



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 12:22 pm BST

PDB ID : 4FFZ
Title : Crystal Structure of DENV1-E111 fab fragment bound to DENV-1 DIII (Western Pacific-74 strain).
Authors : Austin, S.K.; Nelson, C.A.; Fremont, D.H.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2012-06-01
Resolution : 3.80 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 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	:	2.11
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)	:	2.11

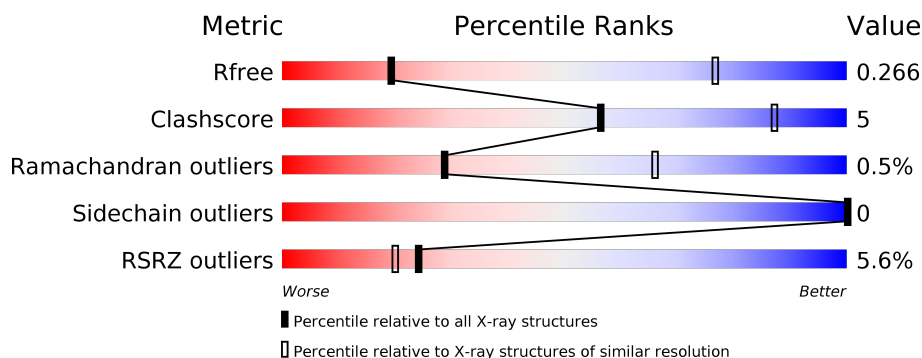
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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 on 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	111	<div> <div>8%</div> <div>77%</div> <div>10%</div> <div>13%</div> </div>
1	X	111	<div> <div>2%</div> <div>79%</div> <div>8%</div> <div>13%</div> </div>
2	L	216	<div> <div>8%</div> <div>88%</div> <div>12%</div> </div>
2	Y	216	<div> <div>3%</div> <div>88%</div> <div>12%</div> </div>
3	H	217	<div> <div>8%</div> <div>82%</div> <div>18%</div> </div>
3	Z	217	<div> <div>2%</div> <div>84%</div> <div>16%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8180 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 Envelope protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	97	Total	C	N	O	S	0	0	0
			745	476	121	145	3			
1	X	97	Total	C	N	O	S	0	0	0
			745	476	121	145	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	289	MET	-	EXPRESSION TAG	UNP P17763
A	290	ALA	-	EXPRESSION TAG	UNP P17763
A	291	SER	-	EXPRESSION TAG	UNP P17763
A	292	MET	-	EXPRESSION TAG	UNP P17763
X	289	MET	-	EXPRESSION TAG	UNP P17763
X	290	ALA	-	EXPRESSION TAG	UNP P17763
X	291	SER	-	EXPRESSION TAG	UNP P17763
X	292	MET	-	EXPRESSION TAG	UNP P17763

- Molecule 2 is a protein called DENV1-E111 fab fragment (light chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	216	Total	C	N	O	S	0	0	0
			1674	1042	280	347	5			
2	Y	216	Total	C	N	O	S	0	0	0
			1674	1042	280	347	5			

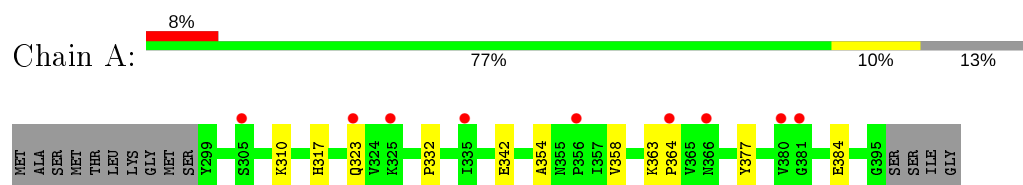
- Molecule 3 is a protein called DENV1-E111 fab fragment (heavy chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	217	Total	C	N	O	S	0	0	0
			1671	1067	277	319	8			
3	Z	217	Total	C	N	O	S	0	0	0
			1671	1067	277	319	8			

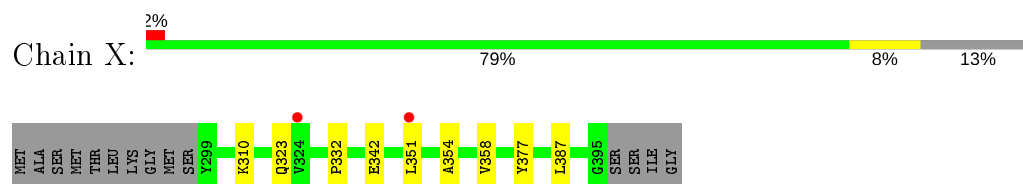
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

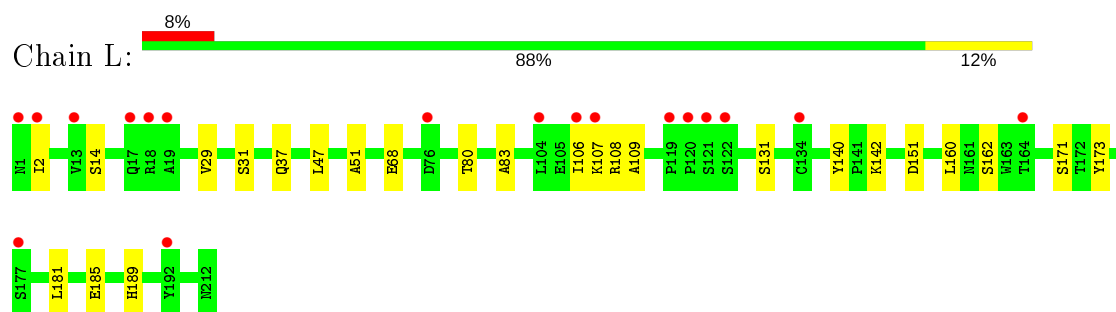
- Molecule 1: Envelope protein E



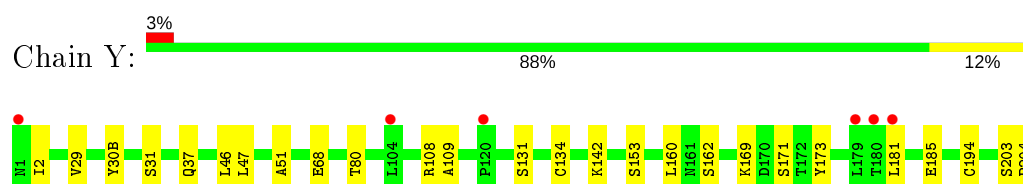
- Molecule 1: Envelope protein E



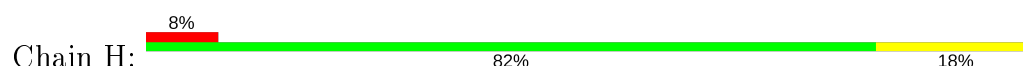
- Molecule 2: DENV1-E111 fab fragment (light chain)

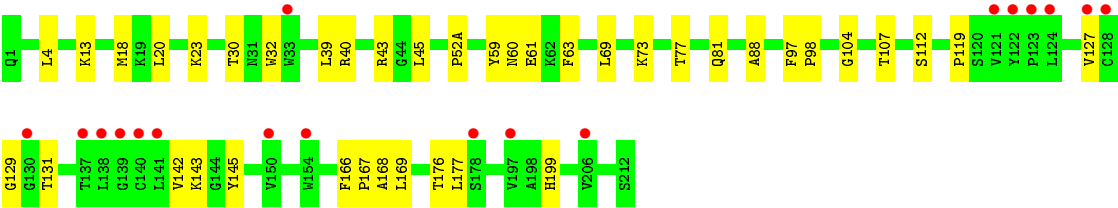


- Molecule 2: DENV1-E111 fab fragment (light chain)

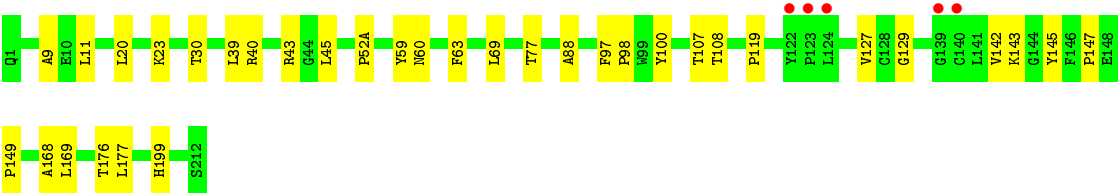
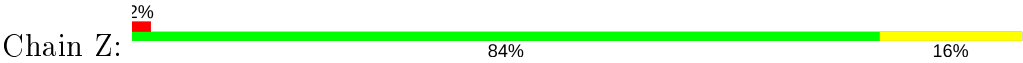


- Molecule 3: DENV1-E111 fab fragment (heavy chain)





● Molecule 3: DENV1-E111 fab fragment (heavy chain)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.86Å 52.01Å 136.40Å 90.00° 107.49° 90.00°	Depositor
Resolution (Å)	43.45 – 3.80 43.45 – 3.79	Depositor EDS
% Data completeness (in resolution range)	97.4 (43.45-3.80) 92.5 (43.45-3.79)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.237 , 0.278 0.231 , 0.266	Depositor DCC
R_{free} test set	553 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	114.3	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 81.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.227 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.305 for h,-k,-h-l	Depositor
Outliers	0 of 11022 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8180	wwPDB-VP
Average B, all atoms (Å ²)	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	0.23	0/760	0.47	0/1027
1	X	0.24	0/760	0.47	0/1027
2	L	0.25	0/1712	0.49	0/2330
2	Y	0.24	0/1712	0.48	0/2330
3	H	0.23	0/1721	0.46	0/2355
3	Z	0.23	0/1721	0.46	0/2355
All	All	0.24	0/8386	0.47	0/11424

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

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	745	0	747	6	0
1	X	745	0	747	6	0
2	L	1674	0	1588	14	0
2	Y	1674	0	1590	16	0
3	H	1671	0	1627	24	1
3	Z	1671	0	1627	24	0
All	All	8180	0	7926	80	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 5.

All (80) 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:Y:162:SER:HB2	3:Z:169:LEU:HD11	1.54	0.89
2:L:162:SER:HB2	3:H:169:LEU:HD11	1.65	0.79
1:A:317:HIS:HB2	2:Y:153:SER:HA	1.67	0.76
3:Z:127:VAL:HG12	3:Z:129:GLY:H	1.51	0.75
3:H:127:VAL:HG12	3:H:129:GLY:H	1.53	0.74
2:Y:160:LEU:HG	3:Z:169:LEU:HD13	1.81	0.63
2:L:14:SER:HA	2:L:107:LYS:HB3	1.81	0.62
2:Y:80:THR:HG23	2:Y:171:SER:OG	2.01	0.61
2:Y:131:SER:OG	3:Z:143:LYS:NZ	2.33	0.61
3:Z:9:ALA:HB2	3:Z:149:PRO:HD2	1.83	0.61
2:L:131:SER:OG	3:H:143:LYS:NZ	2.36	0.58
2:L:80:THR:HG23	2:L:171:SER:OG	2.04	0.57
2:Y:80:THR:HG21	2:Y:169:LYS:C	2.24	0.56
1:X:351:LEU:HD13	2:Y:30(B):TYR:HD2	1.73	0.53
2:Y:37:GLN:HB2	2:Y:47:LEU:HD11	1.90	0.53
3:Z:11:LEU:HB2	3:Z:147:PRO:HG3	1.91	0.52
3:H:143:LYS:HG3	3:H:176:THR:HG22	1.91	0.52
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.90	0.52
1:A:310:LYS:HD3	1:A:323:GLN:HB3	1.91	0.51
1:A:384:GLU:HB2	3:H:32:TRP:CZ2	2.45	0.51
3:H:20:LEU:HD22	3:H:107:THR:HG21	1.93	0.51
3:Z:143:LYS:HG3	3:Z:176:THR:HG22	1.91	0.51
3:H:119:PRO:HB3	3:H:145:TYR:HB3	1.93	0.51
3:Z:20:LEU:HD22	3:Z:107:THR:HG21	1.93	0.50
2:L:160:LEU:HG	3:H:169:LEU:HD13	1.94	0.49
3:Z:119:PRO:HB3	3:Z:145:TYR:HB3	1.94	0.49
3:H:59:TYR:CE1	3:H:69:LEU:HG	2.47	0.49
3:Z:59:TYR:CE1	3:Z:69:LEU:HG	2.48	0.49
1:X:310:LYS:HD3	1:X:323:GLN:HB3	1.95	0.49
3:Z:40:ARG:HG2	3:Z:88:ALA:HB2	1.95	0.48
3:H:40:ARG:HG2	3:H:88:ALA:HB2	1.95	0.48
3:Z:60:ASN:HB3	3:Z:63:PHE:HD2	1.78	0.48
3:H:142:VAL:HB	3:H:177:LEU:HD12	1.96	0.47
3:Z:142:VAL:HB	3:Z:177:LEU:HD12	1.96	0.47
3:H:60:ASN:HB3	3:H:63:PHE:HD2	1.79	0.47
2:L:181:LEU:HD22	2:L:185:GLU:HG2	1.98	0.47
2:Y:203:SER:HA	2:Y:204:PRO:HD3	1.80	0.47
1:X:342:GLU:OE1	1:X:377:TYR:OH	2.16	0.46
3:Z:168:ALA:HA	3:Z:177:LEU:HB3	1.98	0.46
3:H:168:ALA:HA	3:H:177:LEU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:97:PHE:HA	3:H:98:PRO:HA	1.74	0.46
1:A:342:GLU:OE1	1:A:377:TYR:OH	2.18	0.45
2:Y:181:LEU:HD22	2:Y:185:GLU:HG2	1.97	0.45
3:H:13:LYS:HA	3:H:112:SER:O	2.17	0.45
3:Z:108:THR:HB	3:Z:149:PRO:HD3	1.99	0.44
3:H:23:LYS:HG2	3:H:77:THR:OG1	2.18	0.44
3:Z:23:LYS:HG2	3:Z:77:THR:OG1	2.18	0.44
2:L:31:SER:HB2	2:L:51:ALA:HB2	2.00	0.43
3:Z:11:LEU:HD22	3:Z:147:PRO:HD3	2.00	0.43
3:Z:59:TYR:HE1	3:Z:69:LEU:HG	1.83	0.43
3:H:59:TYR:HE1	3:H:69:LEU:HG	1.83	0.43
2:Y:134:CYS:SG	2:Y:194:CYS:SG	3.11	0.43
3:H:119:PRO:HD3	3:H:199:HIS:ND1	2.33	0.43
3:Z:97:PHE:HA	3:Z:98:PRO:HA	1.74	0.42
1:X:332:PRO:HA	1:X:358:VAL:O	2.19	0.42
3:Z:119:PRO:HD3	3:Z:199:HIS:ND1	2.34	0.42
1:A:332:PRO:HA	1:A:358:VAL:O	2.19	0.42
1:A:363:LYS:HA	1:A:364:PRO:HD3	1.93	0.42
2:Y:2:ILE:HD13	2:Y:29:VAL:HG12	2.02	0.42
2:Y:31:SER:HB2	2:Y:51:ALA:HB2	2.00	0.42
1:X:351:LEU:HA	1:X:351:LEU:HD12	1.86	0.42
3:H:40:ARG:HD2	3:H:43:ARG:CZ	2.50	0.42
3:Z:40:ARG:HD2	3:Z:43:ARG:CZ	2.49	0.42
2:L:107:LYS:HA	2:L:140:TYR:CZ	2.55	0.42
2:L:151:ASP:OD2	2:L:189:HIS:ND1	2.45	0.42
2:L:83:ALA:HB2	2:L:106:ILE:HG12	2.02	0.42
2:Y:108:ARG:HG2	2:Y:109:ALA:H	1.84	0.41
3:H:4:LEU:HB2	3:H:104:GLY:HA2	2.03	0.41
3:H:166:PHE:HA	3:H:167:PRO:HD3	1.96	0.41
3:Z:30:THR:HA	3:Z:52(A):PRO:HB2	2.01	0.41
3:Z:39:LEU:HB2	3:Z:45:LEU:HD23	2.02	0.41
2:Y:142:LYS:HA	2:Y:173:TYR:HD2	1.86	0.41
2:L:142:LYS:HA	2:L:173:TYR:HD2	1.86	0.41
3:H:30:THR:HA	3:H:52(A):PRO:HB2	2.01	0.41
3:H:39:LEU:HB2	3:H:45:LEU:HD23	2.01	0.41
2:L:108:ARG:HG2	2:L:109:ALA:H	1.86	0.41
2:L:2:ILE:HD13	2:L:29:VAL:HG12	2.02	0.41
3:H:18:MET:O	3:H:81:GLN:HA	2.22	0.40
2:Y:46:LEU:HD22	3:Z:100:TYR:CD1	2.57	0.40
1:X:387:LEU:HD12	1:X:387:LEU:HA	1.96	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:61:GLU:O	3:H:73:LYS:NZ[2_755]	2.16	0.04

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	95/111 (86%)	90 (95%)	4 (4%)	1 (1%)	14	51
1	X	95/111 (86%)	90 (95%)	4 (4%)	1 (1%)	14	51
2	L	214/216 (99%)	209 (98%)	4 (2%)	1 (0%)	29	66
2	Y	214/216 (99%)	208 (97%)	5 (2%)	1 (0%)	29	66
3	H	215/217 (99%)	210 (98%)	4 (2%)	1 (0%)	29	66
3	Z	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
All	All	1048/1088 (96%)	1016 (97%)	27 (3%)	5 (0%)	29	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	354	ALA
2	L	68	GLU
1	X	354	ALA
2	Y	68	GLU
3	H	131	THR

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	82/93 (88%)	82 (100%)	0	100	100
1	X	82/93 (88%)	82 (100%)	0	100	100
2	L	190/190 (100%)	190 (100%)	0	100	100
2	Y	190/190 (100%)	190 (100%)	0	100	100
3	H	188/188 (100%)	188 (100%)	0	100	100
3	Z	188/188 (100%)	188 (100%)	0	100	100
All	All	920/942 (98%)	920 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
2	L	30(D)	ASN
2	L	124	GLN
2	Y	30(D)	ASN
2	Y	124	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, 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	97/111 (87%)	0.49	9 (9%) 8 7	125, 173, 195, 208	0
1	X	97/111 (87%)	0.24	2 (2%) 63 55	123, 171, 193, 210	0
2	L	216/216 (100%)	0.38	18 (8%) 11 9	127, 162, 206, 235	0
2	Y	216/216 (100%)	0.20	7 (3%) 47 38	124, 160, 205, 232	0
3	H	217/217 (100%)	0.21	18 (8%) 11 9	105, 143, 199, 230	0
3	Z	217/217 (100%)	0.08	5 (2%) 60 52	103, 141, 198, 229	0
All	All	1060/1088 (97%)	0.24	59 (5%) 24 20	103, 156, 202, 235	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	124	LEU	5.8
1	A	366	ASN	4.7
3	H	141	LEU	4.2
3	H	140	CYS	4.0
2	L	13	VAL	3.9
3	H	128	CYS	3.9
2	L	120	PRO	3.7
1	A	381	GLY	3.7
3	H	127	VAL	3.7
3	Z	139	GLY	3.6
3	H	123	PRO	3.6
2	L	18	ARG	3.5
1	A	364	PRO	3.4
2	L	134	CYS	3.3
3	H	138	LEU	3.3
3	H	206	VAL	3.2
2	Y	212	ASN	3.2
2	L	177	SER	3.1
2	L	17	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
3	Z	140	CYS	3.1
1	A	356	PRO	2.9
2	Y	120	PRO	2.9
1	A	380	VAL	2.9
3	H	121	VAL	2.8
3	Z	122	TYR	2.8
2	Y	1	ASN	2.8
3	H	197	VAL	2.7
3	Z	123	PRO	2.7
1	A	335	ILE	2.7
3	H	130	GLY	2.6
3	H	137	THR	2.6
2	Y	180	THR	2.6
1	X	351	LEU	2.5
2	L	2	ILE	2.5
3	H	122	TYR	2.5
2	L	106	ILE	2.4
3	H	178	SER	2.4
1	A	325	LYS	2.3
3	H	154	TRP	2.3
2	L	76	ASP	2.3
2	L	192	TYR	2.3
2	Y	179	LEU	2.3
2	L	164	THR	2.2
2	L	122	SER	2.2
2	L	107	LYS	2.2
3	H	139	GLY	2.2
2	L	19	ALA	2.2
2	Y	181	LEU	2.2
2	L	1	ASN	2.2
1	A	323	GLN	2.1
2	L	104	LEU	2.1
3	H	150	VAL	2.1
2	L	121	SER	2.1
1	X	324	VAL	2.1
2	L	119	PRO	2.1
3	Z	124	LEU	2.1
1	A	305	SER	2.0
3	H	33	TRP	2.0
2	Y	104	LEU	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 carbohydrates 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.