Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2023 – 11:04 PM EDT

PDB ID	:	3PZ6
Title	:	The crystal structure of GlLeuRS-CP1
Authors	:	Liu, R.J.; Du, D.H.; Wang, E.D.
Deposited on	:	2010-12-14
Resolution	:	2.60 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:

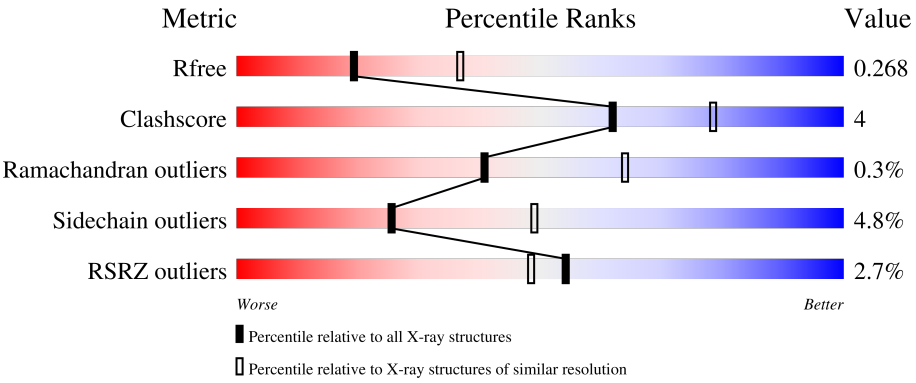
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	311	3% 77% 13% • 10%
1	B	311	5% 77% 12% • 11%
1	C	311	% 71% 11% 18%
1	D	311	% 68% 13% • 18%
1	E	311	% 70% 11% • 18%

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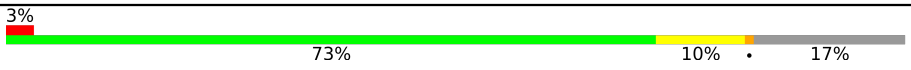
Mol	Chain	Length	Quality of chain
1	F	311	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12091 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 Leucyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2084	1339	339	393	13			
1	B	278	Total	C	N	O	S	0	0	0
			2075	1332	332	398	13			
1	C	256	Total	C	N	O	S	0	0	0
			1934	1241	310	370	13			
1	D	254	Total	C	N	O	S	0	0	0
			1907	1226	308	360	13			
1	E	255	Total	C	N	O	S	0	0	0
			1913	1225	307	368	13			
1	F	259	Total	C	N	O	S	0	0	0
			1948	1248	312	375	13			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	251	GLY	-	expression tag	UNP A8BY54
A	395	SER	CYS	engineered mutation	UNP A8BY54
A	533	SER	CYS	engineered mutation	UNP A8BY54
B	251	GLY	-	expression tag	UNP A8BY54
B	395	SER	CYS	engineered mutation	UNP A8BY54
B	533	SER	CYS	engineered mutation	UNP A8BY54
C	251	GLY	-	expression tag	UNP A8BY54
C	395	SER	CYS	engineered mutation	UNP A8BY54
C	533	SER	CYS	engineered mutation	UNP A8BY54
D	251	GLY	-	expression tag	UNP A8BY54
D	395	SER	CYS	engineered mutation	UNP A8BY54
D	533	SER	CYS	engineered mutation	UNP A8BY54
E	251	GLY	-	expression tag	UNP A8BY54
E	395	SER	CYS	engineered mutation	UNP A8BY54
E	533	SER	CYS	engineered mutation	UNP A8BY54
F	251	GLY	-	expression tag	UNP A8BY54
F	395	SER	CYS	engineered mutation	UNP A8BY54

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Chain	Residue	Modelled	Actual	Comment	Reference
F	533	SER	CYS	engineered mutation	UNP A8BY54

- Molecule 2 is water.

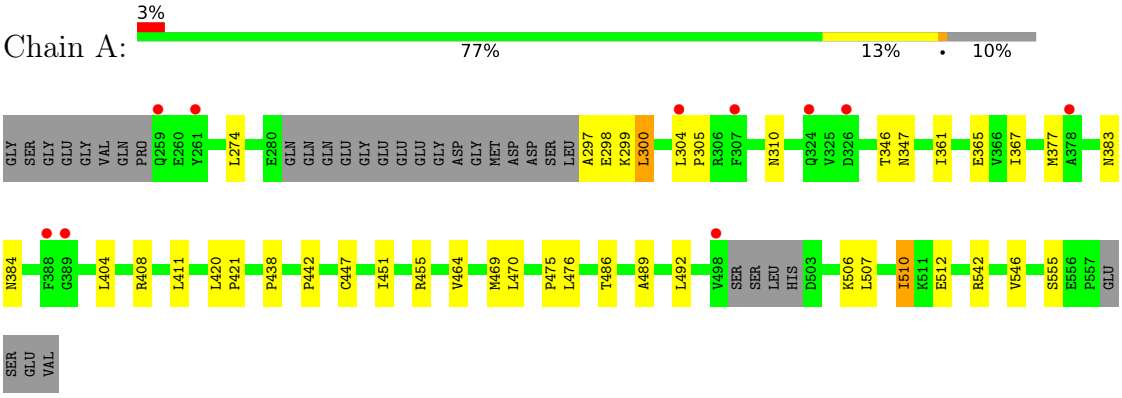
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	42	Total O 42 42	0	0
2	B	37	Total O 37 37	0	0
2	C	26	Total O 26 26	0	0
2	D	30	Total O 30 30	0	0
2	E	50	Total O 50 50	0	0
2	F	45	Total O 45 45	0	0

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.

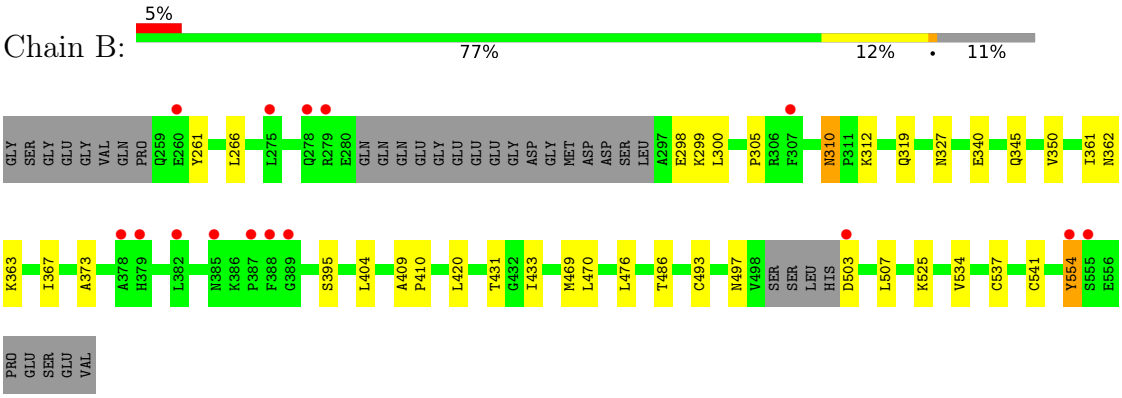
• Molecule 1: Leucyl-tRNA synthetase

Chain A:



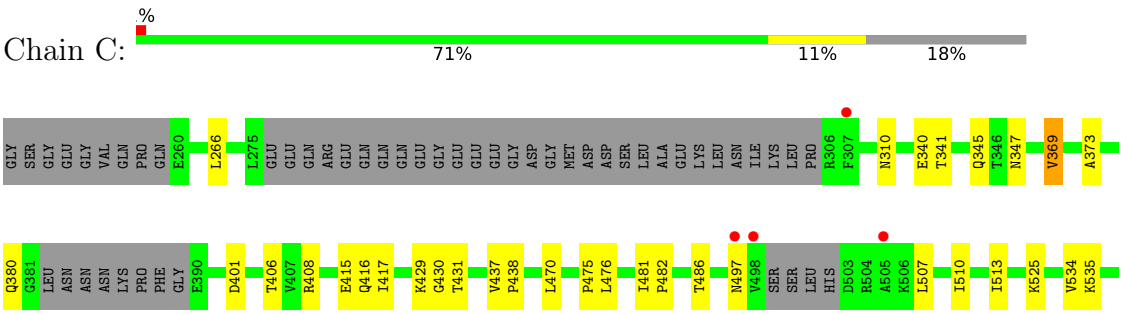
• Molecule 1: Leucyl-tRNA synthetase

Chain B:



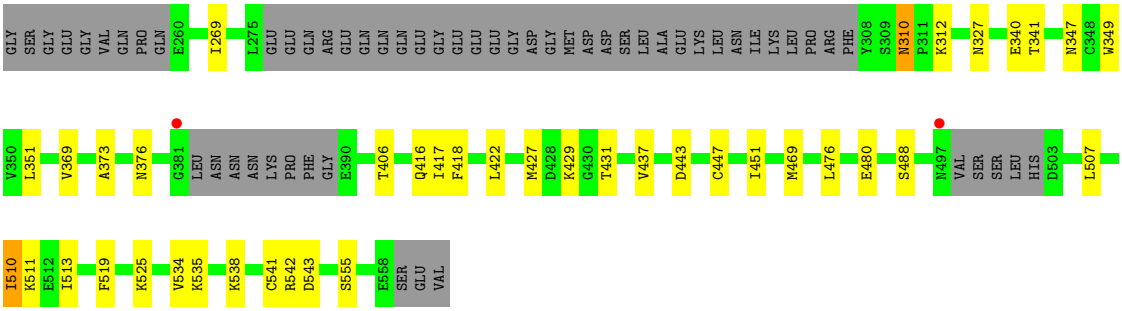
• Molecule 1: Leucyl-tRNA synthetase

Chain C:



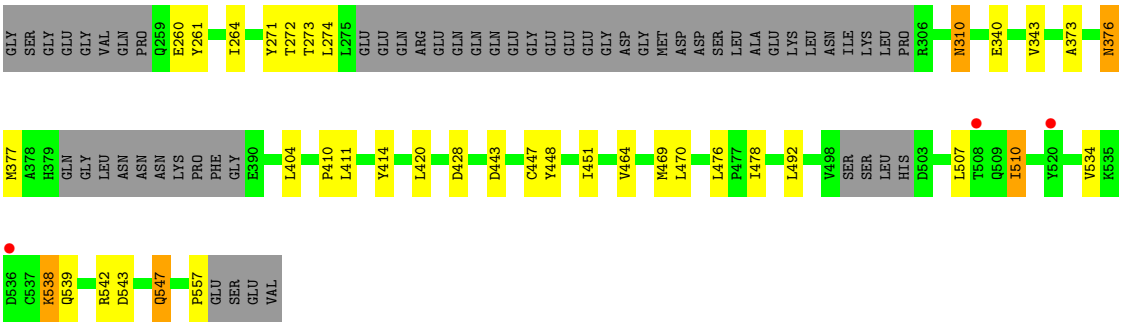
• Molecule 1: Leucyl-tRNA synthetase

Chain D:



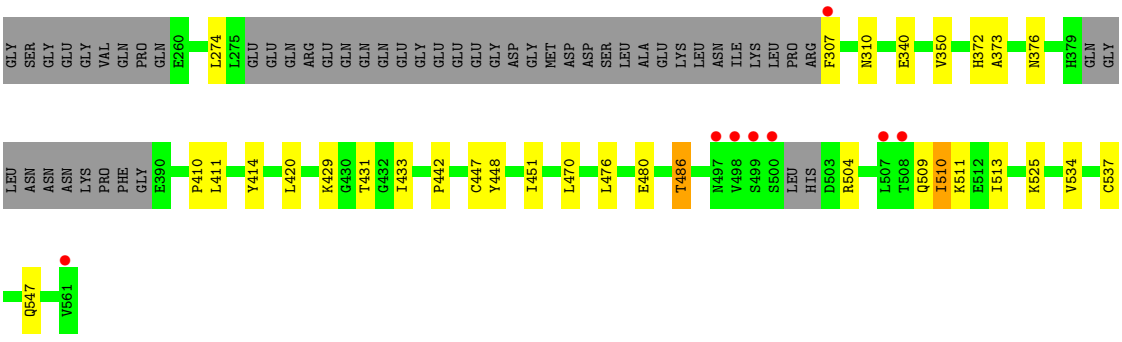
• Molecule 1: Leucyl-tRNA synthetase

Chain E:



• Molecule 1: Leucyl-tRNA synthetase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	232.28Å 72.09Å 111.25Å 90.00° 95.06° 90.00°	Depositor
Resolution (Å)	29.85 – 2.60 29.85 – 2.60	Depositor EDS
% Data completeness (in resolution range)	88.7 (29.85-2.60) 94.2 (29.85-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.10 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.215 , 0.271 0.216 , 0.268	Depositor DCC
R_{free} test set	2693 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	39.9	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 44.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12091	wwPDB-VP
Average B, all atoms (Å^2)	44.0	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 64.89 % 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 7.7187e-06. 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

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	0.37	0/2124	0.55	1/2899 (0.0%)
1	B	0.38	0/2114	0.55	1/2885 (0.0%)
1	C	0.37	0/1970	0.55	1/2684 (0.0%)
1	D	0.39	0/1943	0.51	0/2650
1	E	0.38	0/1948	0.52	0/2657
1	F	0.39	0/1984	0.54	0/2706
All	All	0.38	0/12083	0.54	3/16481 (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	C	557	PRO	N-CA-CB	5.99	110.49	103.30
1	B	305	PRO	N-CA-CB	5.68	110.11	103.30
1	A	305	PRO	N-CA-CB	5.44	109.83	103.30

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	2084	0	2008	18	0
1	B	2075	0	1984	17	0
1	C	1934	0	1875	14	0
1	D	1907	0	1857	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1913	0	1846	22	0
1	F	1948	0	1885	13	0
2	A	42	0	0	1	0
2	B	37	0	0	0	0
2	C	26	0	0	0	0
2	D	30	0	0	1	0
2	E	50	0	0	0	0
2	F	45	0	0	1	0
All	All	12091	0	11455	103	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 4.

All (103) 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:E:376:ASN:HD21	1:E:557:PRO:HD3	1.37	0.88
1:E:507:LEU:HA	1:E:510:ILE:HG22	1.75	0.67
1:F:372:HIS:O	1:F:376:ASN:HB2	1.95	0.66
1:E:414:TYR:CE2	1:E:476:LEU:HD21	2.29	0.66
1:E:271:TYR:O	1:E:274:LEU:HB2	1.96	0.65
1:E:340:GLU:HG3	1:E:534:VAL:HG13	1.79	0.64
1:E:373:ALA:O	1:E:377:MET:HB2	1.96	0.64
1:E:376:ASN:HD21	1:E:557:PRO:CD	2.08	0.64
1:C:340:GLU:HG3	1:C:534:VAL:HG13	1.81	0.62
1:D:310:ASN:HD22	1:D:312:LYS:H	1.48	0.62
1:F:420:LEU:HD11	1:F:470:LEU:HD21	1.82	0.61
1:A:420:LEU:HD11	1:A:470:LEU:HD21	1.83	0.61
1:F:442:PRO:HG2	1:F:511:LYS:HA	1.82	0.61
1:E:448:TYR:CE1	1:E:470:LEU:HD22	2.35	0.61
1:E:414:TYR:HE2	1:E:476:LEU:HD21	1.64	0.60
1:F:414:TYR:CE2	1:F:476:LEU:HD21	2.37	0.59
1:E:447:CYS:O	1:E:451:ILE:HG12	2.02	0.58
1:F:350:VAL:HG12	1:F:433:ILE:HG12	1.84	0.58
1:F:510:ILE:HA	1:F:513:ILE:HD12	1.86	0.58
1:D:480:GLU:HB2	1:D:525:LYS:HD2	1.85	0.57
1:A:506:LYS:O	1:A:510:ILE:HG22	2.05	0.56
1:D:340:GLU:HG3	1:D:534:VAL:HG13	1.87	0.55
1:E:404:LEU:HD21	1:E:464:VAL:HG22	1.91	0.53
1:D:341:THR:HB	1:D:437:VAL:HG11	1.92	0.52
1:A:274:LEU:HD21	1:A:408:ARG:HH22	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:507:LEU:HA	1:D:510:ILE:HG22	1.91	0.51
1:A:420:LEU:CD1	1:A:470:LEU:HD21	2.39	0.51
1:C:341:THR:HB	1:C:437:VAL:HG11	1.93	0.51
1:F:447:CYS:O	1:F:451:ILE:HG12	2.11	0.51
1:F:340:GLU:HG3	1:F:534:VAL:HG13	1.93	0.51
1:E:404:LEU:HD22	1:E:469:MET:SD	2.51	0.50
1:D:510:ILE:HA	1:D:513:ILE:HD12	1.93	0.50
1:C:380:GLN:HE22	1:C:555:SER:H	1.59	0.50
1:B:493:CYS:O	1:B:497:ASN:O	2.29	0.49
1:E:272:THR:C	1:E:274:LEU:H	2.16	0.49
1:B:310:ASN:HD22	1:B:312:LYS:H	1.60	0.49
1:B:525:LYS:HE2	1:B:525:LYS:HA	1.95	0.49
1:C:266:LEU:HD21	1:C:345:GLN:HE22	1.77	0.49
1:D:310:ASN:ND2	1:D:312:LYS:H	2.10	0.49
1:D:542:ARG:NH1	1:D:543:ASP:OD1	2.46	0.48
1:E:376:ASN:ND2	1:E:557:PRO:HD3	2.17	0.48
1:A:361:ILE:HG12	1:A:367:ILE:HG12	1.96	0.48
1:E:310:ASN:C	1:E:310:ASN:HD22	2.17	0.48
1:E:492:LEU:HB2	1:E:510:ILE:HD11	1.95	0.47
1:A:346:THR:OG1	1:A:347:ASN:ND2	2.48	0.47
1:A:489:ALA:HA	1:A:510:ILE:HD11	1.95	0.47
1:F:448:TYR:CE1	1:F:470:LEU:HD22	2.50	0.47
1:D:349:TRP:HB3	1:D:422:LEU:HB3	1.96	0.46
1:D:347:ASN:HA	1:D:417:ILE:HB	1.97	0.46
1:A:486:THR:O	2:A:48:HOH:O	2.20	0.46
1:D:488:SER:HB2	2:D:52:HOH:O	2.15	0.46
1:E:340:GLU:OE1	1:E:538:LYS:HG2	2.15	0.46
1:B:350:VAL:HG12	1:B:433:ILE:HG12	1.98	0.46
1:A:298:GLU:C	1:A:300:LEU:H	2.19	0.46
1:B:362:ASN:OD1	1:B:363:LYS:N	2.49	0.46
1:B:420:LEU:HD11	1:B:470:LEU:HD21	1.98	0.46
1:D:373:ALA:HB2	1:D:431:THR:HA	1.97	0.45
1:B:373:ALA:HB1	1:B:554:TYR:OH	2.17	0.45
1:C:415:GLU:HG2	1:C:416:GLN:OE1	2.16	0.45
1:B:340:GLU:HG3	1:B:534:VAL:HG13	1.98	0.45
1:B:409:ALA:HA	1:B:410:PRO:HD2	1.85	0.45
1:C:438:PRO:HB2	1:C:475:PRO:HG3	1.99	0.45
1:F:480:GLU:HB2	1:F:525:LYS:HD2	1.99	0.45
1:D:519:PHE:HE1	1:D:538:LYS:HD2	1.83	0.44
1:F:373:ALA:HB2	1:F:431:THR:HA	1.99	0.44
1:A:420:LEU:HB3	1:A:421:PRO:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:535:LYS:NZ	1:D:535:LYS:HB3	2.32	0.44
1:C:415:GLU:HG2	1:C:416:GLN:CD	2.38	0.44
1:B:373:ALA:HB2	1:B:431:THR:HA	2.00	0.44
1:C:369:VAL:HG12	1:C:431:THR:HB	2.00	0.43
1:E:543:ASP:O	1:E:547:GLN:HB3	2.18	0.43
1:D:269:ILE:HD12	1:D:406:THR:HB	2.00	0.43
1:A:404:LEU:HD22	1:A:469:MET:SD	2.58	0.43
1:A:542:ARG:O	1:A:546:VAL:HG23	2.19	0.43
1:B:361:ILE:HG12	1:B:367:ILE:HG12	2.00	0.43
1:D:443:ASP:OD2	1:D:511:LYS:HE2	2.19	0.43
1:C:373:ALA:HB2	1:C:430:GLY:O	2.19	0.43
1:F:410:PRO:O	1:F:411:LEU:HB2	2.18	0.43
1:B:261:TYR:HB2	1:B:554:TYR:HB3	2.01	0.42
1:D:418:PHE:CD1	1:D:469:MET:HG2	2.55	0.42
1:B:319:GLN:HE21	1:B:395:SER:HB3	1.84	0.42
1:F:486:THR:O	2:F:98:HOH:O	2.22	0.42
1:C:347:ASN:HA	1:C:417:ILE:HB	2.02	0.42
1:A:442:PRO:HB3	1:A:510:ILE:HD13	2.00	0.42
1:B:266:LEU:HD21	1:B:345:GLN:HE22	1.85	0.42
1:A:492:LEU:HD12	1:A:510:ILE:HG13	2.02	0.41
1:B:298:GLU:C	1:B:300:LEU:H	2.23	0.41
1:E:410:PRO:O	1:E:411:LEU:HB2	2.20	0.41
1:A:447:CYS:O	1:A:451:ILE:HG12	2.20	0.41
1:B:404:LEU:HD22	1:B:469:MET:SD	2.61	0.41
1:B:503:ASP:O	1:B:507:LEU:HB2	2.21	0.41
1:C:510:ILE:HA	1:C:513:ILE:HD12	2.03	0.41
1:E:260:GLU:OE2	1:E:542:ARG:NE	2.49	0.41
1:E:420:LEU:HD11	1:E:470:LEU:HD21	2.02	0.41
1:C:481:ILE:HA	1:C:482:PRO:HD3	1.97	0.40
1:A:438:PRO:HB2	1:A:475:PRO:HG3	2.03	0.40
1:C:507:LEU:HA	1:C:510:ILE:HG22	2.03	0.40
1:D:447:CYS:O	1:D:451:ILE:HG12	2.21	0.40
1:A:297:ALA:O	1:A:299:LYS:N	2.44	0.40
1:D:351:LEU:HB3	1:D:427:MET:HE3	2.04	0.40
1:A:404:LEU:HD21	1:A:464:VAL:HG22	2.03	0.40
1:C:373:ALA:HB2	1:C:431:THR:HA	2.02	0.40
1:E:343:VAL:HG13	1:E:478:ILE:HG21	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	273/311 (88%)	256 (94%)	17 (6%)	0	100	100
1	B	272/311 (88%)	250 (92%)	20 (7%)	2 (1%)	22	43
1	C	248/311 (80%)	234 (94%)	14 (6%)	0	100	100
1	D	246/311 (79%)	228 (93%)	17 (7%)	1 (0%)	34	57
1	E	247/311 (79%)	230 (93%)	16 (6%)	1 (0%)	34	57
1	F	251/311 (81%)	240 (96%)	10 (4%)	1 (0%)	34	57
All	All	1537/1866 (82%)	1438 (94%)	94 (6%)	5 (0%)	41	64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	327	ASN
1	B	327	ASN
1	E	273	THR
1	F	504	ARG
1	B	299	LYS

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	215/271 (79%)	201 (94%)	14 (6%)	17	34
1	B	214/271 (79%)	208 (97%)	6 (3%)	43	69
1	C	205/271 (76%)	193 (94%)	12 (6%)	19	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	200/271 (74%)	191 (96%)	9 (4%)	27 52
1	E	201/271 (74%)	191 (95%)	10 (5%)	24 47
1	F	207/271 (76%)	198 (96%)	9 (4%)	29 54
All	All	1242/1626 (76%)	1182 (95%)	60 (5%)	25 49

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	300	LEU
1	A	304	LEU
1	A	310	ASN
1	A	365	GLU
1	A	377	MET
1	A	383	ASN
1	A	384	ASN
1	A	411	LEU
1	A	455	ARG
1	A	476	LEU
1	A	507	LEU
1	A	510	ILE
1	A	512	GLU
1	A	555	SER
1	B	310	ASN
1	B	476	LEU
1	B	486	THR
1	B	537	CYS
1	B	541	CYS
1	B	554	TYR
1	C	310	ASN
1	C	369	VAL
1	C	401	ASP
1	C	406	THR
1	C	408	ARG
1	C	429	LYS
1	C	470	LEU
1	C	476	LEU
1	C	486	THR
1	C	497	ASN
1	C	525	LYS
1	C	535	LYS
1	D	310	ASN

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Mol	Chain	Res	Type
1	D	369	VAL
1	D	376	ASN
1	D	416	GLN
1	D	429	LYS
1	D	476	LEU
1	D	510	ILE
1	D	541	CYS
1	D	555	SER
1	E	261	TYR
1	E	264	ILE
1	E	310	ASN
1	E	376	ASN
1	E	428	ASP
1	E	443	ASP
1	E	510	ILE
1	E	538	LYS
1	E	539	GLN
1	E	547	GLN
1	F	274	LEU
1	F	307	PHE
1	F	310	ASN
1	F	429	LYS
1	F	486	THR
1	F	509	GLN
1	F	510	ILE
1	F	537	CYS
1	F	547	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	310	ASN
1	A	345	GLN
1	A	347	ASN
1	A	384	ASN
1	A	532	GLN
1	B	310	ASN
1	B	319	GLN
1	B	345	GLN
1	B	347	ASN
1	B	532	GLN
1	C	345	GLN

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Mol	Chain	Res	Type
1	C	347	ASN
1	C	379	HIS
1	C	380	GLN
1	D	310	ASN
1	D	347	ASN
1	D	550	GLN
1	E	310	ASN
1	E	347	ASN
1	E	376	ASN
1	E	532	GLN
1	E	539	GLN
1	E	547	GLN
1	E	548	ASN
1	F	310	ASN
1	F	323	ASN
1	F	347	ASN
1	F	532	GLN
1	F	547	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 (i)

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	279/311 (89%)	-0.03	10 (3%)	42	35	20, 38, 78, 90	0
1	B	278/311 (89%)	0.06	15 (5%)	25	20	20, 40, 81, 93	0
1	C	256/311 (82%)	-0.07	4 (1%)	72	68	24, 43, 70, 90	0
1	D	254/311 (81%)	-0.16	2 (0%)	86	84	23, 44, 70, 89	0
1	E	255/311 (81%)	-0.15	3 (1%)	79	76	23, 39, 66, 85	0
1	F	259/311 (83%)	-0.09	8 (3%)	49	42	22, 42, 74, 83	0
All	All	1581/1866 (84%)	-0.07	42 (2%)	54	48	20, 41, 75, 93	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	388	PHE	5.1
1	C	307	PHE	4.1
1	C	498	VAL	4.1
1	C	497	ASN	3.9
1	A	388	PHE	3.8
1	B	378	ALA	3.7
1	A	307	PHE	3.7
1	B	260	GLU	3.7
1	B	379	HIS	3.7
1	F	497	ASN	3.5
1	F	508	THR	3.3
1	A	378	ALA	3.1
1	A	259	GLN	3.1
1	A	324	GLN	3.1
1	B	554	TYR	2.9
1	D	381	GLY	2.9
1	B	389	GLY	2.8
1	B	387	PRO	2.7
1	A	498	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	520	TYR	2.7
1	B	385	ASN	2.7
1	F	498	VAL	2.6
1	B	382	LEU	2.6
1	F	500	SER	2.6
1	A	326	ASP	2.6
1	E	508	THR	2.6
1	B	307	PHE	2.6
1	F	499	SER	2.5
1	F	561	VAL	2.4
1	B	278	GLN	2.3
1	A	304	LEU	2.3
1	D	497	ASN	2.3
1	B	503	ASP	2.2
1	F	307	PHE	2.2
1	B	275	LEU	2.2
1	F	507	LEU	2.2
1	B	555	SER	2.1
1	E	536	ASP	2.1
1	A	261	TYR	2.1
1	B	279	ARG	2.1
1	C	505	ALA	2.1
1	A	389	GLY	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.