



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:30 AM UTC

PDB ID : 4IZL / pdb_00004izl
Title : Structure Of The N248A Mutant of the PANTON-VALENTINE LEUCOCIDIN S Component from STAPHYLOCOCCUS AUREUS
Authors : Maveyraud, L.; Laventie, B.J.; Prevost, G.; Mourey, L.
Deposited on : 2013-01-30
Resolution : 2.80 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 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

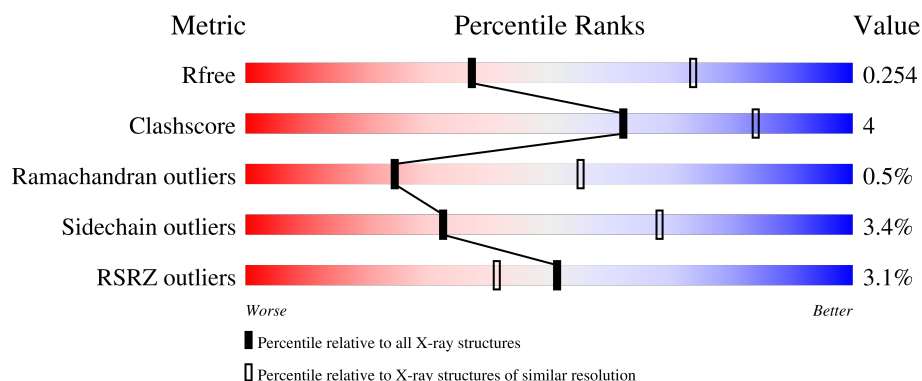
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	292	3% 84% 9% • •
1	B	292	4% 84% 10% • 5%
1	C	292	3% 84% 11% • 5%
1	D	292	% 79% 14% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8815 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 LukS-PV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2210	1394	384	428	4			
1	B	278	Total	C	N	O	S	0	0	0
			2152	1357	370	421	4			
1	C	278	Total	C	N	O	S	0	0	0
			2174	1372	374	424	4			
1	D	277	Total	C	N	O	S	0	0	0
			2183	1373	377	429	4			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP O80066
A	-6	PRO	-	expression tag	UNP O80066
A	-5	LEU	-	expression tag	UNP O80066
A	-4	GLY	-	expression tag	UNP O80066
A	-3	SER	-	expression tag	UNP O80066
A	-2	PRO	-	expression tag	UNP O80066
A	-1	GLU	-	expression tag	UNP O80066
A	0	PHE	-	expression tag	UNP O80066
A	248	ALA	ASN	engineered mutation	UNP O80066
B	-7	GLY	-	expression tag	UNP O80066
B	-6	PRO	-	expression tag	UNP O80066
B	-5	LEU	-	expression tag	UNP O80066
B	-4	GLY	-	expression tag	UNP O80066
B	-3	SER	-	expression tag	UNP O80066
B	-2	PRO	-	expression tag	UNP O80066
B	-1	GLU	-	expression tag	UNP O80066
B	0	PHE	-	expression tag	UNP O80066
B	248	ALA	ASN	engineered mutation	UNP O80066
C	-7	GLY	-	expression tag	UNP O80066
C	-6	PRO	-	expression tag	UNP O80066
C	-5	LEU	-	expression tag	UNP O80066

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLY	-	expression tag	UNP O80066
C	-3	SER	-	expression tag	UNP O80066
C	-2	PRO	-	expression tag	UNP O80066
C	-1	GLU	-	expression tag	UNP O80066
C	0	PHE	-	expression tag	UNP O80066
C	248	ALA	ASN	engineered mutation	UNP O80066
D	-7	GLY	-	expression tag	UNP O80066
D	-6	PRO	-	expression tag	UNP O80066
D	-5	LEU	-	expression tag	UNP O80066
D	-4	GLY	-	expression tag	UNP O80066
D	-3	SER	-	expression tag	UNP O80066
D	-2	PRO	-	expression tag	UNP O80066
D	-1	GLU	-	expression tag	UNP O80066
D	0	PHE	-	expression tag	UNP O80066
D	248	ALA	ASN	engineered mutation	UNP O80066

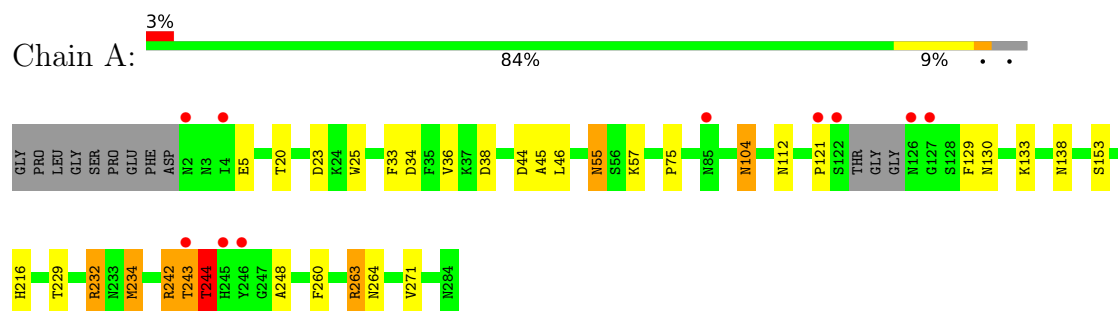
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	24	Total O 24 24	0	0
2	B	12	Total O 12 12	0	0
2	C	25	Total O 25 25	0	0
2	D	35	Total O 35 35	0	0

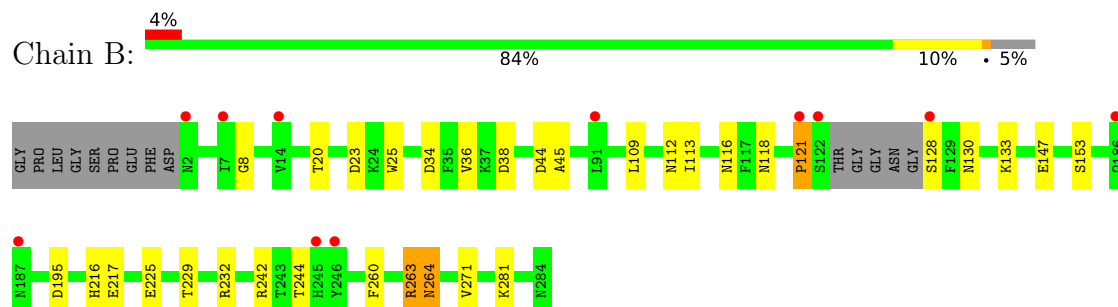
3 Residue-property plots

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 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.

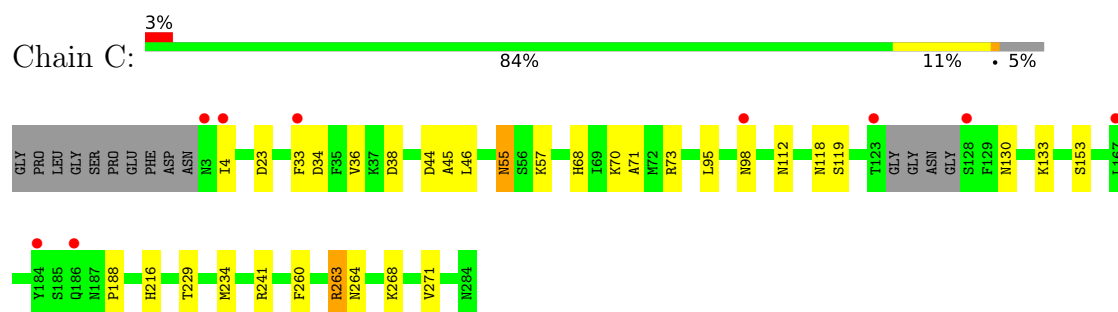
• Molecule 1: LukS-PV



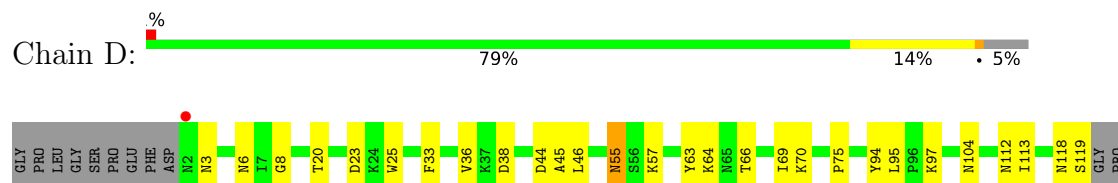
• Molecule 1: LukS-PV

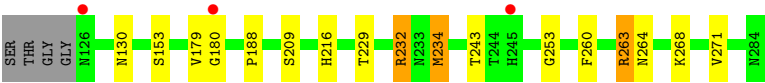


• Molecule 1: LukS-PV



• Molecule 1: LukS-PV





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	93.97Å 93.97Å 309.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.99 – 2.80 46.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.99-2.80) 99.1 (46.99-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.223 , 0.244 0.230 , 0.254	Depositor DCC
R_{free} test set	1772 reflections (3.63%)	wwPDB-VP
Wilson B-factor (Å ²)	53.3	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8815	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.03% 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

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	0.72	1/2266 (0.0%)	1.18	10/3075 (0.3%)
1	B	0.70	0/2207	1.14	8/3001 (0.3%)
1	C	0.68	0/2229	1.14	4/3029 (0.1%)
1	D	0.73	1/2237 (0.0%)	1.15	6/3037 (0.2%)
All	All	0.71	2/8939 (0.0%)	1.15	28/12142 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	234	MET	SD-CE	-9.88	1.54	1.79
1	A	234	MET	SD-CE	-8.65	1.57	1.79

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	ARG	CA-C-N	9.02	137.94	121.70
1	A	242	ARG	C-N-CA	9.02	137.94	121.70
1	D	23	ASP	CA-CB-CG	6.40	119.00	112.60
1	A	129	PHE	CA-CB-CG	6.34	120.14	113.80
1	A	23	ASP	CA-CB-CG	6.18	118.78	112.60
1	B	38	ASP	CA-CB-CG	5.82	118.42	112.60
1	D	38	ASP	CA-CB-CG	5.76	118.36	112.60
1	C	263	ARG	N-CA-C	-5.73	101.02	109.62
1	A	263	ARG	N-CA-C	-5.73	101.03	109.62
1	A	244	THR	N-CA-C	5.70	118.34	110.35
1	A	38	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	244	THR	CA-C-N	5.60	128.10	120.54
1	A	244	THR	C-N-CA	5.60	128.10	120.54
1	D	180	GLY	CA-C-N	5.59	131.75	121.70
1	D	180	GLY	C-N-CA	5.59	131.75	121.70
1	D	263	ARG	N-CA-C	-5.59	101.24	109.62
1	C	38	ASP	CA-CB-CG	5.56	118.16	112.60
1	B	195	ASP	CA-C-N	5.49	128.19	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	195	ASP	C-N-CA	5.49	128.19	120.28
1	A	153	SER	N-CA-C	5.46	117.14	108.79
1	B	264	ASN	CA-CB-CG	5.41	118.01	112.60
1	B	121	PRO	CA-C-N	5.41	131.44	121.70
1	B	121	PRO	C-N-CA	5.41	131.44	121.70
1	B	263	ARG	N-CA-C	-5.41	101.50	109.62
1	D	153	SER	N-CA-C	5.38	117.03	108.79
1	B	153	SER	N-CA-C	5.35	116.98	108.79
1	C	153	SER	N-CA-C	5.13	116.64	108.79
1	C	71	ALA	N-CA-C	5.09	117.41	109.52

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	2210	0	2056	20	0
1	B	2152	0	1947	11	0
1	C	2174	0	2001	14	0
1	D	2183	0	2017	24	0
2	A	24	0	0	0	0
2	B	12	0	0	0	0
2	C	25	0	0	1	0
2	D	35	0	0	0	0
All	All	8815	0	8021	68	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 (68) 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:D:232:ARG:HG3	1:D:234:MET:HE3	1.66	0.78
1:C:95:LEU:HD21	1:C:119:SER:HB2	1.68	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:PRO:HB3	1:D:234:MET:HE1	1.74	0.69
1:A:75:PRO:HB3	1:A:234:MET:HE1	1.74	0.69
1:A:25:TRP:O	1:A:232:ARG:NH2	2.26	0.69
1:C:55:ASN:HD22	1:C:57:LYS:H	1.43	0.66
1:D:66:THR:HG22	1:D:69:ILE:H	1.59	0.66
1:A:55:ASN:HD22	1:A:57:LYS:H	1.42	0.66
1:D:55:ASN:HD22	1:D:57:LYS:H	1.42	0.65
1:A:232:ARG:HG3	1:A:234:MET:HE3	1.79	0.63
1:A:104:ASN:OD1	1:A:138:ASN:ND2	2.36	0.59
1:C:73:ARG:HG2	1:C:234:MET:HE3	1.84	0.58
1:D:25:TRP:O	1:D:232:ARG:NH2	2.37	0.57
1:C:57:LYS:NZ	2:C:322:HOH:O	2.38	0.56
1:B:25:TRP:O	1:B:232:ARG:NH2	2.38	0.55
1:A:75:PRO:HA	1:A:234:MET:HE2	1.88	0.54
1:A:112:ASN:HA	1:A:130:ASN:HD22	1.72	0.54
1:C:68:HIS:HB2	1:C:241:ARG:HB3	1.90	0.53
1:D:75:PRO:HA	1:D:234:MET:HE2	1.90	0.53
1:B:260:PHE:HB3	1:B:263:ARG:HD3	1.90	0.53
1:C:234:MET:HB2	1:C:260:PHE:HB2	1.92	0.52
1:C:70:LYS:HD3	1:C:188:PRO:HA	1.91	0.52
1:B:112:ASN:HA	1:B:130:ASN:HD22	1.75	0.51
1:D:33:PHE:HB3	1:D:46:LEU:HD11	1.93	0.51
1:C:260:PHE:HB3	1:C:263:ARG:HD3	1.93	0.51
1:D:112:ASN:HA	1:D:130:ASN:HD22	1.76	0.50
1:B:229:THR:HG23	1:B:264:ASN:HB3	1.94	0.50
1:A:75:PRO:HA	1:A:234:MET:CE	2.43	0.49
1:A:234:MET:HB2	1:A:260:PHE:HB2	1.94	0.49
1:D:234:MET:HB2	1:D:260:PHE:HB2	1.93	0.49
1:D:232:ARG:CG	1:D:234:MET:HE3	2.41	0.48
1:D:94:TYR:H	1:D:97:LYS:HE2	1.78	0.48
1:A:75:PRO:CB	1:A:234:MET:HE1	2.42	0.48
1:D:75:PRO:HA	1:D:234:MET:CE	2.44	0.48
1:D:95:LEU:HD21	1:D:119:SER:HB2	1.97	0.47
1:D:75:PRO:CB	1:D:234:MET:HE1	2.43	0.47
1:A:242:ARG:HA	1:A:243:THR:CB	2.44	0.47
1:A:232:ARG:CG	1:A:234:MET:HE3	2.45	0.47
1:A:244:THR:HG22	1:A:248:ALA:O	2.15	0.47
1:A:234:MET:HE2	1:A:234:MET:HA	1.97	0.46
1:D:229:THR:HG23	1:D:264:ASN:HB3	1.98	0.46
1:A:260:PHE:HB3	1:A:263:ARG:HD3	1.97	0.46
1:D:260:PHE:HB3	1:D:263:ARG:HD3	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:ASN:HA	1:C:130:ASN:HD22	1.80	0.46
1:B:225:GLU:OE1	1:B:281:LYS:HD3	2.16	0.45
1:B:112:ASN:HB2	1:B:116:ASN:HB2	1.99	0.45
1:D:234:MET:HE2	1:D:234:MET:HA	1.98	0.45
1:C:229:THR:HG23	1:C:264:ASN:HB3	1.99	0.45
1:C:33:PHE:HB3	1:C:46:LEU:HD11	1.99	0.44
1:D:179:VAL:HG21	1:D:253:GLY:HA3	2.00	0.43
1:D:8:GLY:HA3	1:D:113:ILE:HD11	2.01	0.43
1:A:229:THR:HG23	1:A:264:ASN:HB3	2.00	0.43
1:B:8:GLY:HA3	1:B:113:ILE:HD11	1.99	0.43
1:C:44:ASP:HB2	1:C:216:HIS:HB3	2.01	0.43
1:D:44:ASP:HB2	1:D:216:HIS:HB3	2.00	0.43
1:A:44:ASP:HB2	1:A:216:HIS:HB3	2.01	0.43
1:B:118:ASN:HB3	1:D:104:ASN:HB3	2.00	0.43
1:C:36:VAL:HB	1:C:45:ALA:HB3	2.00	0.43
1:D:63:TYR:O	1:D:66:THR:HB	2.19	0.42
1:B:44:ASP:HB2	1:B:216:HIS:HB3	2.00	0.42
1:A:34:ASP:OD2	1:A:133:LYS:HE2	2.20	0.42
1:C:34:ASP:OD2	1:C:133:LYS:HE2	2.19	0.42
1:B:36:VAL:HB	1:B:45:ALA:HB3	2.01	0.42
1:D:70:LYS:HD3	1:D:188:PRO:HA	2.00	0.42
1:A:36:VAL:HB	1:A:45:ALA:HB3	2.01	0.42
1:B:34:ASP:OD2	1:B:133:LYS:HE2	2.21	0.41
1:D:36:VAL:HB	1:D:45:ALA:HB3	2.02	0.41
1:A:33:PHE:HB3	1:A:46:LEU:HD11	2.03	0.41

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	276/292 (94%)	264 (96%)	10 (4%)	2 (1%)	18 47

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	274/292 (94%)	260 (95%)	12 (4%)	2 (1%)	18	47
1	C	274/292 (94%)	261 (95%)	12 (4%)	1 (0%)	30	60
1	D	273/292 (94%)	260 (95%)	12 (4%)	1 (0%)	30	60
All	All	1097/1168 (94%)	1045 (95%)	46 (4%)	6 (0%)	24	55

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	244	THR
1	A	121	PRO
1	A	243	THR
1	D	64	LYS
1	C	98	ASN
1	B	121	PRO

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	236/259 (91%)	229 (97%)	7 (3%)	36	72
1	B	223/259 (86%)	215 (96%)	8 (4%)	31	66
1	C	230/259 (89%)	224 (97%)	6 (3%)	40	75
1	D	234/259 (90%)	224 (96%)	10 (4%)	26	60
All	All	923/1036 (89%)	892 (97%)	31 (3%)	32	68

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	20	THR
1	A	55	ASN
1	A	104	ASN
1	A	232	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	244	THR
1	A	271	VAL
1	B	20	THR
1	B	23	ASP
1	B	109	LEU
1	B	128	SER
1	B	147	GLU
1	B	217	GLU
1	B	242	ARG
1	B	271	VAL
1	C	4	ILE
1	C	23	ASP
1	C	55	ASN
1	C	118	ASN
1	C	268	LYS
1	C	271	VAL
1	D	3	ASN
1	D	6	ASN
1	D	20	THR
1	D	55	ASN
1	D	118	ASN
1	D	209	SER
1	D	232	ARG
1	D	243	THR
1	D	268	LYS
1	D	271	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	6	ASN
1	A	30	ASN
1	A	42	ASN
1	A	55	ASN
1	A	77	GLN
1	A	104	ASN
1	A	116	ASN
1	A	118	ASN
1	A	130	ASN
1	A	138	ASN
1	A	140	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	176	ASN
1	A	238	HIS
1	A	276	HIS
1	B	6	ASN
1	B	30	ASN
1	B	42	ASN
1	B	79	ASN
1	B	130	ASN
1	B	138	ASN
1	B	140	GLN
1	B	176	ASN
1	B	238	HIS
1	B	276	HIS
1	C	6	ASN
1	C	55	ASN
1	C	79	ASN
1	C	112	ASN
1	C	130	ASN
1	C	138	ASN
1	C	140	GLN
1	C	196	ASN
1	C	238	HIS
1	C	276	HIS
1	D	6	ASN
1	D	30	ASN
1	D	32	GLN
1	D	55	ASN
1	D	79	ASN
1	D	104	ASN
1	D	130	ASN
1	D	138	ASN
1	D	140	GLN
1	D	176	ASN
1	D	186	GLN
1	D	196	ASN
1	D	238	HIS

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](#)

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	280/292 (95%)	0.17	10 (3%) 46 37	33, 49, 77, 96	0
1	B	278/292 (95%)	0.38	11 (3%) 42 33	34, 61, 91, 105	0
1	C	278/292 (95%)	0.25	9 (3%) 50 40	37, 58, 85, 112	0
1	D	277/292 (94%)	0.14	4 (1%) 73 64	36, 49, 74, 88	0
All	All	1113/1168 (95%)	0.23	34 (3%) 51 41	33, 55, 84, 112	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	122	SER	6.3
1	A	126	ASN	5.8
1	C	123	THR	4.7
1	B	246	TYR	3.9
1	C	3	ASN	3.7
1	B	122	SER	3.5
1	A	246	TYR	3.4
1	D	126	ASN	3.4
1	A	85	ASN	3.2
1	B	2	ASN	3.0
1	A	245	HIS	3.0
1	B	245	HIS	2.9
1	A	121	PRO	2.9
1	C	128	SER	2.9
1	D	2	ASN	2.8
1	C	98	ASN	2.8
1	A	2	ASN	2.7
1	D	180	GLY	2.6
1	B	128	SER	2.6
1	A	127	GLY	2.6
1	C	167	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	121	PRO	2.4
1	C	184	TYR	2.3
1	A	243	THR	2.3
1	B	7	ILE	2.3
1	C	186	GLN	2.3
1	B	91	LEU	2.2
1	D	245	HIS	2.2
1	B	186	GLN	2.1
1	B	187	ASN	2.0
1	A	4	ILE	2.0
1	C	33	PHE	2.0
1	C	4	ILE	2.0
1	B	14	VAL	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.