



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:23 AM UTC

PDB ID : 8RW9 / pdb_00008rw9
Title : Domains 1 and 2 of Bacillus anthracis Sap S-layer in complex with Nb694
Authors : Sogues, A.; Remaut, H.
Deposited on : 2024-02-02
Resolution : 1.99 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

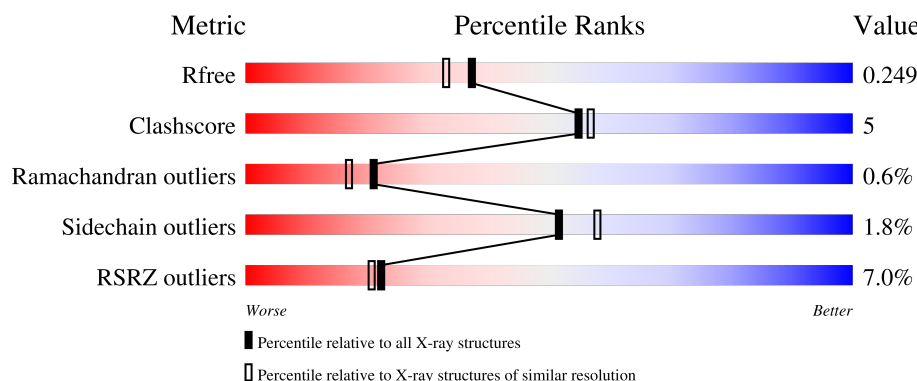
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

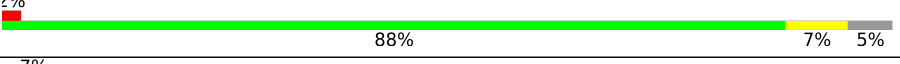
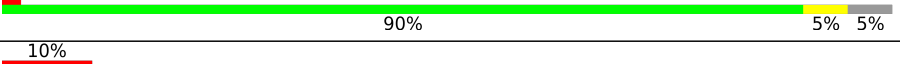
The reported resolution of this entry is 1.99 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	130	
1	B	130	
1	C	130	
1	D	130	
2	E	176	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	176	13% 82% 10% • 6%
2	G	176	7% 88% 7% • 5%
2	H	176	6% 88% 5% • • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9666 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 Nanobody694.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	125	Total	C	N	O	S	0	0	0
			971	613	164	190	4			
1	B	124	Total	C	N	O	S	0	0	0
			961	607	161	189	4			
1	C	123	Total	C	N	O	S	0	0	0
			956	604	161	187	4			
1	D	123	Total	C	N	O	S	0	0	0
			952	602	160	186	4			

- Molecule 2 is a protein called S-layer protein sap.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	167	Total	C	N	O	S	0	0	0
			1225	768	200	256	1			
2	F	166	Total	C	N	O	S	0	0	0
			1233	774	200	258	1			
2	G	168	Total	C	N	O	S	0	0	0
			1234	774	202	257	1			
2	H	167	Total	C	N	O	S	0	0	0
			1241	779	203	258	1			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	208	MET	-	initiating methionine	UNP P49051
E	209	HIS	-	expression tag	UNP P49051
E	210	HIS	-	expression tag	UNP P49051
E	211	HIS	-	expression tag	UNP P49051
E	212	HIS	-	expression tag	UNP P49051
E	213	HIS	-	expression tag	UNP P49051
E	214	HIS	-	expression tag	UNP P49051
F	208	MET	-	initiating methionine	UNP P49051

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	209	HIS	-	expression tag	UNP P49051
F	210	HIS	-	expression tag	UNP P49051
F	211	HIS	-	expression tag	UNP P49051
F	212	HIS	-	expression tag	UNP P49051
F	213	HIS	-	expression tag	UNP P49051
F	214	HIS	-	expression tag	UNP P49051
G	208	MET	-	initiating methionine	UNP P49051
G	209	HIS	-	expression tag	UNP P49051
G	210	HIS	-	expression tag	UNP P49051
G	211	HIS	-	expression tag	UNP P49051
G	212	HIS	-	expression tag	UNP P49051
G	213	HIS	-	expression tag	UNP P49051
G	214	HIS	-	expression tag	UNP P49051
H	208	MET	-	initiating methionine	UNP P49051
H	209	HIS	-	expression tag	UNP P49051
H	210	HIS	-	expression tag	UNP P49051
H	211	HIS	-	expression tag	UNP P49051
H	212	HIS	-	expression tag	UNP P49051
H	213	HIS	-	expression tag	UNP P49051
H	214	HIS	-	expression tag	UNP P49051

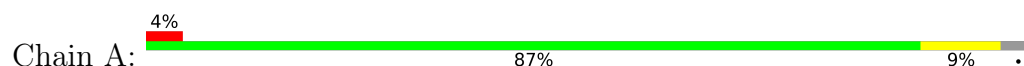
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	96	Total O 96 96	0	0
3	B	79	Total O 79 79	0	0
3	C	88	Total O 88 88	0	0
3	D	116	Total O 116 116	0	0
3	E	137	Total O 137 137	0	0
3	F	118	Total O 118 118	0	0
3	G	136	Total O 136 136	0	0
3	H	123	Total O 123 123	0	0

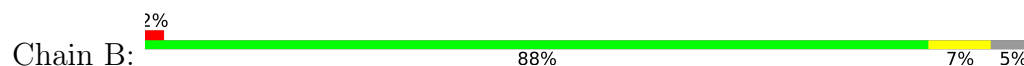
3 Residue-property plots [i](#)

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.

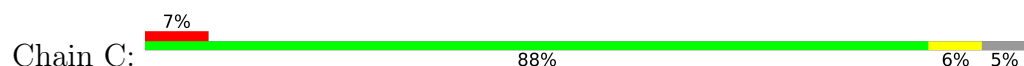
- Molecule 1: Nanobody694



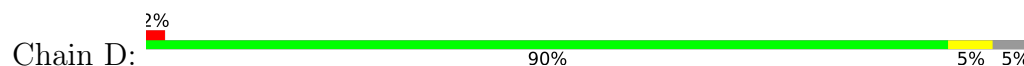
- Molecule 1: Nanobody694



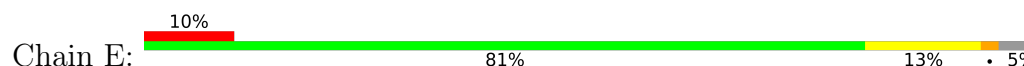
- Molecule 1: Nanobody694



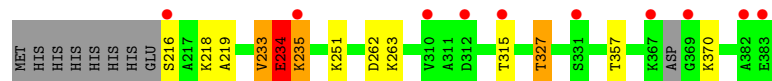
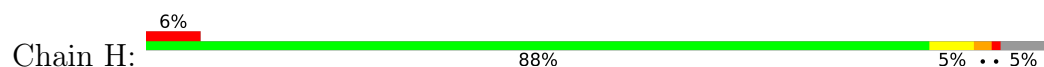
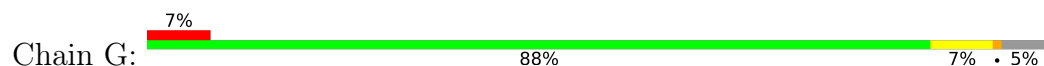
- Molecule 1: Nanobody694



- Molecule 2: S-layer protein sap



Chain F: 13% 82% 10% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	33.41Å 113.97Å 122.70Å 90.71° 96.01° 97.05°	Depositor
Resolution (Å)	42.00 – 1.99 42.00 – 1.99	Depositor EDS
% Data completeness (in resolution range)	96.9 (42.00-1.99) 97.0 (42.00-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.209 , 0.249 0.210 , 0.249	Depositor DCC
R_{free} test set	5986 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	48.4	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.055 for h,-h-k,-h-l 0.000 for -h,h+k,-l 0.000 for -h,-k,h+l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9666	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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	0.33	0/997	0.54	0/1354
1	B	0.31	0/986	0.57	0/1339
1	C	0.30	0/981	0.55	0/1332
1	D	0.37	0/977	0.59	0/1327
2	E	0.40	0/1233	0.70	3/1671 (0.2%)
2	F	0.33	0/1240	0.58	0/1675
2	G	0.33	0/1242	0.56	0/1682
2	H	0.40	0/1248	0.76	2/1685 (0.1%)
All	All	0.35	0/8904	0.62	5/12065 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	234	GLU	CA-C-N	10.67	140.90	121.70
2	H	234	GLU	C-N-CA	10.67	140.90	121.70
2	E	305	ALA	N-CA-C	-8.15	104.33	112.97
2	E	303	GLU	CA-C-N	-6.03	111.91	121.86
2	E	303	GLU	C-N-CA	-6.03	111.91	121.86

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	234	GLU	Peptide

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	971	0	913	11	0
1	B	961	0	906	6	0
1	C	956	0	906	9	0
1	D	952	0	900	5	0
2	E	1225	0	1254	19	0
2	F	1233	0	1280	13	0
2	G	1234	0	1270	15	0
2	H	1241	0	1293	11	0
3	A	96	0	0	2	0
3	B	79	0	0	1	0
3	C	88	0	0	2	0
3	D	116	0	0	1	0
3	E	137	0	0	4	0
3	F	118	0	0	3	0
3	G	136	0	0	4	0
3	H	123	0	0	3	0
All	All	9666	0	8722	84	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 5.

All (84) 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:F:221:THR:HG22	2:F:223:GLN:H	1.19	1.02
2:G:221:THR:HG22	2:G:223:GLN:H	1.31	0.95
2:H:234:GLU:HB2	2:H:235:LYS:HE3	1.51	0.92
2:H:216:SER:N	3:H:401:HOH:O	2.22	0.70
1:D:86:LYS:NZ	3:D:201:HOH:O	2.25	0.69
2:E:304:MET:HE2	2:E:363:ALA:HB2	1.74	0.69
2:F:338:VAL:HG22	2:F:362:LYS:HB3	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:328:GLU:OE1	3:E:401:HOH:O	2.11	0.68
2:E:304:MET:HB2	2:E:376:LYS:NZ	2.08	0.68
2:H:234:GLU:N	2:H:235:LYS:HB2	2.08	0.68
2:E:256:GLU:OE1	3:E:402:HOH:O	2.12	0.67
1:A:124:GLU:N	1:A:124:GLU:OE2	2.28	0.66
2:G:221:THR:CG2	2:G:223:GLN:H	2.08	0.66
2:E:259:LEU:HD13	2:E:263:LYS:HD3	1.77	0.66
2:F:221:THR:HG22	2:F:223:GLN:N	2.03	0.66
2:E:304:MET:HB2	2:E:376:LYS:HZ3	1.60	0.65
2:F:221:THR:HG21	3:F:505:HOH:O	1.96	0.65
2:H:234:GLU:H	2:H:235:LYS:HB2	1.62	0.65
2:H:219:ALA:O	2:H:327:THR:HB	1.97	0.63
2:F:221:THR:HB	2:F:224:LYS:HB2	1.79	0.62
2:G:383:GLU:HA	3:G:407:HOH:O	1.98	0.61
1:A:47:TRP:CD2	1:A:107:GLY:HA2	2.36	0.61
1:A:86:LYS:NZ	3:A:202:HOH:O	2.35	0.58
2:F:366:LYS:HG3	2:F:371:VAL:HG22	1.86	0.58
1:C:47:TRP:CD2	1:C:107:GLY:HA2	2.38	0.58
1:B:47:TRP:CD2	1:B:107:GLY:HA2	2.39	0.57
2:G:221:THR:HB	2:G:224:LYS:HB2	1.85	0.57
2:H:233:VAL:O	2:H:263:LYS:HB3	2.05	0.57
1:A:12:VAL:HG11	1:A:85:LEU:HD13	1.87	0.56
2:G:221:THR:HG22	2:G:223:GLN:N	2.12	0.55
2:E:304:MET:C	2:E:306:ASP:H	2.14	0.55
2:G:357:THR:HG23	2:H:357:THR:HB	1.89	0.55
1:C:47:TRP:CE2	1:C:107:GLY:HA2	2.42	0.55
2:F:344:LYS:HD3	2:F:353:LEU:HD23	1.89	0.55
1:D:47:TRP:CD2	1:D:107:GLY:HA2	2.41	0.54
1:A:30:SER:H	1:C:1:GLN:HE22	1.56	0.54
2:F:218:LYS:HE3	2:F:220:VAL:HG12	1.89	0.54
2:E:344:LYS:O	2:E:351:ILE:O	2.26	0.52
1:A:47:TRP:CE2	1:A:107:GLY:HA2	2.44	0.52
2:F:222:THR:OG1	2:F:330:VAL:HG13	2.10	0.51
2:E:314:PRO:HA	2:E:352:THR:HB	1.92	0.51
1:B:47:TRP:CE2	1:B:107:GLY:HA2	2.46	0.51
2:G:255:LYS:HE2	2:G:271:TYR:CD1	2.46	0.51
2:G:382:ALA:O	2:G:383:GLU:HG2	2.12	0.50
2:F:338:VAL:HG21	2:F:362:LYS:HE2	1.94	0.50
2:E:314:PRO:CA	2:E:352:THR:HB	2.43	0.49
2:G:255:LYS:NZ	3:G:406:HOH:O	2.45	0.49
3:B:256:HOH:O	1:D:1:GLN:HB2	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:311:ALA:C	2:E:313:GLU:H	2.20	0.49
2:H:234:GLU:CB	2:H:235:LYS:HE3	2.35	0.48
1:C:81:GLN:HE21	1:C:83:ASN:ND2	2.10	0.48
2:E:354:ALA:O	2:E:357:THR:HB	2.12	0.48
1:A:20:LEU:HG	1:A:82:MET:HE2	1.96	0.47
1:B:17:SER:OG	1:C:11:LEU:HD12	2.14	0.47
2:G:354:ALA:O	2:G:357:THR:HB	2.15	0.47
2:G:255:LYS:HE2	2:G:271:TYR:CE1	2.51	0.46
1:A:30:SER:H	1:C:1:GLN:NE2	2.14	0.46
1:C:33:PRO:HG3	3:C:203:HOH:O	2.16	0.46
2:E:235:LYS:NZ	3:E:409:HOH:O	2.49	0.46
2:H:218:LYS:NZ	3:H:408:HOH:O	2.49	0.45
2:H:251:LYS:NZ	3:H:410:HOH:O	2.50	0.45
1:C:86:LYS:NZ	3:C:205:HOH:O	2.50	0.45
1:D:47:TRP:CE2	1:D:107:GLY:HA2	2.52	0.45
2:E:308:THR:O	2:E:380:VAL:HA	2.17	0.45
1:A:124:GLU:H	1:A:124:GLU:CD	2.18	0.44
2:G:286:LYS:HA	2:G:286:LYS:HD2	1.60	0.43
2:G:383:GLU:HB3	3:G:442:HOH:O	2.18	0.43
2:G:216:SER:N	3:G:412:HOH:O	2.51	0.43
2:E:314:PRO:N	2:E:352:THR:HB	2.34	0.43
1:B:41:PRO:HA	1:B:42:GLY:HA2	1.67	0.43
1:B:72:ASP:OD2	1:B:75:LYS:HD2	2.19	0.43
1:B:34:MET:HB3	1:B:78:LEU:HD22	2.01	0.42
2:G:346:ASN:HD21	2:G:350:GLU:HB2	1.84	0.42
2:F:383:GLU:HA	3:F:423:HOH:O	2.18	0.42
2:E:304:MET:HE2	2:E:363:ALA:CB	2.47	0.42
1:A:11:LEU:HD11	3:A:270:HOH:O	2.20	0.41
2:H:234:GLU:CA	2:H:235:LYS:HB2	2.50	0.41
2:F:224:LYS:HG2	2:F:269:GLU:HG2	2.03	0.41
2:E:251:LYS:HE3	2:E:251:LYS:HB3	1.78	0.41
2:E:277:LYS:HA	2:E:294:VAL:O	2.21	0.41
1:A:29:PHE:N	1:C:1:GLN:HE22	2.19	0.41
1:D:82:MET:HE1	1:D:120:VAL:HG21	2.03	0.41
2:F:242:LYS:NZ	3:F:407:HOH:O	2.36	0.40
2:E:308:THR:HG21	3:E:426:HOH:O	2.20	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	123/130 (95%)	122 (99%)	1 (1%)	0	100	100
1	B	122/130 (94%)	120 (98%)	2 (2%)	0	100	100
1	C	121/130 (93%)	120 (99%)	1 (1%)	0	100	100
1	D	121/130 (93%)	120 (99%)	1 (1%)	0	100	100
2	E	165/176 (94%)	157 (95%)	6 (4%)	2 (1%)	10	6
2	F	162/176 (92%)	156 (96%)	4 (2%)	2 (1%)	10	6
2	G	166/176 (94%)	163 (98%)	3 (2%)	0	100	100
2	H	163/176 (93%)	158 (97%)	2 (1%)	3 (2%)	6	3
All	All	1143/1224 (93%)	1116 (98%)	20 (2%)	7 (1%)	21	17

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	352	THR
2	H	235	LYS
2	H	262	ASP
2	F	253	LEU
2	E	312	ASP
2	H	370	LYS
2	F	346	ASN

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	102/108 (94%)	101 (99%)	1 (1%)	68	75
1	B	101/108 (94%)	101 (100%)	0	100	100
1	C	101/108 (94%)	101 (100%)	0	100	100
1	D	100/108 (93%)	100 (100%)	0	100	100
2	E	134/150 (89%)	132 (98%)	2 (2%)	57	64
2	F	137/150 (91%)	130 (95%)	7 (5%)	21	19
2	G	135/150 (90%)	132 (98%)	3 (2%)	45	50
2	H	138/150 (92%)	134 (97%)	4 (3%)	37	40
All	All	948/1032 (92%)	931 (98%)	17 (2%)	51	58

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	THR
2	E	357	THR
2	E	380	VAL
2	F	221	THR
2	F	330	VAL
2	F	338	VAL
2	F	344	LYS
2	F	360	THR
2	F	370	LYS
2	F	378	VAL
2	G	221	THR
2	G	357	THR
2	G	379	LYS
2	H	233	VAL
2	H	234	GLU
2	H	315	THR
2	H	327	THR

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	1	GLN
1	A	83	ASN
1	A	112	HIS
1	C	1	GLN
1	C	3	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	39	GLN
1	C	83	ASN
1	C	112	HIS
1	C	116	GLN
1	D	13	GLN
1	D	39	GLN
2	F	223	GLN
2	H	318	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	125/130 (96%)	0.38	5 (4%)	42 41	42, 50, 67, 94	0
1	B	124/130 (95%)	0.45	3 (2%)	59 59	41, 51, 66, 97	0
1	C	123/130 (94%)	0.78	9 (7%)	21 19	43, 55, 67, 86	0
1	D	123/130 (94%)	0.29	2 (1%)	70 70	39, 47, 61, 74	0
2	E	167/176 (94%)	0.77	17 (10%)	12 11	39, 53, 75, 85	0
2	F	166/176 (94%)	0.90	23 (13%)	6 5	44, 60, 78, 118	0
2	G	168/176 (95%)	0.61	12 (7%)	22 20	43, 55, 73, 92	0
2	H	167/176 (94%)	0.56	10 (5%)	27 26	41, 54, 71, 89	0
All	All	1163/1224 (95%)	0.61	81 (6%)	22 21	39, 53, 74, 118	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	305	ALA	9.3
2	E	311	ALA	5.9
2	E	306	ASP	5.7
2	E	352	THR	5.4
2	F	370	LYS	4.4
2	E	308	THR	4.3
2	F	216	SER	4.1
2	F	369	GLY	4.1
2	E	304	MET	3.9
2	E	368	ASP	3.5
1	B	42	GLY	3.4
1	C	42	GLY	3.4
2	F	346	ASN	3.3
2	H	235	LYS	3.2
2	H	369	GLY	3.1
1	A	1	GLN	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	G	368	ASP	3.1
2	H	310	VAL	3.1
2	E	310	VAL	3.0
2	H	383	GLU	3.0
1	C	1	GLN	3.0
2	F	310	VAL	3.0
2	E	312	ASP	2.9
1	C	87	PRO	2.9
1	A	26	GLY	2.9
2	F	341	ALA	2.8
2	G	383	GLU	2.8
2	F	252	VAL	2.7
1	A	125	HIS	2.7
2	F	371	VAL	2.7
2	G	372	VAL	2.7
2	G	313	GLU	2.6
2	F	352	THR	2.6
1	C	123	SER	2.6
2	H	216	SER	2.6
1	A	42	GLY	2.6
1	D	1	GLN	2.6
2	E	358	SER	2.6
1	D	42	GLY	2.6
2	F	351	ILE	2.5
2	H	367	LYS	2.5
2	F	347	ALA	2.5
2	F	345	ILE	2.5
2	F	312	ASP	2.5
1	C	52	ASN	2.4
2	F	365	TYR	2.4
2	E	381	SER	2.4
2	F	311	ALA	2.3
2	E	309	VAL	2.3
2	H	312	ASP	2.3
2	E	376	LYS	2.3
2	F	299	ALA	2.3
2	F	342	ALA	2.3
2	G	221	THR	2.2
1	B	124	GLU	2.2
2	F	217	ALA	2.2
2	G	370	LYS	2.2
2	E	357	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	353	LEU	2.2
2	F	297	LEU	2.2
2	E	356	GLY	2.2
2	F	343	GLU	2.2
2	G	247	ALA	2.2
1	C	20	LEU	2.1
2	E	347	ALA	2.1
1	C	2	VAL	2.1
1	B	11	LEU	2.1
1	C	18	LEU	2.1
1	C	13	GLN	2.1
2	G	342	ALA	2.1
1	A	27	PHE	2.1
2	G	312	ASP	2.1
2	G	352	THR	2.0
2	F	338	VAL	2.0
2	G	338	VAL	2.0
2	F	354	ALA	2.0
2	F	373	ALA	2.0
2	H	382	ALA	2.0
2	H	331	SER	2.0
2	G	337	PHE	2.0
2	H	315	THR	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.