



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 11:01 am BST

PDB ID : 4IZL
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtrriage (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

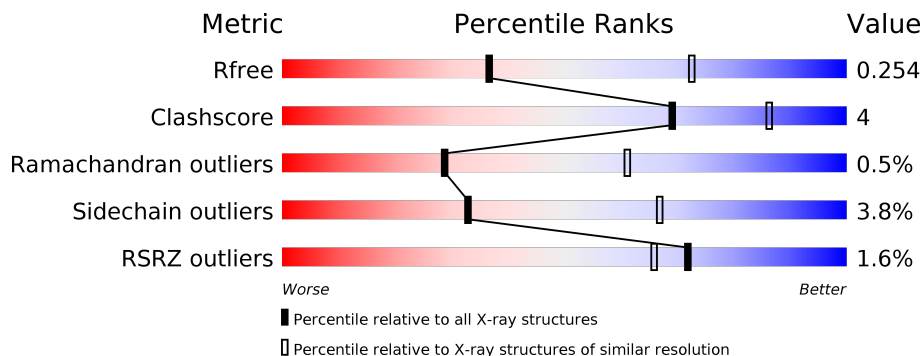
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 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	292	 0% 86% 8% • •
1	B	292	 2% 85% 10% • 5%
1	C	292	 3% 85% 10% • 5%
1	D	292	 0% 81% 13% • 5%

2 Entry composition [i](#)

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

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

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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

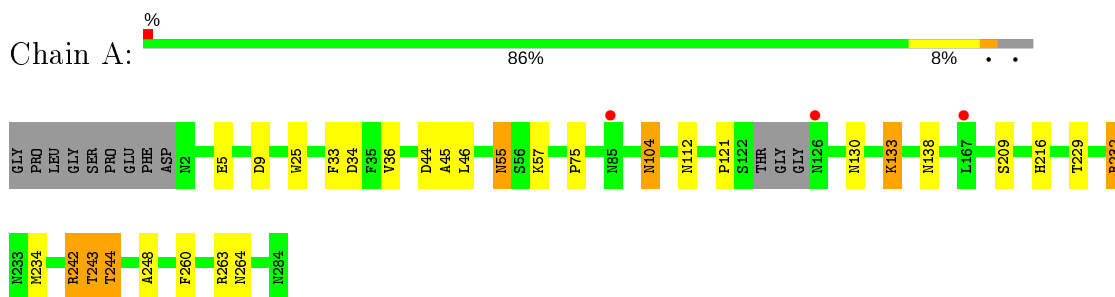
- Molecule 2 is water.

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

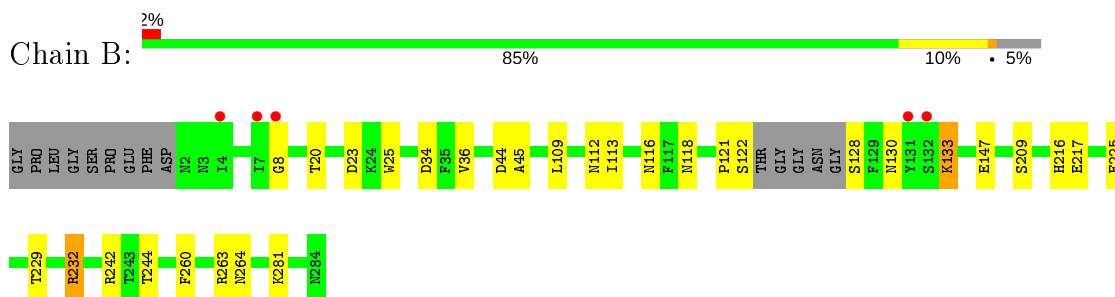
3 Residue-property plots [i](#)

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.

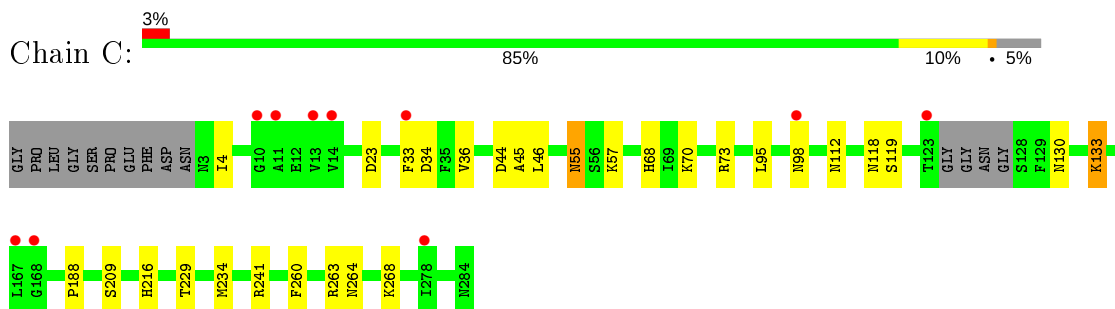
- Molecule 1: LukS-PV



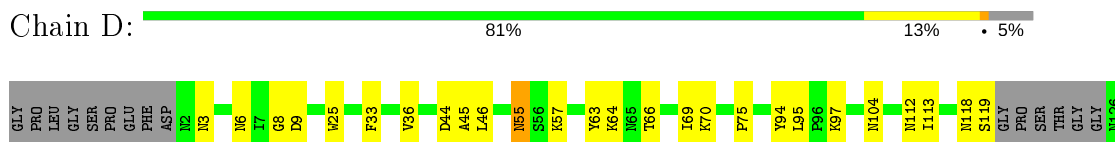
- Molecule 1: LukS-PV

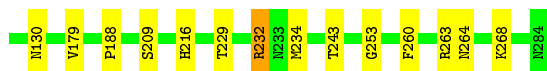


- Molecule 1: LukS-PV



- 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 46.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.99-2.80) 99.1 (46.98-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.81Å)	Xtrriage
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 (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	53.3	Xtrriage
Anisotropy	0.344	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 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	0.40	0/2266	0.68	1/3075 (0.0%)
1	B	0.39	0/2207	0.65	0/3001
1	C	0.38	0/2229	0.66	0/3029
1	D	0.41	0/2237	0.66	0/3037
All	All	0.40	0/8939	0.66	1/12142 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	ARG	C-N-CA	6.50	137.94	121.70

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	2210	0	2056	16	0
1	B	2152	0	1947	11	0
1	C	2174	0	2001	14	0
1	D	2183	0	2017	22	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8815	0	8021	62	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 (62) 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:75:PRO:HA	1:D:234:MET:HE2	1.59	0.85
1:A:75:PRO:HA	1:A:234:MET:HE2	1.57	0.84
1:C:95:LEU:HD21	1:C:119:SER:HB2	1.68	0.76
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:104:ASN:OD1	1:A:138:ASN:ND2	2.36	0.59
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:D:75:PRO:HB3	1:D:234:MET:HE1	1.89	0.55
1:A:112:ASN:HA	1:A:130:ASN:HD22	1.72	0.54
1:A:75:PRO:HB3	1:A:234:MET:HE1	1.89	0.54
1:C:68:HIS:HB2	1:C:241:ARG:HB3	1.90	0.53
1:A:75:PRO:CA	1:A:234:MET:HE2	2.36	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:232:ARG:HG3	1:D:234:MET:HE3	1.92	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: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:94:TYR:H	1:D:97:LYS:HE2	1.78	0.48
1:D:95:LEU:HD21	1:D:119:SER:HB2	1.97	0.47
1:A:242:ARG:HA	1:A:243:THR:CB	2.44	0.47
1:D:75:PRO:CA	1:D:234:MET:HE2	2.37	0.47
1:A:244:THR:HG22	1:A:248:ALA:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:232:ARG:HD2	1:D:234:MET:HE1	1.97	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
1:C:73:ARG:HG2	1:C:234:MET:CE	2.51	0.40

There are no symmetry-related clashes.

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	276/292 (94%)	264 (96%)	10 (4%)	2 (1%)	22	53
1	B	274/292 (94%)	260 (95%)	12 (4%)	2 (1%)	22	53
1	C	274/292 (94%)	261 (95%)	12 (4%)	1 (0%)	34	66
1	D	273/292 (94%)	260 (95%)	12 (4%)	1 (0%)	34	66
All	All	1097/1168 (94%)	1045 (95%)	46 (4%)	6 (0%)	29	61

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 [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	236/259 (91%)	228 (97%)	8 (3%)	37	71
1	B	223/259 (86%)	212 (95%)	11 (5%)	25	57
1	C	230/259 (89%)	223 (97%)	7 (3%)	41	75
1	D	234/259 (90%)	225 (96%)	9 (4%)	33	67
All	All	923/1036 (89%)	888 (96%)	35 (4%)	33	67

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	9	ASP
1	A	55	ASN
1	A	104	ASN
1	A	133	LYS

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Mol	Chain	Res	Type
1	A	209	SER
1	A	232	ARG
1	A	244	THR
1	B	20	THR
1	B	23	ASP
1	B	109	LEU
1	B	122	SER
1	B	128	SER
1	B	133	LYS
1	B	147	GLU
1	B	209	SER
1	B	217	GLU
1	B	232	ARG
1	B	242	ARG
1	C	4	ILE
1	C	23	ASP
1	C	55	ASN
1	C	118	ASN
1	C	133	LYS
1	C	209	SER
1	C	268	LYS
1	D	3	ASN
1	D	6	ASN
1	D	9	ASP
1	D	55	ASN
1	D	118	ASN
1	D	209	SER
1	D	232	ARG
1	D	243	THR
1	D	268	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	42	ASN
1	A	55	ASN
1	A	79	ASN
1	A	104	ASN
1	A	130	ASN
1	A	138	ASN
1	A	176	ASN

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Mol	Chain	Res	Type
1	A	276	HIS
1	B	42	ASN
1	B	79	ASN
1	B	118	ASN
1	B	130	ASN
1	B	176	ASN
1	B	238	HIS
1	B	276	HIS
1	C	55	ASN
1	C	79	ASN
1	C	112	ASN
1	C	130	ASN
1	C	176	ASN
1	C	238	HIS
1	C	276	HIS
1	D	30	ASN
1	D	55	ASN
1	D	79	ASN
1	D	130	ASN
1	D	176	ASN
1	D	186	GLN
1	D	276	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	280/292 (95%)	-0.12	3 (1%) 80 75	33, 49, 77, 96	0
1	B	278/292 (95%)	0.10	5 (1%) 68 61	34, 61, 91, 105	0
1	C	278/292 (95%)	0.07	10 (3%) 42 32	37, 58, 85, 112	0
1	D	277/292 (94%)	-0.19	0 100 100	36, 49, 74, 88	0
All	All	1113/1168 (95%)	-0.04	18 (1%) 72 66	33, 55, 84, 112	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	167	LEU	5.1
1	B	4	ILE	3.2
1	C	278	ILE	3.2
1	C	10	GLY	3.2
1	A	126	ASN	3.2
1	B	7	ILE	3.1
1	A	167	LEU	2.7
1	C	11	ALA	2.6
1	C	33	PHE	2.6
1	B	8	GLY	2.4
1	C	123	THR	2.3
1	B	132	SER	2.3
1	C	13	VAL	2.3
1	C	14	VAL	2.3
1	B	131	TYR	2.3
1	A	85	ASN	2.2
1	C	98	ASN	2.2
1	C	168	GLY	2.2

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.