



Full wwPDB EM Validation Report ⓘ

Mar 8, 2025 – 12:15 pm GMT

PDB ID : 8S8B
EMDB ID : EMD-19800
Title : Phenylalanyl-tRNA Synthetase Domain Swap: evolutionary advantage?
Authors : Real-Hohn, A.; Ross, J.J.; Stefania, V.; Burga, A.; Dong, G.
Deposited on : 2024-03-06
Resolution : 2.80 Å(reported)
Based on initial model : .

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : **FAILED**
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

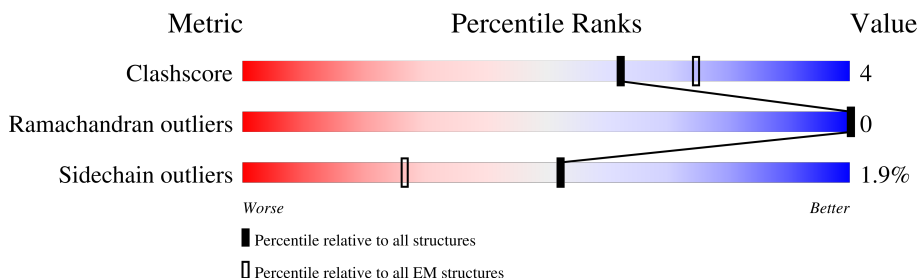
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	496	<div> <div>55%</div> <div>8%</div> <div>37%</div> </div>
1	B	496	<div> <div>55%</div> <div>8%</div> <div>37%</div> </div>
2	C	590	<div> <div>87%</div> <div>12%</div> <div>.</div> </div>
2	D	590	<div> <div>88%</div> <div>12%</div> <div>.</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14396 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Phenylalanyl-tRNA Synthetase alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	312	Total	C	N	O	S	0	0
			2525	1627	427	461	10		
1	B	312	Total	C	N	O	S	0	0
			2525	1627	427	461	10		

- Molecule 2 is a protein called Phenylalanyl-tRNA Synthetase beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	589	Total	C	N	O	S	0	0
			4672	2981	787	885	19		
2	D	589	Total	C	N	O	S	0	0
			4672	2981	787	885	19		

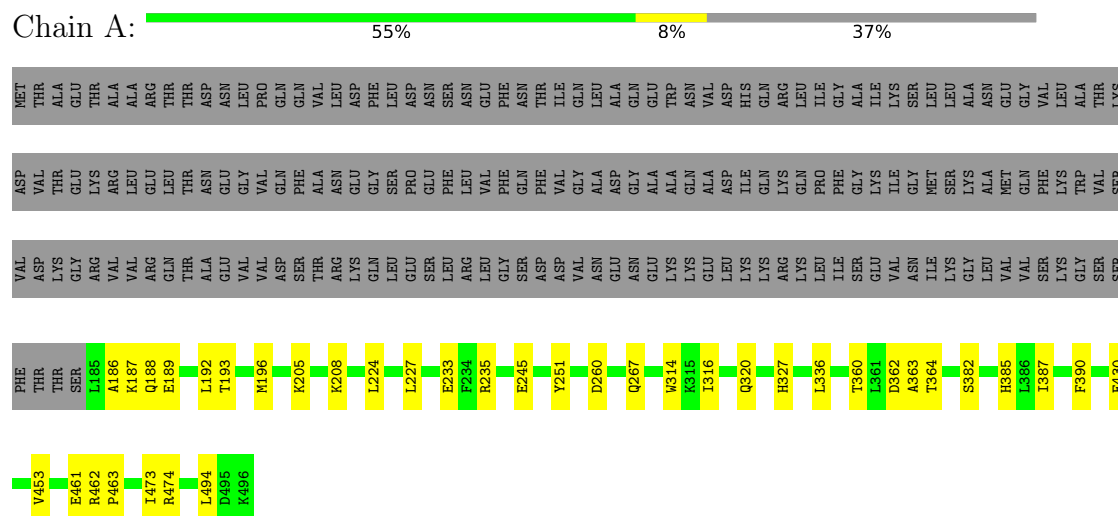
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Mg	0
			1	1	
3	B	1	Total	Mg	0
			1	1	

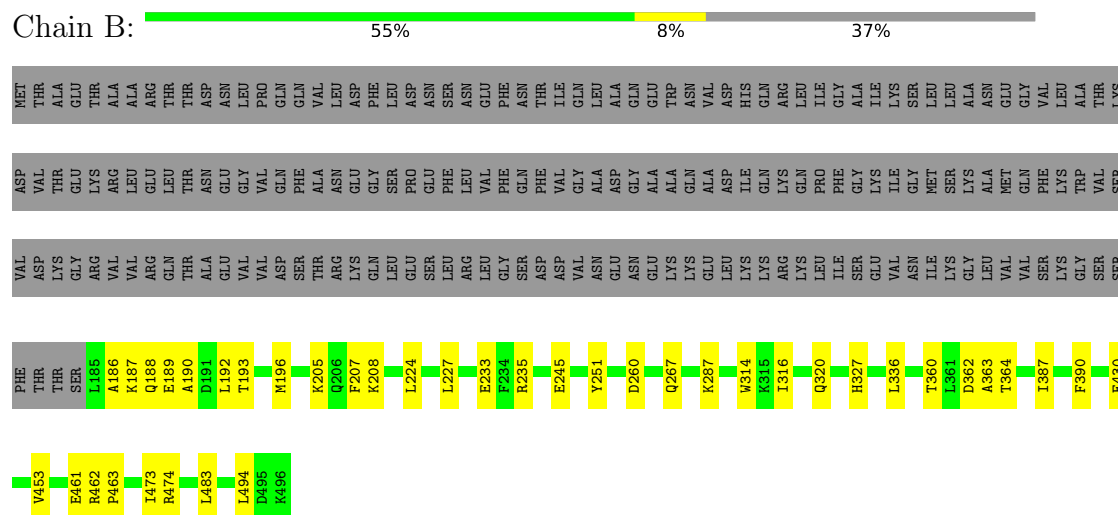
3 Residue-property plots

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. 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. 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.

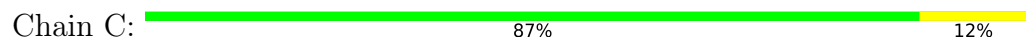
• Molecule 1: Phenylalanyl-tRNA Synthetase alpha subunit

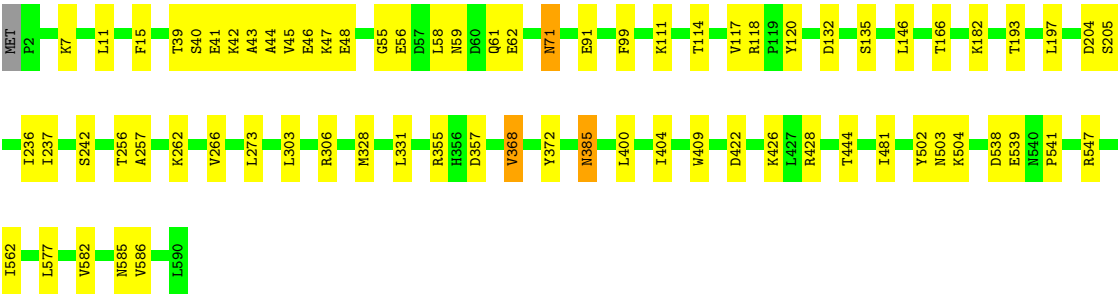


• Molecule 1: Phenylalanyl-tRNA Synthetase alpha subunit

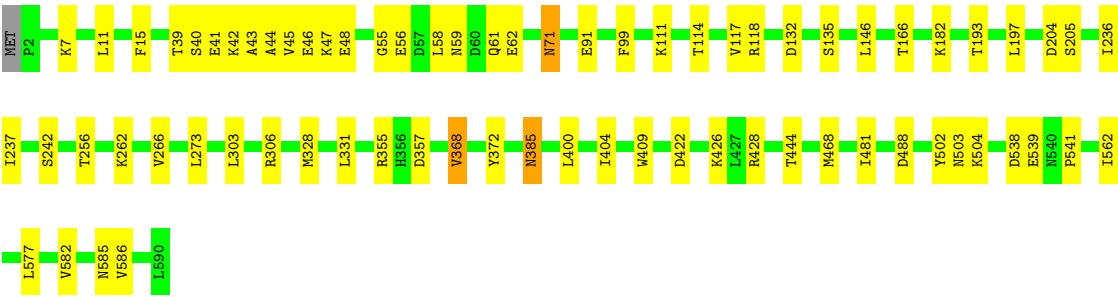
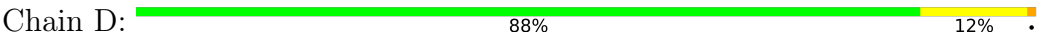


• Molecule 2: Phenylalanyl-tRNA Synthetase beta subunit





● Molecule 2: Phenylalanyl-tRNA Synthetase beta subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	178962	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Patch CTF	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.26	0/2594	0.46	0/3504
1	B	0.26	0/2594	0.46	0/3504
2	C	0.25	0/4763	0.47	0/6452
2	D	0.25	0/4763	0.47	0/6452
All	All	0.25	0/14714	0.47	0/19912

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	2525	0	2473	20	0
1	B	2525	0	2473	23	0
2	C	4672	0	4725	41	0
2	D	4672	0	4725	40	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	14396	0	14396	117	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 (117) 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)
2:D:44:ALA:O	2:D:48:GLU:HB2	1.90	0.71
2:C:44:ALA:O	2:C:48:GLU:HB2	1.90	0.70
2:C:7:LYS:NZ	2:C:41:GLU:OE1	2.27	0.68
2:D:7:LYS:NZ	2:D:41:GLU:OE1	2.27	0.68
1:B:193:THR:H	1:B:196:MET:HE3	1.59	0.67
1:A:193:THR:H	1:A:196:MET:HE3	1.61	0.66
2:C:306:ARG:NH2	2:C:355:ARG:O	2.29	0.66
2:D:306:ARG:NH2	2:D:355:ARG:O	2.29	0.66
2:C:197:LEU:HD21	2:C:237:ILE:HD11	1.79	0.65
2:D:197:LEU:HD21	2:D:237:ILE:HD11	1.79	0.64
1:A:267:GLN:O	2:D:262:LYS:NZ	2.24	0.63
1:B:267:GLN:O	2:C:262:LYS:NZ	2.28	0.61
2:D:182:LYS:HB2	2:D:193:THR:HG22	1.84	0.60
2:C:46:GLU:HA	2:C:55:GLY:H	1.67	0.60
2:D:538:ASP:OD1	2:D:539:GLU:N	2.35	0.59
1:B:188:GLN:HB3	1:B:208:LYS:N	2.17	0.59
2:C:182:LYS:HB2	2:C:193:THR:HG22	1.84	0.59
1:A:188:GLN:HB3	1:A:208:LYS:N	2.17	0.59
2:C:538:ASP:OD1	2:C:539:GLU:N	2.35	0.58
1:B:190:ALA:HA	2:C:547:ARG:HH21	1.68	0.57
1:A:430:GLU:O	1:A:462:ARG:NH1	2.35	0.57
2:D:46:GLU:HA	2:D:55:GLY:H	1.67	0.56
2:C:118:ARG:NH2	2:C:256:THR:O	2.38	0.56
2:D:118:ARG:NH2	2:D:256:THR:O	2.39	0.56
2:D:40:SER:O	2:D:44:ALA:N	2.34	0.56
2:D:562:ILE:HB	2:D:582:VAL:HG23	1.88	0.56
2:D:331:LEU:HD21	2:D:372:TYR:HB2	1.88	0.56
2:C:40:SER:O	2:C:44:ALA:N	2.34	0.56
1:B:430:GLU:O	1:B:462:ARG:NH1	2.35	0.55
2:D:204:ASP:OD1	2:D:205:SER:N	2.34	0.55
2:C:132:ASP:H	2:C:135:SER:HG	1.55	0.55
2:D:132:ASP:H	2:D:135:SER:HG	1.55	0.55
2:D:45:VAL:HG21	2:D:58:LEU:HD13	1.89	0.54
2:C:331:LEU:HD21	2:C:372:TYR:HB2	1.88	0.54
2:C:562:ILE:HB	2:C:582:VAL:HG23	1.88	0.54
2:D:146:LEU:HD13	2:D:266:VAL:HG13	1.88	0.54
2:C:146:LEU:HD13	2:C:266:VAL:HG13	1.88	0.54
2:C:502:TYR:CZ	2:C:577:LEU:HB2	2.43	0.54
1:A:362:ASP:OD2	1:A:364:THR:OG1	2.23	0.54
2:C:45:VAL:HG21	2:C:58:LEU:HD13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:ASP:OD2	1:B:364:THR:OG1	2.23	0.53
2:D:502:TYR:CZ	2:D:577:LEU:HB2	2.43	0.53
2:D:428:ARG:NH1	2:D:541:PRO:O	2.42	0.53
2:C:204:ASP:OD1	2:C:205:SER:N	2.34	0.52
2:C:385:ASN:HD22	2:C:385:ASN:H	1.57	0.52
2:C:428:ARG:NH1	2:C:541:PRO:O	2.42	0.52
2:D:59:ASN:ND2	2:D:61:GLN:OE1	2.43	0.52
2:C:40:SER:HA	2:C:62:GLU:HA	1.92	0.52
2:C:503:ASN:OD1	2:C:504:LYS:N	2.42	0.52
2:D:40:SER:HA	2:D:62:GLU:HA	1.92	0.52
2:C:59:ASN:ND2	2:C:61:GLN:OE1	2.43	0.51
2:C:328:MET:HG3	2:C:368:VAL:HG21	1.93	0.51
2:D:385:ASN:H	2:D:385:ASN:HD22	1.57	0.51
1:B:251:TYR:HD2	2:D:481:ILE:HD11	1.76	0.51
2:D:422:ASP:HA	2:D:426:LYS:HD2	1.93	0.50
2:D:328:MET:HG3	2:D:368:VAL:HG21	1.93	0.50
2:C:422:ASP:HA	2:C:426:LYS:HD2	1.93	0.50
2:C:71:ASN:HD22	2:C:71:ASN:H	1.60	0.49
2:D:503:ASN:OD1	2:D:504:LYS:N	2.42	0.49
2:D:71:ASN:H	2:D:71:ASN:HD22	1.60	0.49
2:D:166:THR:HG21	2:D:242:SER:HA	1.95	0.48
1:B:260:ASP:OD2	1:B:314:TRP:NE1	2.44	0.48
2:D:585:ASN:OD1	2:D:586:VAL:N	2.47	0.47
1:A:260:ASP:OD2	1:A:314:TRP:NE1	2.44	0.47
2:C:117:VAL:HG12	2:C:118:ARG:HG2	1.96	0.47
2:D:117:VAL:HG12	2:D:118:ARG:HG2	1.96	0.47
2:C:585:ASN:OD1	2:C:586:VAL:N	2.47	0.47
1:B:483:LEU:HB2	2:D:468:MET:SD	2.55	0.47
2:C:166:THR:HG21	2:C:242:SER:HA	1.95	0.47
1:A:251:TYR:HD2	2:C:481:ILE:HD11	1.80	0.46
1:A:316:ILE:O	1:A:320:GLN:HG2	2.16	0.46
2:D:42:LYS:HG3	2:D:56:GLU:HA	1.97	0.46
1:B:316:ILE:O	1:B:320:GLN:HG2	2.16	0.46
2:D:111:LYS:O	2:D:114:THR:OG1	2.30	0.46
2:C:236:ILE:HG22	2:C:237:ILE:HG12	1.98	0.46
1:B:462:ARG:HB3	1:B:463:PRO:HD3	1.98	0.45
1:A:462:ARG:HB3	1:A:463:PRO:HD3	1.98	0.45
2:C:42:LYS:HG3	2:C:56:GLU:HA	1.98	0.45
1:A:461:GLU:HG2	1:A:473:ILE:HD11	1.98	0.45
2:D:236:ILE:HG22	2:D:237:ILE:HG12	1.98	0.45
2:C:400:LEU:O	2:C:404:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:400:LEU:O	2:D:404:ILE:HG13	2.17	0.45
1:B:186:ALA:C	1:B:188:GLN:H	2.20	0.45
1:A:186:ALA:C	1:A:188:GLN:H	2.20	0.44
1:B:430:GLU:OE1	1:B:462:ARG:NH2	2.47	0.44
1:B:187:LYS:O	1:B:189:GLU:N	2.51	0.44
1:B:461:GLU:HG2	1:B:473:ILE:HD11	1.98	0.44
2:D:43:ALA:O	2:D:47:LYS:HG2	2.18	0.44
2:D:357:ASP:N	2:D:357:ASP:OD1	2.47	0.44
1:B:196:MET:SD	1:B:205:LYS:HD2	2.58	0.44
1:B:363:ALA:HA	1:B:474:ARG:HH12	1.82	0.44
1:A:363:ALA:HA	1:A:474:ARG:HH12	1.82	0.44
1:A:187:LYS:O	1:A:189:GLU:N	2.51	0.43
2:C:111:LYS:O	2:C:114:THR:OG1	2.30	0.43
2:C:43:ALA:O	2:C:47:LYS:HG2	2.18	0.43
1:A:382:SER:OG	1:A:385:HIS:ND1	2.47	0.43
1:B:336:LEU:HD21	1:B:453:VAL:HG11	2.00	0.43
1:B:387:ILE:HA	1:B:390:PHE:CE2	2.54	0.43
2:C:197:LEU:HD12	2:C:197:LEU:HA	1.89	0.43
2:C:357:ASP:OD1	2:C:357:ASP:N	2.48	0.43
1:A:196:MET:SD	1:A:205:LYS:HD2	2.58	0.43
1:A:387:ILE:HA	1:A:390:PHE:CE2	2.54	0.42
2:C:11:LEU:HD22	2:C:15:PHE:HE2	1.84	0.42
2:D:11:LEU:HD22	2:D:15:PHE:HE2	1.84	0.42
1:A:336:LEU:HD21	1:A:453:VAL:HG11	2.00	0.42
2:C:42:LYS:N	2:C:59:ASN:O	2.53	0.42
1:A:387:ILE:HA	1:A:390:PHE:CZ	2.55	0.42
1:B:387:ILE:HA	1:B:390:PHE:CZ	2.55	0.42
1:A:235:ARG:NH1	1:A:245:GLU:OE1	2.53	0.41
2:D:99:PHE:HE1	2:D:303:LEU:HD23	1.85	0.41
2:C:99:PHE:HE1	2:C:303:LEU:HD23	1.85	0.41
1:B:235:ARG:NH1	1:B:245:GLU:OE1	2.53	0.41
1:B:287:LYS:HG3	2:D:488:ASP:OD1	2.19	0.41
1:B:188:GLN:HB3	1:B:207:PHE:C	2.42	0.41
2:D:42:LYS:N	2:D:59:ASN:O	2.53	0.40
1:A:430:GLU:OE1	1:A:462:ARG:NH2	2.47	0.40
2:C:120:TYR:HB2	2:C:257:ALA:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	310/496 (62%)	301 (97%)	9 (3%)	0	100	100
1	B	310/496 (62%)	301 (97%)	9 (3%)	0	100	100
2	C	587/590 (100%)	568 (97%)	19 (3%)	0	100	100
2	D	587/590 (100%)	569 (97%)	18 (3%)	0	100	100
All	All	1794/2172 (83%)	1739 (97%)	55 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	271/429 (63%)	264 (97%)	7 (3%)	41	75
1	B	271/429 (63%)	264 (97%)	7 (3%)	41	75
2	C	515/516 (100%)	507 (98%)	8 (2%)	58	85
2	D	515/516 (100%)	507 (98%)	8 (2%)	58	85
All	All	1572/1890 (83%)	1542 (98%)	30 (2%)	52	82

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	LEU
1	A	224	LEU

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Mol	Chain	Res	Type
1	A	227	LEU
1	A	233	GLU
1	A	327	HIS
1	A	360	THR
1	A	494	LEU
1	B	192	LEU
1	B	224	LEU
1	B	227	LEU
1	B	233	GLU
1	B	327	HIS
1	B	360	THR
1	B	494	LEU
2	C	39	THR
2	C	71	ASN
2	C	91	GLU
2	C	273	LEU
2	C	368	VAL
2	C	385	ASN
2	C	409	TRP
2	C	444	THR
2	D	39	THR
2	D	71	ASN
2	D	91	GLU
2	D	273	LEU
2	D	368	VAL
2	D	385	ASN
2	D	409	TRP
2	D	444	THR

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

Mol	Chain	Res	Type
1	A	311	ASN
2	C	71	ASN
2	C	385	ASN
2	D	71	ASN
2	D	385	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.