



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 10:30 AM UTC

PDB ID : 8P5O / pdb_00008p5o
Title : Proline activating adenylation domain of gramicidin S synthetase 2 - GrsB1-Acore
Authors : Stephan, P.; Basquin, J.; Caputi, L.; O'Connor, S.E.; Kries, H.
Deposited on : 2023-05-24
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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

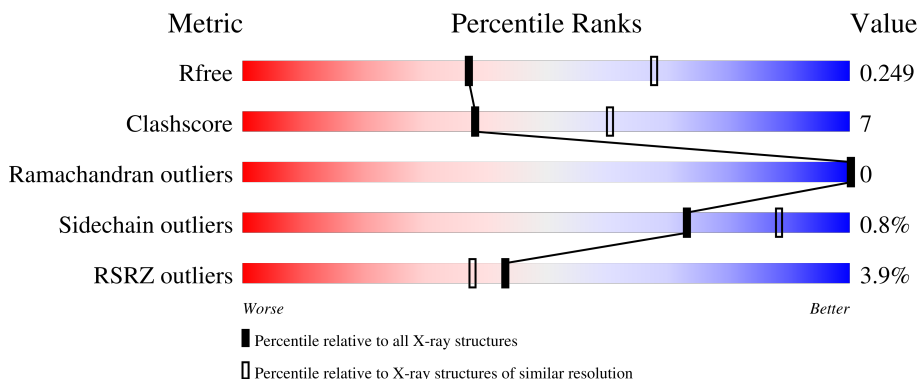
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

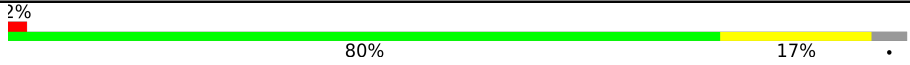
The reported resolution of this entry is 2.60 Å.

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 $\leq 5\%$. 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	405	
1	B	405	
1	C	405	
1	D	405	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12855 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 Gramicidin S synthase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3210	2068	535	598	9			
1	B	390	Total	C	N	O	S	0	0	0
			3206	2065	534	598	9			
1	C	390	Total	C	N	O	S	0	0	0
			3204	2062	535	598	9			
1	D	388	Total	C	N	O	S	0	0	0
			3187	2050	532	596	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P0C063
A	2	PRO	-	expression tag	UNP P0C063
B	1	GLY	-	expression tag	UNP P0C063
B	2	PRO	-	expression tag	UNP P0C063
C	1	GLY	-	expression tag	UNP P0C063
C	2	PRO	-	expression tag	UNP P0C063
D	1	GLY	-	expression tag	UNP P0C063
D	2	PRO	-	expression tag	UNP P0C063

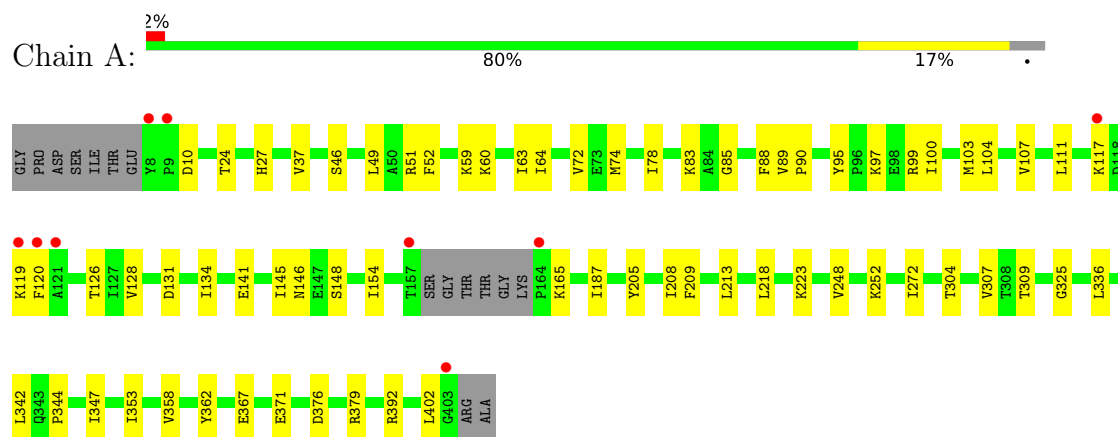
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	O	0	0
			7	7		
2	B	23	Total	O	0	0
			23	23		
2	C	13	Total	O	0	0
			13	13		
2	D	5	Total	O	0	0
			5	5		

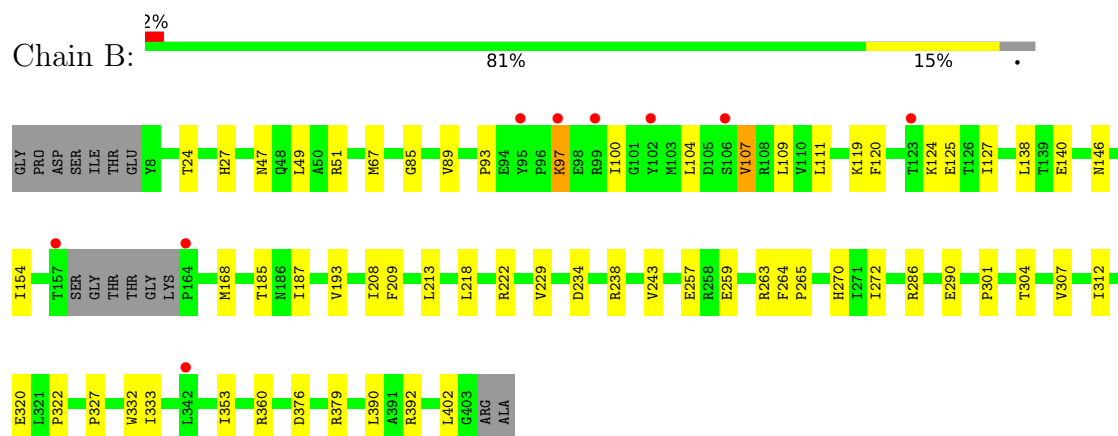
3 Residue-property plots [i](#)

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.

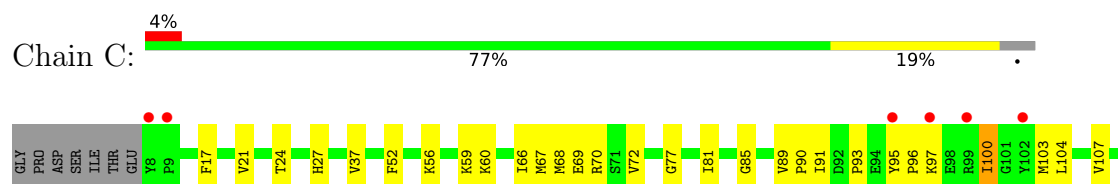
• Molecule 1: Gramicidin S synthase 2

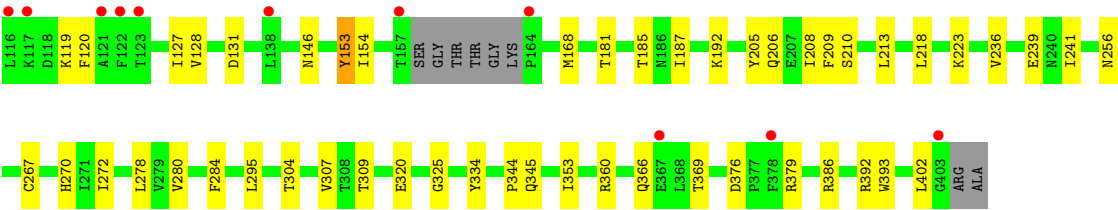


• Molecule 1: Gramicidin S synthase 2

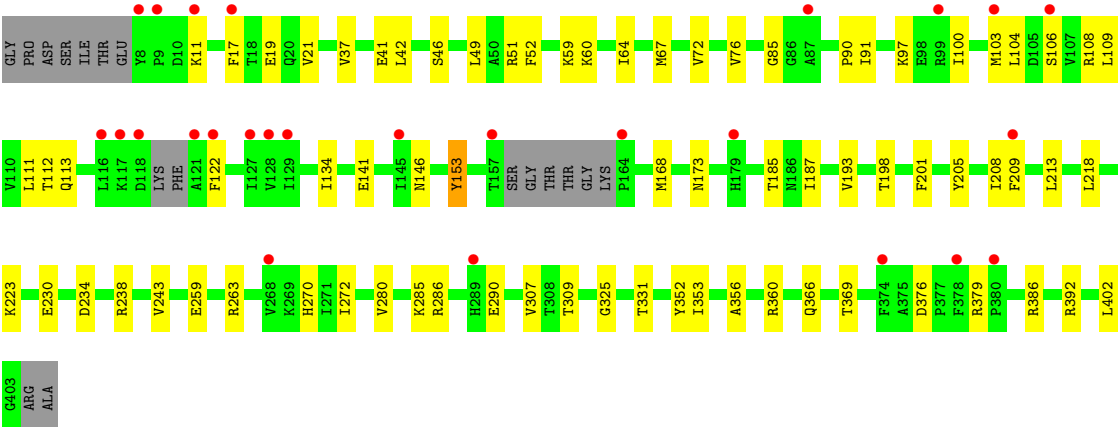
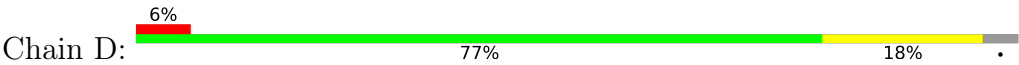


• Molecule 1: Gramicidin S synthase 2





● Molecule 1: Gramicidin S synthase 2



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	195.02Å 195.02Å 346.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.46 – 2.60 60.46 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (60.46-2.60) 89.6 (60.46-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.58 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.19rc6_4061	Depositor
R, R_{free}	0.223 , 0.249 0.222 , 0.249	Depositor DCC
R_{free} test set	2000 reflections (2.56%)	wwPDB-VP
Wilson B-factor (Å ²)	56.6	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12855	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.09	0/3286	0.27	0/4450
1	B	0.14	0/3282	0.31	0/4446
1	C	0.10	0/3279	0.28	0/4441
1	D	0.11	0/3261	0.29	0/4416
All	All	0.11	0/13108	0.29	0/17753

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	3210	0	3173	39	0
1	B	3206	0	3162	36	0
1	C	3204	0	3166	52	0
1	D	3187	0	3141	51	0
2	A	7	0	0	0	0
2	B	23	0	0	0	0
2	C	13	0	0	1	0
2	D	5	0	0	0	0
All	All	12855	0	12642	175	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 7.

All (175) 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:C:59:LYS:HD2	1:C:60:LYS:H	1.48	0.78
1:B:97:LYS:HA	1:B:100:ILE:HG12	1.70	0.73
1:B:327:PRO:HG3	1:B:333:ILE:HG12	1.68	0.73
1:C:345:GLN:NE2	2:C:501:HOH:O	2.25	0.69
1:D:11:LYS:NZ	1:D:19:GLU:OE2	2.26	0.68
1:D:91:ILE:HG12	1:D:103:MET:HE2	1.76	0.68
1:A:304:THR:HG22	1:A:358:VAL:HA	1.78	0.65
1:D:108:ARG:HG3	1:D:109:LEU:HD23	1.81	0.63
1:D:37:VAL:HG13	1:D:41:GLU:HB2	1.81	0.63
1:D:59:LYS:HD3	1:D:60:LYS:H	1.63	0.63
1:C:37:VAL:HG21	1:C:72:VAL:HG11	1.80	0.63
1:C:187:ILE:HD13	1:C:272:ILE:HD11	1.81	0.63
1:B:107:VAL:O	1:B:124:LYS:HE2	2.00	0.62
1:C:223:LYS:H	1:C:223:LYS:HD2	1.65	0.61
1:D:97:LYS:HA	1:D:100:ILE:HG12	1.83	0.61
1:B:168:MET:HE3	1:B:360:ARG:HB3	1.83	0.60
1:C:95:TYR:HD2	1:C:103:MET:HE1	1.66	0.60
1:C:334:TYR:OH	1:C:379:ARG:NH1	2.34	0.60
1:C:185:THR:HG22	1:C:187:ILE:H	1.67	0.60
1:B:138:LEU:HB3	1:B:140:GLU:OE1	2.02	0.59
1:A:97:LYS:HA	1:A:100:ILE:HG12	1.85	0.59
1:B:67:MET:HE3	1:B:93:PRO:HA	1.86	0.58
1:A:187:ILE:HD13	1:A:272:ILE:HD11	1.86	0.56
1:D:67:MET:HB2	1:D:91:ILE:HB	1.86	0.56
1:D:64:ILE:HD12	1:D:109:LEU:HG	1.87	0.56
1:D:100:ILE:HG22	1:D:104:LEU:HD21	1.88	0.55
1:B:392:ARG:HG3	1:B:402:LEU:HD11	1.88	0.55
1:C:208:ILE:HG12	1:C:218:LEU:HD21	1.88	0.55
1:D:392:ARG:HG3	1:D:402:LEU:HD11	1.88	0.55
1:B:307:VAL:HG21	1:B:353:ILE:HD13	1.89	0.54
1:D:112:THR:OG1	1:D:113:GLN:N	2.38	0.54
1:D:185:THR:HG22	1:D:187:ILE:H	1.72	0.54
1:A:51:ARG:NH2	1:A:141:GLU:O	2.41	0.53
1:C:91:ILE:HG21	1:C:100:ILE:HG23	1.90	0.53
1:B:24:THR:HB	1:B:27:HIS:CG	2.44	0.53
1:C:168:MET:HE3	1:C:360:ARG:HB3	1.88	0.53
1:D:208:ILE:HG12	1:D:218:LEU:HD21	1.90	0.53
1:A:74:MET:O	1:A:78:ILE:HG13	2.08	0.53
1:C:376:ASP:HB3	1:C:379:ARG:O	2.08	0.53
1:C:392:ARG:HG3	1:C:402:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:PHE:HE1	1:C:127:ILE:HD13	1.73	0.53
1:C:96:PRO:O	1:C:100:ILE:HG12	2.08	0.52
1:C:104:LEU:HD12	1:C:107:VAL:HG11	1.91	0.52
1:D:193:VAL:HG22	1:D:243:VAL:HB	1.91	0.52
1:D:100:ILE:O	1:D:104:LEU:HD22	2.09	0.52
1:D:234:ASP:O	1:D:238:ARG:HG3	2.09	0.52
1:B:109:LEU:HD13	1:B:127:ILE:HD12	1.91	0.52
1:C:307:VAL:HG21	1:C:353:ILE:HD13	1.90	0.52
1:B:301:PRO:HG2	1:B:304:THR:HG22	1.91	0.52
1:D:376:ASP:HB3	1:D:379:ARG:O	2.09	0.52
1:A:208:ILE:HG12	1:A:218:LEU:HD21	1.90	0.51
1:D:307:VAL:HG21	1:D:353:ILE:HD13	1.91	0.51
1:C:89:VAL:HG22	1:C:154:ILE:HB	1.92	0.51
1:D:51:ARG:NH2	1:D:141:GLU:O	2.43	0.51
1:C:119:LYS:HB3	1:C:120:PHE:CD1	2.45	0.51
1:D:230:GLU:OE2	1:D:263:ARG:NE	2.37	0.51
1:C:59:LYS:HD2	1:C:60:LYS:N	2.23	0.51
1:D:49:LEU:HD21	1:D:111:LEU:HD21	1.93	0.51
1:B:100:ILE:O	1:B:104:LEU:HD22	2.10	0.51
1:C:345:GLN:HA	1:C:393:TRP:HB2	1.92	0.51
1:A:89:VAL:HG22	1:A:154:ILE:HB	1.93	0.51
1:B:234:ASP:O	1:B:238:ARG:HG3	2.11	0.50
1:D:168:MET:HE3	1:D:360:ARG:HD2	1.92	0.50
1:A:336:LEU:HD23	1:A:342:LEU:HD23	1.93	0.50
1:B:208:ILE:HG12	1:B:218:LEU:HD21	1.94	0.50
1:D:52:PHE:CG	1:D:134:ILE:HG12	2.47	0.50
1:A:46:SER:OG	1:A:83:LYS:NZ	2.43	0.50
1:D:42:LEU:O	1:D:46:SER:OG	2.25	0.50
1:C:59:LYS:CD	1:C:60:LYS:H	2.21	0.49
1:D:67:MET:HE1	1:D:122:PHE:HZ	1.77	0.49
1:C:56:LYS:HG3	1:C:127:ILE:HD11	1.95	0.49
1:C:236:VAL:HG13	1:C:241:ILE:HB	1.94	0.49
1:C:66:ILE:HG13	1:C:68:MET:HE3	1.94	0.49
1:D:187:ILE:HD13	1:D:272:ILE:HD11	1.94	0.49
1:A:307:VAL:HG21	1:A:353:ILE:HD13	1.95	0.49
1:D:49:LEU:HD13	1:D:134:ILE:HD13	1.94	0.48
1:D:352:TYR:CZ	1:D:386:ARG:HG3	2.48	0.48
1:B:67:MET:HE1	1:B:120:PHE:CE1	2.49	0.48
1:B:47:ASN:O	1:B:51:ARG:HG3	2.14	0.48
1:B:125:GLU:OE1	1:B:125:GLU:N	2.44	0.48
1:B:187:ILE:HD13	1:B:272:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:GLU:HB3	1:C:223:LYS:HE3	1.96	0.48
1:C:77:GLY:O	1:C:81:ILE:HG13	2.13	0.48
1:A:376:ASP:HB3	1:A:379:ARG:O	2.14	0.48
1:B:390:LEU:HD21	1:C:256:ASN:HD21	1.77	0.48
1:A:128:VAL:HG23	1:A:131:ASP:HB2	1.96	0.47
1:C:70:ARG:H	1:C:223:LYS:CE	2.27	0.47
1:A:344:PRO:HD2	1:A:347:ILE:HD12	1.96	0.47
1:A:37:VAL:HG21	1:A:72:VAL:HG11	1.97	0.47
1:B:187:ILE:HA	1:B:270:HIS:CD2	2.50	0.47
1:C:67:MET:HE2	1:C:93:PRO:HA	1.96	0.47
1:B:376:ASP:HB3	1:B:379:ARG:O	2.15	0.47
1:A:10:ASP:OD1	1:A:148:SER:HB2	2.15	0.47
1:A:90:PRO:HB3	1:A:205:TYR:OH	2.15	0.47
1:D:106:SER:O	1:D:106:SER:OG	2.33	0.46
1:D:209:PHE:O	1:D:213:LEU:HB2	2.16	0.46
1:D:173:ASN:ND2	1:D:356:ALA:O	2.39	0.46
1:B:49:LEU:HD21	1:B:111:LEU:HD21	1.97	0.46
1:D:67:MET:HE2	1:D:67:MET:HB3	1.71	0.46
1:D:259:GLU:HG3	1:D:263:ARG:NH1	2.31	0.46
1:C:280:VAL:HG13	1:C:284:PHE:HB3	1.98	0.46
1:A:100:ILE:HG22	1:A:104:LEU:HD21	1.98	0.46
1:C:192:LYS:HE2	1:C:239:GLU:O	2.15	0.46
1:B:259:GLU:OE2	1:B:263:ARG:NH2	2.49	0.45
1:C:366:GLN:HA	1:C:369:THR:HB	1.97	0.45
1:A:248:VAL:HG12	1:A:252:LYS:HD2	1.97	0.45
1:C:128:VAL:HG23	1:C:131:ASP:HB2	1.99	0.45
1:D:72:VAL:O	1:D:76:VAL:HG23	2.16	0.45
1:D:366:GLN:HA	1:D:369:THR:HB	1.97	0.45
1:C:206:GLN:O	1:C:210:SER:OG	2.23	0.45
1:C:24:THR:HB	1:C:27:HIS:CG	2.52	0.45
1:D:59:LYS:HD3	1:D:60:LYS:N	2.31	0.45
1:B:209:PHE:O	1:B:213:LEU:HB2	2.17	0.45
1:C:304:THR:HG21	1:C:353:ILE:HD13	1.98	0.45
1:B:100:ILE:HG22	1:B:104:LEU:HD21	1.98	0.44
1:B:119:LYS:HB3	1:B:120:PHE:CD1	2.52	0.44
1:B:97:LYS:H	1:B:97:LYS:HG2	1.55	0.44
1:C:181:THR:O	1:C:185:THR:HB	2.17	0.44
1:B:286:ARG:O	1:B:290:GLU:HB2	2.17	0.44
1:D:17:PHE:O	1:D:21:VAL:HG23	2.17	0.44
1:A:95:TYR:CD2	1:A:103:MET:HE1	2.52	0.44
1:A:342:LEU:HD11	1:C:344:PRO:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:VAL:HG22	1:B:154:ILE:HB	1.99	0.43
1:B:332:TRP:C	1:B:333:ILE:HD13	2.43	0.43
1:D:286:ARG:O	1:D:290:GLU:HB2	2.18	0.43
1:A:49:LEU:HD21	1:A:111:LEU:HD21	2.01	0.43
1:A:209:PHE:O	1:A:213:LEU:HB2	2.19	0.43
1:C:90:PRO:HB3	1:C:205:TYR:OH	2.17	0.43
1:A:117:LYS:HG2	1:A:126:THR:HG21	2.01	0.43
1:A:63:ILE:HG22	1:A:107:VAL:HG22	2.00	0.43
1:A:392:ARG:HG3	1:A:402:LEU:HD11	2.00	0.43
1:C:85:GLY:HA2	1:C:146:ASN:OD1	2.18	0.43
1:C:104:LEU:O	1:C:107:VAL:HG12	2.19	0.43
1:C:100:ILE:HG12	1:C:100:ILE:H	1.67	0.42
1:C:209:PHE:O	1:C:213:LEU:HB2	2.19	0.42
1:D:90:PRO:HB3	1:D:205:TYR:OH	2.19	0.42
1:A:59:LYS:HG3	1:A:60:LYS:H	1.83	0.42
1:A:85:GLY:HA3	1:A:145:ILE:HD11	2.02	0.42
1:C:17:PHE:O	1:C:21:VAL:HG23	2.19	0.42
1:D:309:THR:O	1:D:325:GLY:HA3	2.18	0.42
1:B:257:GLU:OE2	1:C:386:ARG:NH1	2.52	0.42
1:C:95:TYR:CD2	1:C:103:MET:HE1	2.51	0.42
1:C:187:ILE:HA	1:C:270:HIS:CD2	2.54	0.42
1:D:37:VAL:HG21	1:D:72:VAL:HG11	2.02	0.42
1:D:85:GLY:HA2	1:D:146:ASN:OD1	2.19	0.42
1:A:52:PHE:CG	1:A:134:ILE:HG12	2.55	0.42
1:A:100:ILE:O	1:A:104:LEU:HD22	2.20	0.42
1:C:278:LEU:HD21	1:C:295:LEU:HD21	2.01	0.42
1:A:24:THR:HB	1:A:27:HIS:CG	2.54	0.42
1:D:307:VAL:HB	1:D:331:THR:HG21	2.01	0.42
1:B:312:ILE:HD11	1:B:322:PRO:HG3	2.02	0.41
1:C:309:THR:O	1:C:325:GLY:HA3	2.20	0.41
1:A:99:ARG:HG3	1:A:103:MET:HE3	2.01	0.41
1:D:64:ILE:HD13	1:D:108:ARG:HB3	2.02	0.41
1:A:367:GLU:O	1:A:371:GLU:HG3	2.20	0.41
1:B:304:THR:HG21	1:B:353:ILE:HD13	2.02	0.41
1:A:223:LYS:HB3	1:A:223:LYS:HE2	1.83	0.41
1:B:264:PHE:HA	1:B:265:PRO:HD3	1.92	0.41
1:C:153:TYR:C	1:C:153:TYR:CD1	2.99	0.41
1:B:85:GLY:HA2	1:B:146:ASN:OD1	2.20	0.41
1:A:64:ILE:O	1:A:88:PHE:HA	2.20	0.41
1:D:223:LYS:HB3	1:D:223:LYS:HE2	1.92	0.41
1:D:280:VAL:HG12	1:D:285:LYS:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:GLY:HA2	1:A:146:ASN:OD1	2.21	0.41
1:D:187:ILE:HA	1:D:270:HIS:CD2	2.55	0.41
1:D:153:TYR:CD1	1:D:153:TYR:C	2.99	0.41
1:A:165:LYS:HD2	1:A:362:TYR:CE1	2.56	0.41
1:D:198:THR:HB	1:D:201:PHE:CE2	2.56	0.41
1:A:119:LYS:HB3	1:A:120:PHE:CD1	2.56	0.40
1:A:309:THR:O	1:A:325:GLY:HA3	2.22	0.40
1:C:153:TYR:C	1:C:153:TYR:HD1	2.29	0.40
1:B:193:VAL:HG22	1:B:243:VAL:HB	2.03	0.40
1:D:153:TYR:C	1:D:153:TYR:HD1	2.30	0.40
1:A:49:LEU:HD13	1:A:134:ILE:HD13	2.03	0.40
1:D:67:MET:CE	1:D:122:PHE:HZ	2.34	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 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	386/405 (95%)	382 (99%)	4 (1%)	0	100	100
1	B	386/405 (95%)	379 (98%)	7 (2%)	0	100	100
1	C	386/405 (95%)	380 (98%)	6 (2%)	0	100	100
1	D	382/405 (94%)	378 (99%)	4 (1%)	0	100	100
All	All	1540/1620 (95%)	1519 (99%)	21 (1%)	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 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	357/368 (97%)	357 (100%)	0	100	100
1	B	356/368 (97%)	350 (98%)	6 (2%)	53	78
1	C	356/368 (97%)	351 (99%)	5 (1%)	59	81
1	D	354/368 (96%)	353 (100%)	1 (0%)	86	94
All	All	1423/1472 (97%)	1411 (99%)	12 (1%)	73	88

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	97	LYS
1	B	107	VAL
1	B	185	THR
1	B	222	ARG
1	B	229	VAL
1	B	320	GLU
1	C	97	LYS
1	C	100	ILE
1	C	153	TYR
1	C	267	CYS
1	C	320	GLU
1	D	153	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	ASN
1	A	231	GLN
1	A	341	GLN
1	A	345	GLN
1	B	179	HIS
1	B	291	HIS
1	B	366	GLN
1	B	381	ASN
1	C	47	ASN
1	C	289	HIS
1	C	292	ASN

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Mol	Chain	Res	Type
1	D	179	HIS
1	D	340	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 oligosaccharides 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

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, 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	390/405 (96%)	0.11	9 (2%) 61 55	47, 66, 95, 118	0
1	B	390/405 (96%)	0.12	9 (2%) 61 55	50, 62, 82, 100	0
1	C	390/405 (96%)	0.40	17 (4%) 39 33	53, 75, 103, 123	0
1	D	388/405 (95%)	0.71	26 (6%) 24 19	53, 86, 115, 135	0
All	All	1558/1620 (96%)	0.34	61 (3%) 43 38	47, 70, 106, 135	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	164	PRO	5.9
1	D	164	PRO	5.1
1	C	164	PRO	5.0
1	D	121	ALA	4.7
1	B	164	PRO	4.5
1	D	157	THR	4.4
1	D	9	PRO	4.3
1	C	157	THR	4.0
1	C	122	PHE	3.9
1	C	116	LEU	3.6
1	B	106	SER	3.4
1	C	403	GLY	3.2
1	D	289	HIS	3.2
1	A	157	THR	3.2
1	C	121	ALA	3.0
1	D	116	LEU	3.0
1	C	102	TYR	3.0
1	A	9	PRO	2.9
1	B	157	THR	2.8
1	D	87	ALA	2.8
1	D	117	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	380	PRO	2.7
1	C	97	LYS	2.7
1	C	9	PRO	2.7
1	D	8	TYR	2.7
1	A	120	PHE	2.7
1	A	121	ALA	2.6
1	B	97	LYS	2.6
1	B	102	TYR	2.6
1	D	99	ARG	2.6
1	D	129	ILE	2.5
1	C	123	THR	2.5
1	C	95	TYR	2.5
1	D	209	PHE	2.5
1	B	95	TYR	2.5
1	D	128	VAL	2.5
1	D	374	PHE	2.4
1	C	138	LEU	2.4
1	C	367	GLU	2.4
1	D	268	VAL	2.4
1	D	122	PHE	2.4
1	D	127	ILE	2.3
1	A	117	LYS	2.3
1	C	378	PHE	2.3
1	D	17	PHE	2.3
1	A	8	TYR	2.3
1	C	117	LYS	2.2
1	D	118	ASP	2.2
1	D	11	LYS	2.2
1	C	8	TYR	2.2
1	D	145	ILE	2.2
1	D	179	HIS	2.2
1	B	99	ARG	2.1
1	C	99	ARG	2.1
1	A	119	LYS	2.1
1	B	123	THR	2.1
1	D	106	SER	2.1
1	B	342	LEU	2.1
1	A	403	GLY	2.1
1	D	378	PHE	2.1
1	D	103	MET	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 oligosaccharides 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.