	2.46	0.63
1:B:283:LEU:HB3	1:B:289:LEU:HD12	1.79	0.63
1:A:175:ASP:HB3	1:A:383:SER:HB3	1.80	0.63
1:A:77:PHE:CE1	1:A:386:VAL:HG21	2.33	0.63
1:B:149:ARG:C	1:B:149:ARG:CD	2.66	0.62
1:B:417:GLN:H	1:B:417:GLN:HE21	1.48	0.61
1:A:453:GLN:HA	1:A:456:GLU:HG3	1.83	0.61
1:B:288:LYS:NZ	1:B:288:LYS:CD	2.62	0.61
1:A:204:ILE:HD12	1:A:340:LEU:HD11	1.82	0.61
1:B:415:SER:HB2	1:B:466:ILE:O	2.02	0.60
1:A:492:GLU:H	1:A:492:GLU:CD	2.05	0.59
1:B:62:THR:HG22	1:B:170:GLU:HB3	1.85	0.59
1:A:313:GLY:O	1:A:314:ILE:HD13	2.03	0.59
1:A:195:MET:HE1	1:A:209:VAL:CG1	2.33	0.59
1:B:139:LEU:HD21	1:B:147:ILE:HG21	1.84	0.59
1:B:479:ARG:HG3	1:B:486:GLU:HG3	1.85	0.58
1:B:139:LEU:HD21	1:B:147:ILE:CG2	2.33	0.58
1:B:149:ARG:HD3	1:B:149:ARG:C	2.23	0.58
1:B:155:VAL:CG2	1:B:173:GLN:HB2	2.33	0.58
1:A:235:CYS:HA	1:A:238:VAL:CG2	2.33	0.58
1:B:232:ARG:HA	1:B:235:CYS:SG	2.43	0.57
1:B:221:PHE:HB3	1:B:226:VAL:CG2	2.34	0.57
1:B:175:ASP:HB3	1:B:383:SER:HB3	1.86	0.57
1:B:492:GLU:OE2	1:B:492:GLU:N	2.30	0.57
1:A:195:MET:HG3	1:A:382:LEU:HD23	1.85	0.57
1:A:453:GLN:HA	1:A:456:GLU:CG	2.35	0.57
1:A:367:VAL:CA	1:A:367:VAL:HG12	2.33	0.56
1:B:156:TYR:CE1	1:B:170:GLU:HG3	2.41	0.56
1:B:232:ARG:HA	1:B:235:CYS:HG	1.70	0.56
1:A:117:LEU:HA	1:B:117:LEU:HA	1.86	0.56
1:A:367:VAL:CA	1:A:367:VAL:HG13	2.33	0.56
1:B:492:GLU:H	1:B:492:GLU:CD	2.09	0.56
1:A:199:LEU:HB3	1:A:207:PHE:CE2	2.40	0.56
1:B:321:ASP:C	1:B:323:SER:H	2.08	0.56
1:B:424:ARG:O	1:B:428:VAL:HG22	2.05	0.55
1:A:129:TYR:CD1	1:A:130:ASP:HB2	2.41	0.55
1:B:280:VAL:HG12	1:B:320:PHE:CD2	2.42	0.55
1:A:368:GLY:O	1:A:370:PHE:N	2.40	0.55
1:B:219:GLY:HA3	1:B:295:ALA:HB2	1.89	0.55
1:B:410:GLN:HG3	1:B:437:LYS:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:CYS:SG	1:B:174:CYS:O	2.64	0.55
1:A:445:ASN:ND2	1:A:445:ASN:N	2.55	0.54
1:B:321:ASP:OD1	1:B:323:SER:HB3	2.08	0.54
1:A:235:CYS:HA	1:A:238:VAL:HG22	1.90	0.54
1:B:203:GLN:O	1:B:205:GLY:N	2.33	0.54
1:A:410:GLN:HG3	1:A:437:LYS:HB2	1.90	0.54
1:B:271:VAL:HG13	1:B:323:SER:HB2	1.90	0.53
1:A:183:ASP:HB3	1:A:184:PRO:HD2	1.90	0.53
1:A:246:TRP:CZ2	1:A:268:GLY:HA3	2.44	0.53
1:B:445:ASN:HD22	1:B:445:ASN:N	2.06	0.53
1:A:176:PHE:C	1:A:176:PHE:CD2	2.82	0.53
1:B:283:LEU:HA	1:B:286:ASP:HB2	1.91	0.52
1:B:156:TYR:CZ	1:B:170:GLU:HG3	2.45	0.52
1:B:471:LEU:C	1:B:473:ASP:H	2.12	0.52
1:B:389:ILE:O	1:B:393:VAL:HG23	2.10	0.52
1:B:475:VAL:CG1	1:B:488:ASP:HB2	2.39	0.52
1:B:172:TYR:HB3	1:B:386:VAL:HG11	1.92	0.52
1:B:147:ILE:HG22	1:B:179:ALA:HB3	1.92	0.52
1:B:128:ARG:NH2	1:B:153:ALA:HB1	2.25	0.52
1:A:424:ARG:O	1:A:428:VAL:HG22	2.11	0.51
1:A:195:MET:HG3	1:A:382:LEU:HD22	1.90	0.51
1:A:133:VAL:HG13	1:A:370:PHE:HE1	1.76	0.51
1:B:277:VAL:HG22	1:B:306:PHE:CD1	2.46	0.51
1:A:280:VAL:HG12	1:A:320:PHE:CD2	2.46	0.51
1:B:148:LYS:HG3	1:B:178:ILE:HG12	1.93	0.51
1:A:246:TRP:CZ2	1:A:268:GLY:CA	2.94	0.50
1:A:492:GLU:N	1:A:492:GLU:OE2	2.44	0.50
1:A:215:ARG:HH11	1:A:298:GLY:HA2	1.76	0.50
1:A:424:ARG:HB3	1:A:440:LEU:HD11	1.94	0.50
1:B:221:PHE:HB3	1:B:226:VAL:HG22	1.92	0.50
1:B:244:VAL:CG1	1:B:245:SER:H	2.16	0.50
1:B:187:PRO:HA	1:B:190:GLU:HB3	1.94	0.50
1:A:308:TYR:HA	1:A:311:LEU:HD12	1.93	0.50
1:B:135:PHE:HB2	1:B:149:ARG:NH1	2.27	0.50
1:A:79:VAL:HG13	1:A:201:SER:HB3	1.94	0.50
1:A:371:ASP:OD1	1:A:374:GLY:N	2.44	0.50
1:A:217:LEU:HA	1:A:220:MET:HE1	1.95	0.49
1:A:367:VAL:HG12	1:A:367:VAL:C	2.32	0.49
1:A:87:HIS:ND1	1:A:190:GLU:OE1	2.39	0.49
1:A:252:GLU:O	1:A:256:GLU:N	2.37	0.48
1:A:442:TYR:OH	1:B:190:GLU:OE2	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ARG:HH22	1:A:329:ASP:HB3	1.77	0.48
1:B:330:TYR:O	1:B:363:TYR:HB2	2.13	0.48
1:A:79:VAL:CG1	1:A:201:SER:HB3	2.43	0.47
1:A:244:VAL:CG1	1:A:248:GLU:OE2	2.62	0.47
1:A:429:SER:HA	1:A:432:TRP:CE3	2.49	0.47
1:B:254:VAL:HA	1:B:258:GLY:HA2	1.96	0.47
1:A:274:HIS:HA	1:A:279:LEU:HD22	1.95	0.47
1:A:386:VAL:HG22	1:A:390:PHE:CZ	2.50	0.47
1:B:115:TYR:OH	1:B:169:ARG:HD3	2.15	0.47
1:A:367:VAL:CG1	1:A:367:VAL:C	2.82	0.46
1:B:445:ASN:ND2	1:B:445:ASN:N	2.63	0.46
1:A:290:SER:HA	1:A:296:LEU:HD13	1.97	0.46
1:B:244:VAL:CG1	1:B:245:SER:N	2.77	0.46
1:B:479:ARG:HB2	1:B:486:GLU:HG2	1.98	0.46
1:A:452:LEU:O	1:A:456:GLU:HG2	2.17	0.45
1:A:149:ARG:HD3	1:A:149:ARG:C	2.36	0.45
1:A:442:TYR:O	1:B:182:PHE:HB3	2.17	0.45
1:A:190:GLU:OE2	1:B:442:TYR:OH	2.34	0.45
1:A:195:MET:HE3	1:A:195:MET:HB3	1.84	0.45
1:B:493:ASP:N	1:B:493:ASP:OD1	2.50	0.45
1:A:182:PHE:CD2	1:B:442:TYR:HB2	2.52	0.44
1:B:221:PHE:HB3	1:B:226:VAL:HG21	1.99	0.44
1:A:306:PHE:CZ	1:A:318:ILE:HD11	2.51	0.44
1:A:62:THR:HG21	1:B:97:PHE:HE1	1.81	0.44
1:A:115:TYR:OH	1:A:169:ARG:HD3	2.16	0.44
1:B:149:ARG:HD3	1:B:150:TYR:CA	2.47	0.44
1:A:415:SER:OG	1:A:424:ARG:NH1	2.51	0.44
1:B:178:ILE:HD11	1:B:190:GLU:HG2	1.99	0.44
1:A:244:VAL:HG12	1:A:248:GLU:OE2	2.17	0.44
1:B:176:PHE:CD2	1:B:176:PHE:C	2.90	0.44
1:A:202:LEU:CD1	1:A:389:ILE:HD13	2.47	0.44
1:A:183:ASP:OD1	1:B:442:TYR:O	2.36	0.44
1:A:132:THR:O	1:A:135:PHE:HB3	2.18	0.44
1:B:417:GLN:HE21	1:B:417:GLN:N	2.15	0.44
1:B:89:ALA:HA	1:B:148:LYS:O	2.18	0.44
1:A:279:LEU:O	1:A:283:LEU:HG	2.18	0.44
1:B:283:LEU:O	1:B:286:ASP:HB3	2.18	0.43
1:B:424:ARG:HG2	1:B:466:ILE:HD12	2.00	0.43
1:B:429:SER:HA	1:B:432:TRP:CE3	2.53	0.43
1:A:436:ILE:CD1	1:A:495:VAL:HG13	2.48	0.43
1:B:99:LEU:O	1:B:102:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LEU:HB3	1:A:129:TYR:HE2	1.83	0.43
1:A:436:ILE:HD12	1:A:495:VAL:HG13	2.00	0.43
1:A:68:ARG:O	1:A:72:VAL:HG23	2.19	0.43
1:B:326:ARG:O	1:B:328:LEU:N	2.52	0.43
1:A:492:GLU:N	1:A:492:GLU:CD	2.72	0.42
1:A:442:TYR:HB2	1:B:182:PHE:CD2	2.53	0.42
1:A:494:LEU:O	1:A:498:ILE:HB	2.19	0.42
1:B:475:VAL:HG13	1:B:488:ASP:HB2	2.01	0.42
1:B:410:GLN:O	1:B:461:PRO:HD2	2.18	0.42
1:A:424:ARG:HB3	1:A:440:LEU:CD1	2.49	0.42
1:A:262:GLU:O	1:A:266:ARG:HG3	2.19	0.42
1:B:230:LYS:O	1:B:231:PHE:C	2.58	0.42
1:A:99:LEU:O	1:A:100:LYS:C	2.58	0.42
1:B:377:VAL:HA	1:B:378:PRO:HD3	1.83	0.42
1:B:61:GLY:O	1:B:168:TYR:HD1	2.02	0.42
1:A:149:ARG:HG2	1:A:150:TYR:N	2.35	0.42
1:B:211:VAL:O	1:B:320:PHE:HD1	2.03	0.41
1:B:188:ASP:HA	1:B:380:VAL:HG21	2.02	0.41
1:B:90:GLU:O	1:B:149:ARG:HA	2.21	0.41
1:A:226:VAL:HG23	1:A:227:SER:O	2.19	0.41
1:A:96:VAL:O	1:A:128:ARG:HG2	2.19	0.41
1:A:246:TRP:CH2	1:A:268:GLY:HA2	2.55	0.41
1:B:57:LYS:HE2	1:B:60:LYS:N	2.35	0.41
1:A:190:GLU:O	1:A:194:ILE:HG13	2.21	0.41
1:A:73:ARG:HA	1:A:390:PHE:CE1	2.55	0.41
1:A:424:ARG:HA	1:A:466:ILE:HD12	2.03	0.41
1:A:131:LEU:HD12	1:A:131:LEU:HA	1.85	0.41
1:B:496:GLU:O	1:B:500:ARG:HB2	2.21	0.40
1:B:199:LEU:HB3	1:B:207:PHE:CE2	2.56	0.40
1:B:410:GLN:CG	1:B:437:LYS:HB2	2.49	0.40
1:A:211:VAL:HG22	1:A:336:TYR:HB3	2.03	0.40
1:A:117:LEU:HD13	1:A:125:LEU:HB2	2.03	0.40
1:B:57:LYS:HG2	1:B:58:THR:H	1.87	0.40
1:A:64:ASP:OD1	1:B:137:ARG:NH2	2.55	0.40
1:A:244:VAL:HG12	1:A:245:SER:H	1.86	0.40
1:A:302:LEU:HA	1:A:302:LEU:HD23	1.95	0.40
1:B:260:ALA:HB3	1:B:263:VAL:HG23	2.02	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	419/517 (81%)	382 (91%)	28 (7%)	9 (2%)	9	38
1	B	418/517 (81%)	372 (89%)	34 (8%)	12 (3%)	6	30
All	All	837/1034 (81%)	754 (90%)	62 (7%)	21 (2%)	7	33

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	PRO
1	B	59	PRO
1	B	204	ILE
1	B	502	THR
1	A	120	GLN
1	A	369	MET
1	A	419	LYS
1	B	120	GLN
1	B	184	PRO
1	B	327	GLY
1	A	256	GLU
1	A	315	ASP
1	B	104	MET
1	B	368	GLY
1	A	502	THR
1	B	322	LEU
1	A	372	PRO
1	A	385	GLY
1	B	231	PHE
1	B	256	GLU
1	B	401	GLU

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	326/444 (73%)	279 (86%)	47 (14%)	4 17
1	B	330/444 (74%)	279 (84%)	51 (16%)	3 14
All	All	656/888 (74%)	558 (85%)	98 (15%)	4 16

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ASP
1	A	96	VAL
1	A	97	PHE
1	A	125	LEU
1	A	149	ARG
1	A	155	VAL
1	A	158	ARG
1	A	172	TYR
1	A	175	ASP
1	A	176	PHE
1	A	183	ASP
1	A	184	PRO
1	A	188	ASP
1	A	190	GLU
1	A	191	CYS
1	A	199	LEU
1	A	226	VAL
1	A	232	ARG
1	A	235	CYS
1	A	238	VAL
1	A	242	ASP
1	A	244	VAL
1	A	290	SER
1	A	307	GLU
1	A	310	THR
1	A	318	ILE
1	A	319	SER

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Mol	Chain	Res	Type
1	A	329	ASP
1	A	334	VAL
1	A	340	LEU
1	A	356	SER
1	A	370	PHE
1	A	371	ASP
1	A	382	LEU
1	A	393	VAL
1	A	409	THR
1	A	428	VAL
1	A	440	LEU
1	A	445	ASN
1	A	456	GLU
1	A	457	GLU
1	A	475	VAL
1	A	478	LEU
1	A	484	ARG
1	A	492	GLU
1	A	498	ILE
1	A	501	ARG
1	B	96	VAL
1	B	97	PHE
1	B	102	THR
1	B	120	GLN
1	B	124	LEU
1	B	125	LEU
1	B	131	LEU
1	B	141	MET
1	B	149	ARG
1	B	155	VAL
1	B	160	ASN
1	B	174	CYS
1	B	175	ASP
1	B	177	ASP
1	B	181	ASN
1	B	183	ASP
1	B	188	ASP
1	B	190	GLU
1	B	199	LEU
1	B	204	ILE
1	B	208	LEU
1	B	228	ASP

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Mol	Chain	Res	Type
1	B	232	ARG
1	B	238	VAL
1	B	240	LYS
1	B	242	ASP
1	B	247	GLU
1	B	262	GLU
1	B	277	VAL
1	B	307	GLU
1	B	318	ILE
1	B	323	SER
1	B	334	VAL
1	B	340	LEU
1	B	366	LEU
1	B	371	ASP
1	B	386	VAL
1	B	409	THR
1	B	410	GLN
1	B	417	GLN
1	B	428	VAL
1	B	429	SER
1	B	436	ILE
1	B	441	LEU
1	B	457	GLU
1	B	478	LEU
1	B	484	ARG
1	B	492	GLU
1	B	493	ASP
1	B	501	ARG
1	B	502	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	445	ASN
1	B	120	GLN
1	B	417	GLN
1	B	445	ASN
1	B	451	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	427/517 (82%)	-0.21	0 100 100	74, 92, 122, 157	0
1	B	426/517 (82%)	0.14	21 (4%) 33 14	77, 112, 199, 246	0
All	All	853/1034 (82%)	-0.03	21 (2%) 61 39	74, 98, 177, 246	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	261	PRO	5.1
1	B	253	MET	5.1
1	B	220	MET	4.5
1	B	289	LEU	4.0
1	B	238	VAL	3.8
1	B	271	VAL	3.6
1	B	242	ASP	3.4
1	B	247	GLU	3.3
1	B	254	VAL	2.9
1	B	245	SER	2.7
1	B	105	GLY	2.7
1	B	251	ASN	2.5
1	B	252	GLU	2.5
1	B	213	ASP	2.4
1	B	235	CYS	2.2
1	B	262	GLU	2.1
1	B	120	GLN	2.1
1	B	237	SER	2.1
1	B	243	LYS	2.1
1	B	97	PHE	2.0
1	B	466	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.