



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 03:58 AM EDT

PDB ID : 6FBM
Title : Crystal structure of GNIP1Aa from Chromobacterium piscinae
Authors : Freigang, J.; Zaitseva, J.
Deposited on : 2017-12-19
Resolution : 2.50 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)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

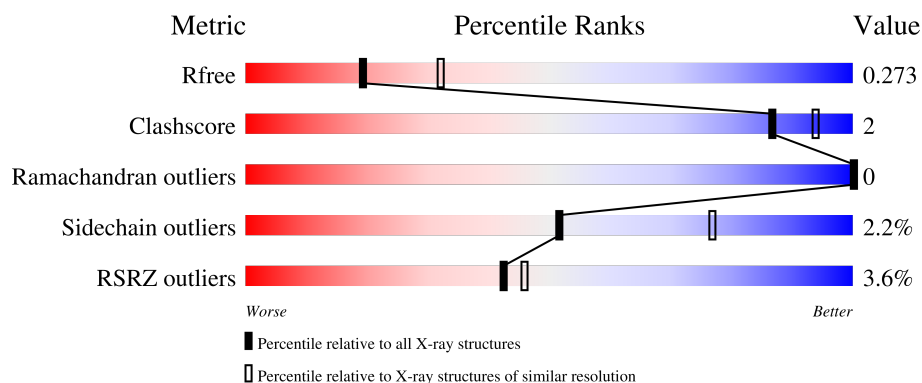
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	536	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>6%</div> <div></div> </div> <div>• •</div> </div>
1	B	536	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div></div> </div> <div>•</div> </div>
1	C	536	<div> <div>4%</div> <div> <div></div> <div>92%</div> <div>5%</div> <div></div> </div> <div>•</div> </div>
1	D	536	<div> <div>5%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div></div> </div> <div>• •</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16588 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 Gram-negative insecticidal protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	521	Total	C	N	O	S	0	0	0
			4034	2527	695	785	27			
1	B	521	Total	C	N	O	S	0	0	0
			4034	2527	695	785	27			
1	C	521	Total	C	N	O	S	0	0	0
			4034	2527	695	785	27			
1	D	521	Total	C	N	O	S	0	0	0
			4034	2527	695	785	27			

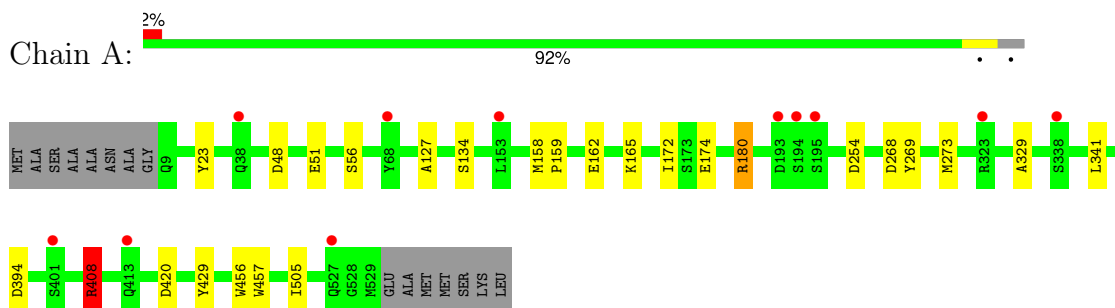
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	120	Total	O	0	0
			120	120		
2	B	116	Total	O	0	0
			116	116		
2	C	105	Total	O	0	0
			105	105		
2	D	111	Total	O	0	0
			111	111		

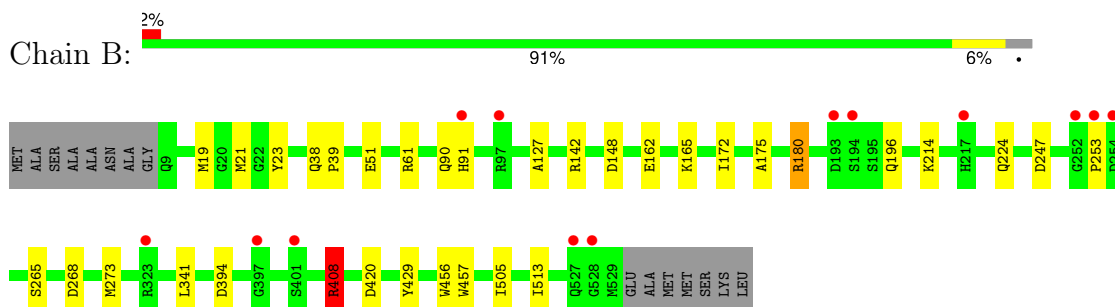
3 Residue-property plots [i](#)

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.

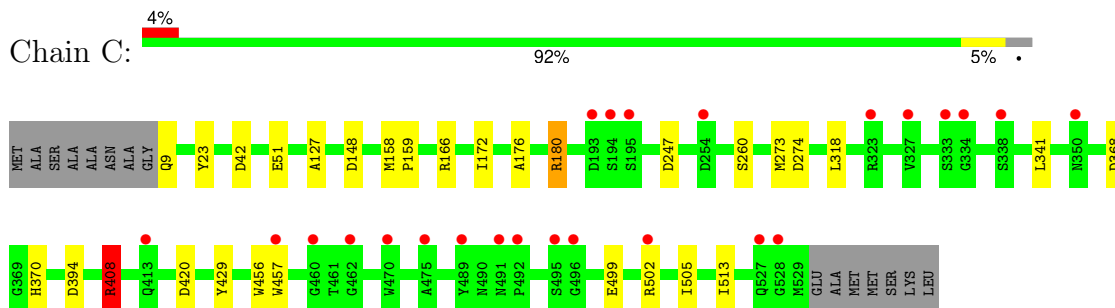
- Molecule 1: Gram-negative insecticidal protein



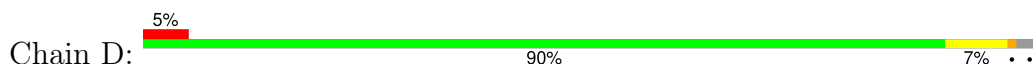
- Molecule 1: Gram-negative insecticidal protein

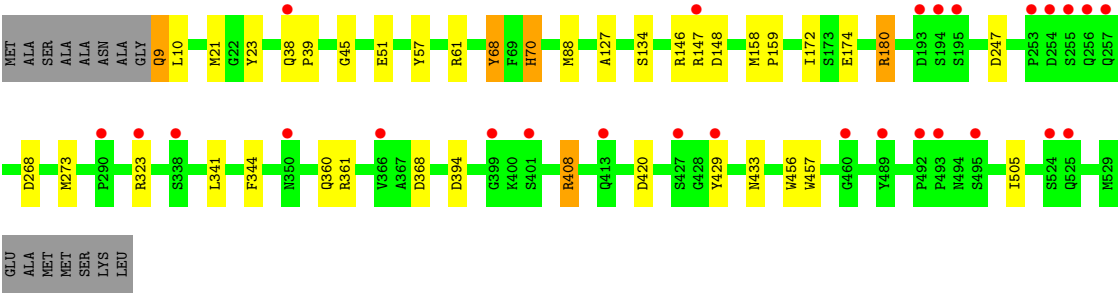


- Molecule 1: Gram-negative insecticidal protein



- Molecule 1: Gram-negative insecticidal protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.68Å 143.19Å 209.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.99 – 2.50 14.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.7 (14.99-2.50) 97.2 (14.99-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0158 2016/10/03	Depositor
R, R_{free}	0.230 , 0.271 0.233 , 0.273	Depositor DCC
R_{free} test set	4016 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 29.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	16588	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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 46.11 % 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 1.1995e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	0.59	0/4129	0.78	4/5589 (0.1%)
1	B	0.61	1/4129 (0.0%)	0.79	5/5589 (0.1%)
1	C	0.63	0/4129	0.80	5/5589 (0.1%)
1	D	0.62	0/4129	0.81	5/5589 (0.1%)
All	All	0.61	1/16516 (0.0%)	0.80	19/22356 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	265	SER	CB-OG	6.08	1.50	1.42

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	D	57	TYR	CB-CG-CD1	-7.25	116.65	121.00
1	D	57	TYR	CB-CG-CD2	6.77	125.06	121.00
1	A	408	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	B	408	ARG	NE-CZ-NH2	6.33	123.47	120.30
1	A	180	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	C	408	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	C	408	ARG	NE-CZ-NH2	6.22	123.41	120.30
1	D	268	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	408	ARG	NE-CZ-NH1	-5.97	117.31	120.30
1	C	180	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	B	408	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	C	42	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	B	180	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	B	268	ASP	CB-CG-OD2	5.38	123.14	118.30
1	D	68	TYR	CA-CB-CG	5.37	123.61	113.40
1	D	180	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	C	166	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	A	268	ASP	CB-CG-OD2	5.08	122.88	118.30

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	4034	0	3895	15	0
1	B	4034	0	3895	15	0
1	C	4034	0	3895	18	1
1	D	4034	0	3895	19	1
2	A	120	0	0	2	0
2	B	116	0	0	0	0
2	C	105	0	0	2	0
2	D	111	0	0	0	0
All	All	16588	0	15580	65	1

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 2.

All (65) 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:499:GLU:OE2	1:C:502:ARG:NH2	2.19	0.76
1:B:196:GLN:HB3	1:B:224:GLN:HE21	1.59	0.68
1:C:499:GLU:CD	1:C:502:ARG:NH2	2.52	0.63
1:C:370:HIS:CE1	2:C:698:HOH:O	2.52	0.63
1:C:370:HIS:HE1	2:C:698:HOH:O	1.83	0.59
1:B:408:ARG:HD3	1:B:505:ILE:HD11	1.85	0.57
1:C:408:ARG:HD3	1:C:505:ILE:HD11	1.84	0.57
1:D:408:ARG:HD3	1:D:505:ILE:HD11	1.85	0.56
1:A:408:ARG:HD3	1:A:505:ILE:HD11	1.85	0.56
1:A:269:TYR:OH	1:D:45:GLY:HA3	2.06	0.55
1:C:158:MET:HE2	1:C:159:PRO:HD2	1.89	0.55
1:C:499:GLU:OE1	1:C:502:ARG:NH2	2.40	0.55
1:B:90:GLN:HB3	1:B:91:HIS:ND1	2.23	0.54
1:D:9:GLN:HE21	1:D:9:GLN:N	2.06	0.54
1:D:180:ARG:HD3	1:D:273:MET:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:ARG:HD3	1:C:273:MET:O	2.11	0.51
1:C:127:ALA:HB1	1:C:273:MET:HE3	1.92	0.51
1:D:127:ALA:HB1	1:D:273:MET:CE	2.40	0.51
1:C:127:ALA:HB1	1:C:273:MET:CE	2.41	0.51
1:B:127:ALA:HB1	1:B:273:MET:CE	2.41	0.50
1:B:180:ARG:HD3	1:B:273:MET:O	2.12	0.50
1:D:127:ALA:HB1	1:D:273:MET:HE3	1.92	0.50
1:A:127:ALA:HB1	1:A:273:MET:CE	2.42	0.50
1:A:134:SER:HB3	1:A:174:GLU:HG3	1.94	0.49
1:A:180:ARG:HD3	1:A:273:MET:O	2.11	0.49
1:A:254:ASP:OD2	1:B:253:PRO:O	2.30	0.49
1:B:180:ARG:HB2	1:B:273:MET:HE2	1.94	0.49
1:A:180:ARG:HB2	1:A:273:MET:HE2	1.95	0.49
1:B:196:GLN:HB3	1:B:224:GLN:NE2	2.27	0.49
1:D:394:ASP:HB2	1:D:429:TYR:CE1	2.49	0.48
1:A:165:LYS:HE3	2:A:718:HOH:O	2.13	0.48
1:B:394:ASP:HB2	1:B:429:TYR:CE1	2.49	0.47
1:D:344:PHE:CE1	1:D:360:GLN:NE2	2.83	0.47
1:D:408:ARG:HG2	1:D:420:ASP:OD1	2.14	0.47
1:A:394:ASP:HB2	1:A:429:TYR:CE1	2.49	0.47
1:D:68:TYR:HB3	1:D:70:HIS:CE1	2.50	0.46
1:B:408:ARG:HG2	1:B:420:ASP:OD1	2.15	0.46
1:C:408:ARG:HG2	1:C:420:ASP:OD1	2.15	0.46
1:A:408:ARG:HG2	1:A:420:ASP:OD1	2.15	0.46
1:C:394:ASP:HB2	1:C:429:TYR:CE1	2.49	0.46
1:D:21:MET:HE2	1:D:39:PRO:HA	1.98	0.45
1:D:341:LEU:HB2	1:D:456:TRP:CD1	2.51	0.45
1:C:23:TYR:CD1	1:C:172:ILE:HD11	2.52	0.45
1:D:134:SER:HB3	1:D:174:GLU:HG3	1.97	0.45
1:B:127:ALA:HB1	1:B:273:MET:HE3	1.99	0.45
1:C:341:LEU:HB2	1:C:456:TRP:CD1	2.52	0.45
1:B:341:LEU:HB2	1:B:456:TRP:CD1	2.52	0.44
1:A:341:LEU:HB2	1:A:456:TRP:CD1	2.52	0.44
1:D:23:TYR:CD1	1:D:172:ILE:HD11	2.52	0.44
1:D:158:MET:HE2	1:D:159:PRO:HD2	1.99	0.44
1:A:23:TYR:CD1	1:A:172:ILE:HD11	2.53	0.44
1:C:180:ARG:HB2	1:C:273:MET:HE2	2.00	0.44
1:D:180:ARG:HB2	1:D:273:MET:HE2	2.00	0.43
1:B:23:TYR:CD1	1:B:172:ILE:HD11	2.53	0.43
1:A:329:ALA:HB1	2:A:611:HOH:O	2.18	0.43
1:A:158:MET:HE2	1:A:159:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:MET:CE	1:B:175:ALA:HB3	2.48	0.43
1:C:499:GLU:OE2	1:C:502:ARG:CZ	2.67	0.42
1:C:318:LEU:HD12	1:C:513:ILE:HD11	2.02	0.42
1:A:127:ALA:HB1	1:A:273:MET:HE3	2.01	0.41
1:C:176:ALA:HB3	1:C:274:ASP:HB3	2.01	0.41
1:B:21:MET:HE2	1:B:39:PRO:HA	2.02	0.41
1:D:360:GLN:HG2	1:D:368:ASP:OD2	2.21	0.41
1:D:344:PHE:CD1	1:D:360:GLN:NE2	2.88	0.40
1:D:10:LEU:HD12	1:D:45:GLY:HA2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:ASP:O	1:D:361:ARG:O[3_646]	2.17	0.03

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	519/536 (97%)	504 (97%)	15 (3%)	0	100	100
1	B	519/536 (97%)	504 (97%)	15 (3%)	0	100	100
1	C	519/536 (97%)	505 (97%)	14 (3%)	0	100	100
1	D	519/536 (97%)	503 (97%)	16 (3%)	0	100	100
All	All	2076/2144 (97%)	2016 (97%)	60 (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 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	436/445 (98%)	430 (99%)	6 (1%)	67	86
1	B	436/445 (98%)	425 (98%)	11 (2%)	47	73
1	C	436/445 (98%)	429 (98%)	7 (2%)	62	84
1	D	436/445 (98%)	422 (97%)	14 (3%)	39	65
All	All	1744/1780 (98%)	1706 (98%)	38 (2%)	52	77

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	A	51	GLU
1	A	56	SER
1	A	162	GLU
1	A	408	ARG
1	A	457	TRP
1	B	38	GLN
1	B	51	GLU
1	B	61	ARG
1	B	148	ASP
1	B	162	GLU
1	B	165	LYS
1	B	214	LYS
1	B	247	ASP
1	B	408	ARG
1	B	457	TRP
1	B	513	ILE
1	C	9	GLN
1	C	51	GLU
1	C	148	ASP
1	C	247	ASP
1	C	260	SER
1	C	408	ARG
1	C	457	TRP

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Mol	Chain	Res	Type
1	D	9	GLN
1	D	38	GLN
1	D	51	GLU
1	D	61	ARG
1	D	70	HIS
1	D	88	MET
1	D	146	ARG
1	D	147	ARG
1	D	148	ASP
1	D	247	ASP
1	D	323	ARG
1	D	408	ARG
1	D	433	ASN
1	D	457	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	224	GLN
1	C	9	GLN
1	C	370	HIS
1	D	70	HIS

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 monosaccharides 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	521/536 (97%)	-0.08	11 (2%) 63 66	9, 21, 46, 72	0
1	B	521/536 (97%)	0.02	13 (2%) 57 61	8, 25, 49, 78	0
1	C	521/536 (97%)	0.14	24 (4%) 32 34	6, 24, 58, 85	0
1	D	521/536 (97%)	0.17	27 (5%) 27 29	7, 29, 60, 95	0
All	All	2084/2144 (97%)	0.06	75 (3%) 42 46	6, 25, 55, 95	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	254	ASP	6.3
1	C	492	PRO	5.1
1	B	194	SER	4.1
1	D	350	ASN	4.0
1	C	495	SER	3.6
1	D	255	SER	3.6
1	A	194	SER	3.5
1	D	253	PRO	3.5
1	D	195	SER	3.3
1	C	528	GLY	3.3
1	C	338	SER	3.3
1	C	475	ALA	3.1
1	B	91	HIS	3.1
1	C	489	TYR	3.1
1	A	195	SER	3.1
1	B	323	ARG	3.0
1	B	252	GLY	2.9
1	B	528	GLY	2.8
1	C	333	SER	2.8
1	D	401	SER	2.8
1	C	193	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	217	HIS	2.7
1	B	397	GLY	2.7
1	C	334	GLY	2.7
1	C	527	GLN	2.7
1	B	527	GLN	2.7
1	D	429	TYR	2.7
1	C	413	GLN	2.7
1	C	194	SER	2.6
1	C	350	ASN	2.6
1	C	460	GLY	2.6
1	B	193	ASP	2.6
1	D	366	VAL	2.6
1	C	254	ASP	2.6
1	B	253	PRO	2.6
1	D	427	SER	2.6
1	D	492	PRO	2.6
1	C	502	ARG	2.6
1	D	193	ASP	2.6
1	D	194	SER	2.5
1	A	413	GLN	2.5
1	B	97	ARG	2.5
1	D	524	SER	2.4
1	C	457	TRP	2.4
1	A	153	LEU	2.4
1	A	527	GLN	2.4
1	D	493	PRO	2.4
1	A	401	SER	2.4
1	C	462	GLY	2.4
1	B	254	ASP	2.4
1	C	323	ARG	2.3
1	D	257	GLN	2.3
1	D	38	GLN	2.3
1	D	413	GLN	2.2
1	A	338	SER	2.2
1	D	338	SER	2.2
1	A	38	GLN	2.2
1	C	195	SER	2.2
1	D	399	GLY	2.1
1	A	68	TYR	2.1
1	A	193	ASP	2.1
1	C	491	ASN	2.1
1	D	256	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	147	ARG	2.1
1	D	323	ARG	2.1
1	D	495	SER	2.1
1	D	489	TYR	2.1
1	B	401	SER	2.1
1	C	496	GLY	2.1
1	D	525	GLN	2.1
1	C	470	TRP	2.1
1	D	290	PRO	2.0
1	C	327	VAL	2.0
1	D	460	GLY	2.0
1	A	323	ARG	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.