



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 12:30 AM EDT

PDB ID : 2QK7
Title : A covalent S-F heterodimer of staphylococcal gamma-hemolysin
Authors : Roblin, P.; Guillet, V.; Maveyraud, L.; Mourey, L.
Deposited on : 2007-07-10
Resolution : 2.40 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	:	2.23.2
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)	:	2.23.2

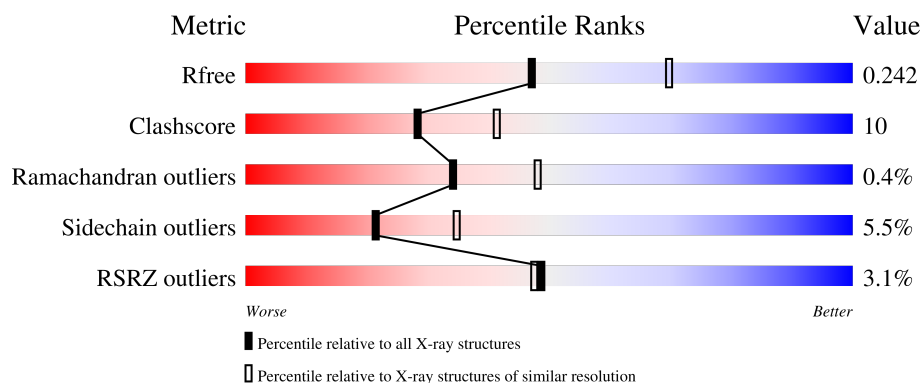
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	288	<div> <div>5%</div> <div> <div></div> <div>70%</div> <div>17%</div> <div>•</div> <div>10%</div> </div> </div>
2	B	307	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>•</div> <div>7%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4476 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 Gamma-hemolysin component A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			1999	1274	331	390	4			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP P0A074
A	-6	PRO	-	expression tag	UNP P0A074
A	-5	LEU	-	expression tag	UNP P0A074
A	-4	GLY	-	expression tag	UNP P0A074
A	-3	SER	-	expression tag	UNP P0A074
A	-2	PRO	-	expression tag	UNP P0A074
A	-1	GLU	-	expression tag	UNP P0A074
A	0	PHE	-	expression tag	UNP P0A074
A	28	CYS	THR	engineered mutation	UNP P0A074
A	217	LYS	ARG	SEE REMARK 999	UNP P0A074

- Molecule 2 is a protein called Gamma-hemolysin component B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	287	Total	C	N	O	S	0	0	0
			2304	1463	390	447	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	GLY	-	expression tag	UNP P0A077
B	-6	PRO	-	expression tag	UNP P0A077
B	-5	LEU	-	expression tag	UNP P0A077
B	-4	GLY	-	expression tag	UNP P0A077
B	-3	SER	-	expression tag	UNP P0A077
B	-2	PRO	-	expression tag	UNP P0A077

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLU	-	expression tag	UNP P0A077
B	0	PHE	-	expression tag	UNP P0A077
B	56	ALA	THR	SEE REMARK 999	UNP P0A077
B	63	TYR	PHE	SEE REMARK 999	UNP P0A077
B	64	GLU	VAL	SEE REMARK 999	UNP P0A077
B	156	CYS	ASN	engineered mutation	UNP P0A077

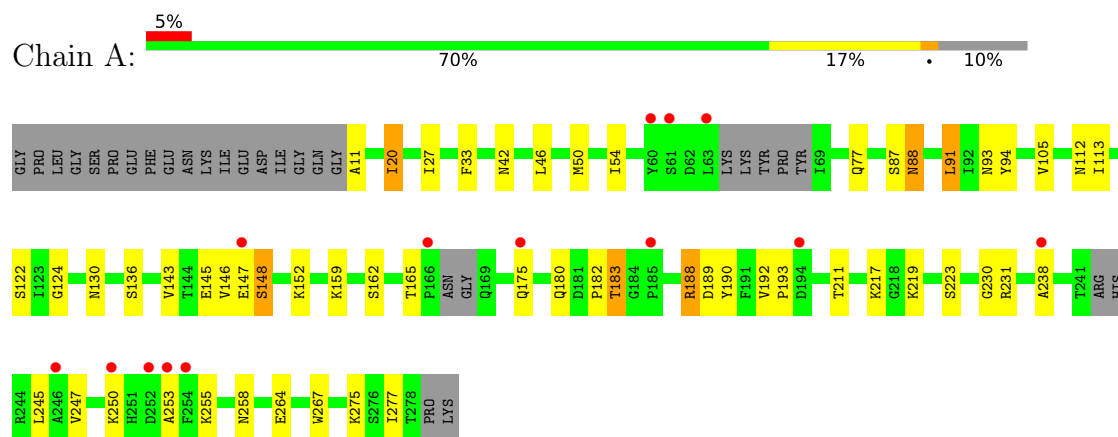
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	49	Total O 49 49	0	0
3	B	124	Total O 124 124	0	0

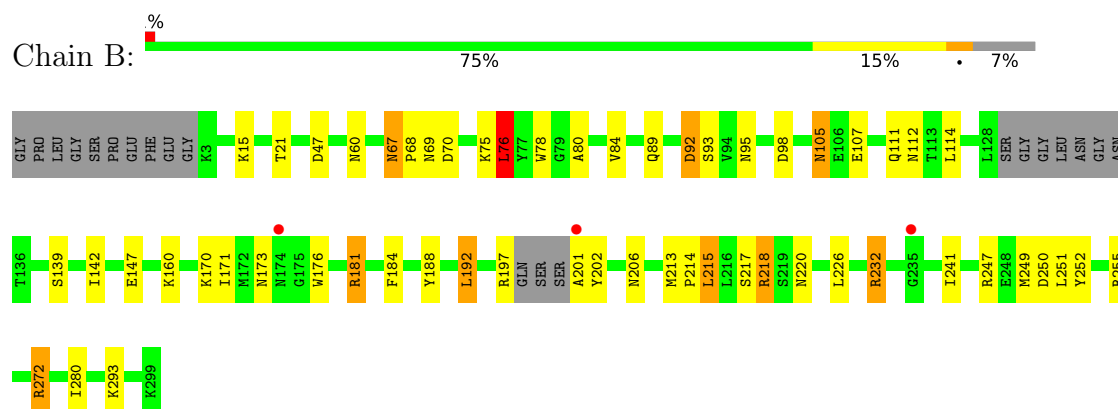
3 Residue-property plots [i](#)

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: Gamma-hemolysin component A



• Molecule 2: Gamma-hemolysin component B



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	140.00Å 140.00Å 73.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.40 50.55 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.40) 100.0 (50.55-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.16 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.180 , 0.239 0.185 , 0.242	Depositor DCC
R_{free} test set	1625 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.034 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4476	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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	1.02	0/2041	0.96	3/2769 (0.1%)
2	B	1.23	3/2359 (0.1%)	1.14	14/3193 (0.4%)
All	All	1.14	3/4400 (0.1%)	1.06	17/5962 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	ALA	CA-CB	7.50	1.68	1.52
2	B	184	PHE	CE2-CZ	5.84	1.48	1.37
2	B	84	VAL	CB-CG1	5.38	1.64	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	272	ARG	NE-CZ-NH2	-19.24	110.68	120.30
2	B	181	ARG	NE-CZ-NH2	-11.65	114.47	120.30
2	B	272	ARG	NE-CZ-NH1	11.34	125.97	120.30
2	B	181	ARG	NE-CZ-NH1	9.73	125.16	120.30
2	B	76	LEU	CB-CG-CD1	8.38	125.24	111.00
2	B	272	ARG	CD-NE-CZ	7.87	134.62	123.60
2	B	272	ARG	CG-CD-NE	-7.72	95.59	111.80
2	B	215	LEU	CA-CB-CG	7.14	131.72	115.30
1	A	188	ARG	NE-CZ-NH1	6.86	123.73	120.30
2	B	192	LEU	CA-CB-CG	5.91	128.90	115.30
2	B	170	LYS	CD-CE-NZ	-5.69	98.62	111.70
2	B	218	ARG	NE-CZ-NH1	-5.69	117.46	120.30
2	B	215	LEU	CB-CG-CD1	5.61	120.54	111.00
2	B	215	LEU	CB-CG-CD2	-5.36	101.89	111.00
2	B	92	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	231	ARG	CG-CD-NE	-5.08	101.13	111.80
1	A	91	LEU	CA-CB-CG	5.03	126.87	115.30

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	1999	0	1871	35	0
2	B	2304	0	2183	47	0
3	A	49	0	0	0	0
3	B	124	0	0	3	0
All	All	4476	0	4054	82	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 10.

All (82) 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:B:76:LEU:HD23	2:B:76:LEU:O	1.76	0.85
2:B:80:ALA:HB1	2:B:181:ARG:HD3	1.56	0.84
2:B:76:LEU:CD2	2:B:252:TYR:HB3	2.06	0.84
2:B:76:LEU:HD23	2:B:76:LEU:C	1.98	0.83
1:A:113:ILE:H	1:A:130:ASN:HD22	1.33	0.76
2:B:60:ASN:HA	2:B:220:ASN:HD22	1.50	0.75
2:B:76:LEU:HD21	2:B:252:TYR:HB3	1.68	0.73
2:B:75:LYS:HD2	2:B:251:LEU:HD11	1.70	0.72
1:A:33:PHE:HB3	1:A:46:LEU:HD11	1.71	0.72
2:B:147:GLU:HG2	3:B:329:HOH:O	1.90	0.72
1:A:230:GLY:HA3	1:A:258:ASN:HD22	1.54	0.71
1:A:88:ASN:ND2	1:A:219:LYS:O	2.23	0.69
1:A:183:THR:HG22	1:A:189:ASP:HB3	1.75	0.69
1:A:113:ILE:H	1:A:130:ASN:ND2	1.91	0.69
1:A:42:ASN:O	1:A:217:LYS:HG3	1.94	0.68
1:A:188:ARG:HH21	1:A:193:PRO:HA	1.59	0.67
1:A:77:GLN:HE21	1:A:159:LYS:HG2	1.58	0.67
2:B:70:ASP:O	2:B:202:TYR:HB3	1.98	0.64
2:B:181:ARG:HD2	2:B:250:ASP:OD1	1.97	0.63
1:A:112:ASN:HA	1:A:130:ASN:HD22	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:MET:HE1	2:B:272:ARG:HG2	1.82	0.61
1:A:188:ARG:NH2	1:A:193:PRO:HA	2.16	0.61
1:A:146:VAL:O	1:A:148:SER:N	2.35	0.59
1:A:230:GLY:HA3	1:A:258:ASN:ND2	2.17	0.58
2:B:60:ASN:HA	2:B:220:ASN:ND2	2.17	0.58
2:B:105:ASN:HD22	2:B:105:ASN:C	2.07	0.58
2:B:249:MET:CE	2:B:272:ARG:HG2	2.33	0.58
2:B:171:ILE:HD13	2:B:214:PRO:HG2	1.86	0.57
1:A:77:GLN:HE21	1:A:159:LYS:CG	2.17	0.57
2:B:105:ASN:ND2	2:B:107:GLU:H	2.04	0.56
2:B:67:ASN:HD22	2:B:68:PRO:CD	2.18	0.56
2:B:67:ASN:HD22	2:B:68:PRO:N	2.04	0.55
1:A:11:ALA:HB2	1:A:113:ILE:HD12	1.87	0.55
1:A:188:ARG:NH2	1:A:192:VAL:O	2.40	0.54
2:B:241:ILE:HG12	2:B:280:ILE:HD11	1.90	0.54
2:B:67:ASN:ND2	2:B:69:ASN:H	2.07	0.53
1:A:113:ILE:N	1:A:130:ASN:HD22	2.04	0.53
2:B:93:SER:HB2	2:B:232:ARG:HG3	1.91	0.53
1:A:264:GLU:HB2	1:A:275:LYS:HD2	1.91	0.52
2:B:67:ASN:ND2	2:B:68:PRO:HD2	2.26	0.51
2:B:80:ALA:CB	2:B:181:ARG:HD3	2.34	0.51
1:A:219:LYS:O	1:A:219:LYS:HG2	2.11	0.51
2:B:249:MET:HE1	2:B:272:ARG:CG	2.40	0.51
2:B:67:ASN:HD22	2:B:68:PRO:HD2	1.76	0.50
2:B:78:TRP:HE3	2:B:217:SER:HB3	1.77	0.50
2:B:89:GLN:HB2	2:B:92:ASP:OD1	2.12	0.50
2:B:173:ASN:O	2:B:176:TRP:HB2	2.12	0.50
2:B:249:MET:CE	2:B:272:ARG:CG	2.89	0.50
2:B:67:ASN:HD22	2:B:67:ASN:C	2.15	0.50
1:A:105:VAL:O	1:A:136:SER:HA	2.12	0.50
1:A:94:TYR:CE1	1:A:146:VAL:HG11	2.47	0.49
1:A:182:PRO:HG3	1:A:190:TYR:CD2	2.48	0.49
2:B:142:ILE:CG2	2:B:226:LEU:HG	2.44	0.48
1:A:27:ILE:HG12	1:A:54:ILE:HG23	1.96	0.48
1:A:250:LYS:HD3	1:A:253:ALA:HA	1.96	0.48
1:A:112:ASN:HA	1:A:130:ASN:ND2	2.28	0.47
2:B:293:LYS:NZ	3:B:417:HOH:O	2.41	0.47
2:B:95:ASN:ND2	2:B:160:LYS:HE2	2.29	0.47
2:B:67:ASN:HD22	2:B:69:ASN:H	1.63	0.47
2:B:202:TYR:N	2:B:202:TYR:CD2	2.83	0.47
2:B:213:MET:HB2	2:B:218:ARG:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:ASP:OD2	2:B:47:ASP:N	2.48	0.46
2:B:111:GLN:C	2:B:112:ASN:HD22	2.19	0.46
2:B:142:ILE:HG23	2:B:226:LEU:HG	1.97	0.46
2:B:188:TYR:CE2	2:B:197:ARG:HB3	2.51	0.45
1:A:122:SER:OG	1:A:124:GLY:O	2.32	0.45
2:B:114:LEU:C	2:B:114:LEU:HD23	2.36	0.45
1:A:183:THR:HG22	1:A:189:ASP:CB	2.46	0.45
1:A:11:ALA:HB2	1:A:113:ILE:CD1	2.47	0.44
1:A:11:ALA:CB	1:A:113:ILE:CD1	2.95	0.44
2:B:105:ASN:HD21	2:B:107:GLU:HB2	1.81	0.44
2:B:181:ARG:CD	2:B:250:ASP:OD1	2.63	0.44
1:A:20:ILE:HD11	1:A:277:ILE:CG1	2.49	0.43
1:A:223:SER:HB2	1:A:267:TRP:HE1	1.84	0.43
1:A:238:ALA:HB1	1:A:245:LEU:HD11	2.00	0.42
1:A:94:TYR:HE1	1:A:146:VAL:HG11	1.85	0.42
2:B:78:TRP:CE3	2:B:217:SER:HB3	2.54	0.41
2:B:220:ASN:HB2	3:B:377:HOH:O	2.19	0.41
1:A:175:GLN:NE2	1:A:247:VAL:O	2.48	0.41
2:B:60:ASN:O	2:B:247:ARG:HD3	2.21	0.41
2:B:89:GLN:O	2:B:160:LYS:HD2	2.22	0.40
1:A:50:MET:CE	1:A:211:THR:HG23	2.51	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	251/288 (87%)	235 (94%)	14 (6%)	2 (1%)	19	29
2	B	281/307 (92%)	262 (93%)	19 (7%)	0	100	100
All	All	532/595 (89%)	497 (93%)	33 (6%)	2 (0%)	34	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	GLU
1	A	148	SER

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	206/255 (81%)	193 (94%)	13 (6%)	18	28
2	B	246/268 (92%)	234 (95%)	12 (5%)	25	40
All	All	452/523 (86%)	427 (94%)	25 (6%)	21	35

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ILE
1	A	87	SER
1	A	88	ASN
1	A	91	LEU
1	A	93	ASN
1	A	143	VAL
1	A	145	GLU
1	A	152	LYS
1	A	162	SER
1	A	165	THR
1	A	180	GLN
1	A	183	THR
1	A	255	LYS
2	B	15	LYS
2	B	21	THR
2	B	67	ASN
2	B	76	LEU
2	B	98	ASP
2	B	105	ASN
2	B	139	SER
2	B	192	LEU

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Mol	Chain	Res	Type
2	B	206	ASN
2	B	215	LEU
2	B	232	ARG
2	B	255	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	32	GLN
1	A	77	GLN
1	A	79	ASN
1	A	88	ASN
1	A	93	ASN
1	A	130	ASN
1	A	169	GLN
1	A	180	GLN
1	A	206	ASN
1	A	258	ASN
2	B	34	GLN
2	B	67	ASN
2	B	69	ASN
2	B	95	ASN
2	B	103	ASN
2	B	104	GLN
2	B	105	ASN
2	B	158	ASN
2	B	220	ASN
2	B	233	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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	259/288 (89%)	0.28	14 (5%) 25 24	34, 54, 71, 79	0
2	B	287/307 (93%)	-0.20	3 (1%) 82 80	29, 40, 56, 68	0
All	All	546/595 (91%)	0.03	17 (3%) 49 47	29, 45, 69, 79	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	235	GLY	4.6
1	A	254	PHE	4.0
1	A	253	ALA	3.8
1	A	63	LEU	3.7
1	A	175	GLN	3.0
1	A	238	ALA	3.0
1	A	147	GLU	2.9
1	A	246	ALA	2.8
1	A	185	PRO	2.7
1	A	60	TYR	2.5
1	A	166	PRO	2.5
1	A	250	LYS	2.3
1	A	194	ASP	2.2
1	A	252	ASP	2.2
1	A	61	SER	2.1
2	B	201	ALA	2.0
2	B	174	ASN	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.