



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:03 AM GMT

PDB ID : 2PV3
Title : Crystallographic Structure of SurA fragment lacking the second peptidyl-prolyl isomerase domain complexed with peptide NFTLKFWDFIRK
Authors : Xu, X.; McKay, D.B.
Deposited on : 2007-05-09
Resolution : 3.39 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

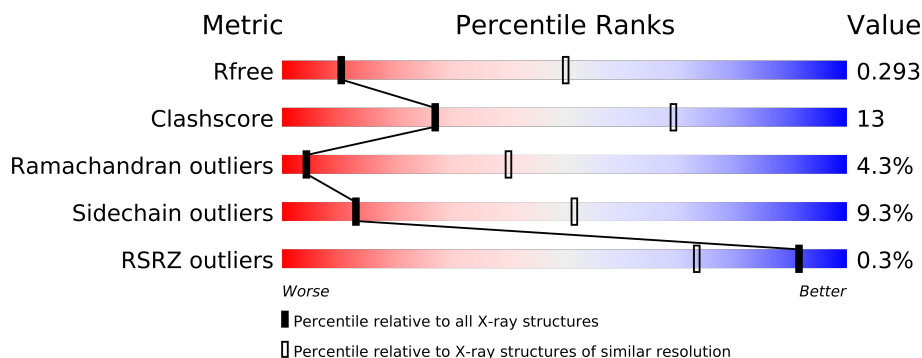
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.39 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}	66092	1017 (3.52-3.28)
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)
RSRZ outliers	66119	1017 (3.52-3.28)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	299	
1	B	299	
2	C	12	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4529 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Chaperone surA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2217	1364	412	429	12			
1	B	284	Total	C	N	O	S	0	0	0
			2217	1364	412	429	12			

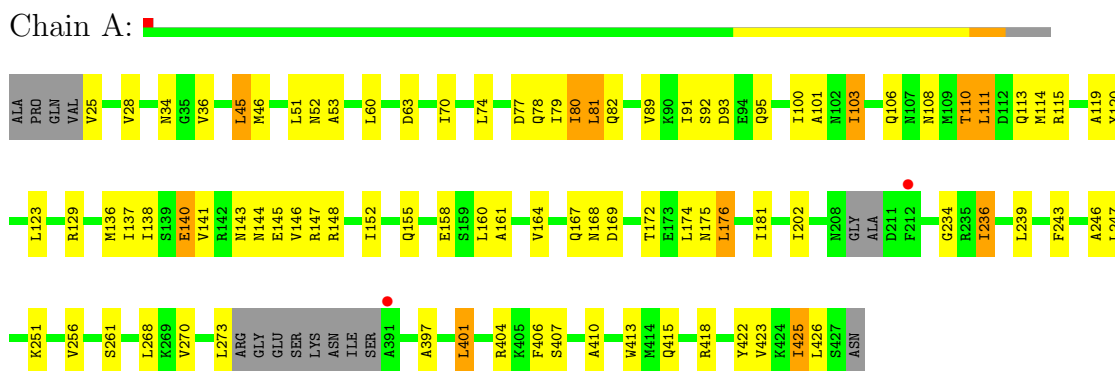
- Molecule 2 is a protein called C-peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	0	0	0
			95	68	13	14			

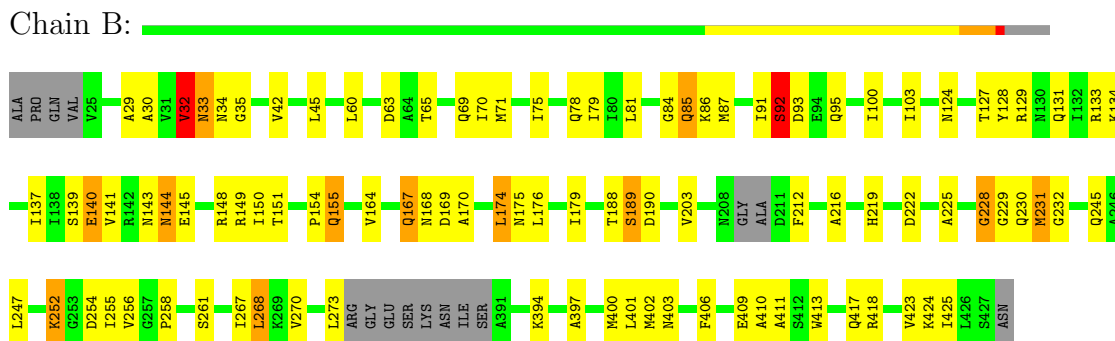
3 Residue-property plots

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



- Molecule 1: Chaperone surA



- Molecule 2: C-peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	148.33Å 148.33Å 188.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.39 41.76 – 3.39	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.00-3.39) 98.3 (41.76-3.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.284 , 0.299 0.278 , 0.293	Depositor DCC
R_{free} test set	1690 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	123.9	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 199.0	EDS
Estimated twinning fraction	0.008 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 33271 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4529	wwPDB-VP
Average B, all atoms (Å ²)	177.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.46	1/2238 (0.0%)	0.63	0/3013
1	B	0.52	2/2238 (0.1%)	0.65	0/3013
2	C	0.70	0/99	0.68	0/133
All	All	0.49	3/4575 (0.1%)	0.64	0/6159

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	228	GLY	N-CA	9.95	1.60	1.46
1	A	25	VAL	CA-CB	5.35	1.66	1.54
1	B	228	GLY	CA-C	5.32	1.60	1.51

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2217	0	2231	62	0
1	B	2217	0	2231	54	0
2	C	95	0	91	6	0
All	All	4529	0	4553	118	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (118) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:81:LEU:HD13	1:A:137:ILE:HD11	1.50	0.92
1:A:80:ILE:HD11	1:A:138:ILE:HG23	1.64	0.78
1:B:45:LEU:HD23	1:B:70:ILE:HG23	1.69	0.75
1:A:167:GLN:O	1:A:169:ASP:N	2.22	0.72
1:B:84:GLY:O	1:B:87:MET:O	2.12	0.67
1:B:229:GLY:O	1:B:231:MET:HG2	1.96	0.65
1:A:81:LEU:HD12	1:A:81:LEU:O	1.97	0.64
1:A:91:ILE:HD13	1:A:136:MET:HB3	1.78	0.64
1:A:146:VAL:HG11	1:A:410:ALA:HA	1.82	0.61
1:A:89:VAL:HG21	1:A:141:VAL:CG1	2.31	0.61
1:B:203:VAL:HG13	1:B:255:ILE:HG21	1.81	0.61
1:B:29:ALA:HB1	1:B:71:MET:HE1	1.82	0.60
1:A:45:LEU:HD11	1:A:70:ILE:HG23	1.82	0.60
1:A:155:GLN:H	1:B:95:GLN:HE22	1.50	0.60
1:A:89:VAL:HG21	1:A:141:VAL:HG12	1.84	0.59
1:B:267:ILE:C	1:B:268:LEU:HD23	2.23	0.59
1:A:155:GLN:H	1:B:95:GLN:NE2	2.00	0.59
1:B:33:ASN:O	1:B:35:GLY:N	2.38	0.57
1:A:45:LEU:HD11	1:A:70:ILE:HG12	1.85	0.57
1:B:268:LEU:HD23	1:B:268:LEU:N	2.20	0.57
1:B:167:GLN:O	1:B:169:ASP:N	2.37	0.56
1:A:91:ILE:CD1	1:A:136:MET:HB3	2.35	0.56
1:A:46:MET:HA	1:A:70:ILE:HD13	1.87	0.56
1:A:103:ILE:HA	1:A:106:GLN:HB2	1.87	0.56
2:C:7:TRP:O	2:C:9:ILE:N	2.33	0.56
1:A:77:ASP:O	1:A:81:LEU:HB2	2.06	0.56
1:B:401:LEU:O	1:B:402:MET:C	2.44	0.55
1:B:133:ARG:O	1:B:137:ILE:HG12	2.05	0.55
1:A:174:LEU:HD21	1:A:247:LEU:HD13	1.87	0.55
1:B:32:VAL:C	1:B:33:ASN:O	2.44	0.55
1:A:77:ASP:O	1:A:81:LEU:CB	2.55	0.54
1:A:92:SER:HB3	1:A:95:GLN:HG3	1.90	0.54
1:B:203:VAL:HG21	1:B:258:PRO:HD3	1.90	0.54
1:B:124:ASN:O	1:B:127:THR:OG1	2.16	0.54
1:B:174:LEU:HD21	1:B:270:VAL:HG13	1.90	0.53
2:C:7:TRP:C	2:C:9:ILE:H	2.12	0.53
1:A:110:THR:OG1	1:A:111:LEU:N	2.41	0.53
1:B:91:ILE:O	1:B:92:SER:C	2.46	0.52
1:A:161:ALA:HA	1:A:164:VAL:HG12	1.89	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:119:ALA:HA	1:A:123:LEU:O	2.10	0.52
1:B:229:GLY:O	1:B:230:GLN:C	2.46	0.52
1:A:181:ILE:HD11	1:A:202:ILE:HD12	1.91	0.52
1:B:229:GLY:O	1:B:231:MET:CG	2.58	0.52
1:A:169:ASP:HA	1:A:172:THR:OG1	2.10	0.52
1:B:150:ILE:HD11	1:B:406:PHE:HA	1.92	0.51
1:A:413:TRP:CG	1:A:413:TRP:O	2.63	0.51
1:A:91:ILE:HG13	1:A:137:ILE:HG22	1.92	0.51
1:A:80:ILE:HD11	1:A:138:ILE:HA	1.93	0.51
1:B:247:LEU:CD2	1:B:256:VAL:HG21	2.41	0.50
1:B:155:GLN:NE2	1:B:155:GLN:H	2.09	0.50
1:A:45:LEU:HD12	1:A:45:LEU:C	2.32	0.50
1:A:425:ILE:HD12	1:A:425:ILE:H	1.76	0.50
1:B:254:ASP:O	1:B:270:VAL:HG23	2.11	0.49
1:A:80:ILE:HD11	1:A:138:ILE:CG2	2.39	0.49
1:A:143:ASN:O	1:A:145:GLU:N	2.45	0.49
1:A:100:ILE:HA	1:A:103:ILE:HD12	1.93	0.49
1:A:70:ILE:HG22	1:A:74:LEU:HD12	1.92	0.49
1:A:110:THR:HG23	1:A:113:GLN:HB2	1.95	0.49
1:B:155:GLN:NE2	1:B:155:GLN:N	2.61	0.49
1:B:252:LYS:H	1:B:273:LEU:HD11	1.78	0.48
1:A:397:ALA:O	1:A:401:LEU:HD22	2.14	0.48
1:A:406:PHE:C	1:A:406:PHE:CD2	2.87	0.48
1:A:243:PHE:CD1	1:A:268:LEU:HD11	2.47	0.48
1:A:53:ALA:CB	1:A:60:LEU:HD11	2.44	0.48
1:A:236:ILE:HD11	1:A:247:LEU:HB2	1.95	0.48
1:B:60:LEU:HD12	1:B:60:LEU:N	2.28	0.47
1:B:228:GLY:C	1:B:230:GLN:H	2.18	0.47
1:B:410:ALA:O	1:B:413:TRP:N	2.48	0.47
1:A:80:ILE:CD1	1:A:138:ILE:HG23	2.41	0.47
2:C:2:PHE:O	2:C:3:THR:C	2.54	0.46
1:B:179:ILE:HD13	1:B:212:PHE:CZ	2.50	0.46
1:B:30:ALA:HB1	1:B:424:LYS:O	2.14	0.46
1:B:143:ASN:O	1:B:144:ASN:C	2.53	0.46
1:A:28:VAL:HG12	1:A:426:LEU:HD12	1.97	0.45
1:B:145:GLU:O	1:B:148:ARG:HB2	2.17	0.45
1:B:203:VAL:HG13	1:B:255:ILE:CG2	2.46	0.45
1:A:146:VAL:CG1	1:A:410:ALA:HA	2.47	0.44
1:B:149:ARG:HB2	1:B:409:GLU:HG2	1.99	0.44
1:A:418:ARG:NH2	1:A:423:VAL:HG21	2.33	0.44
1:B:100:ILE:CD1	1:B:129:ARG:HG3	2.47	0.44
1:A:80:ILE:HD11	1:A:138:ILE:CA	2.48	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:267:ILE:C	1:B:268:LEU:CD2	2.86	0.44
1:B:65:THR:O	1:B:69:GLN:HG2	2.17	0.44
1:A:239:LEU:CD1	1:A:247:LEU:HD12	2.48	0.44
1:A:28:VAL:CG1	1:A:426:LEU:HD12	2.48	0.44
1:A:174:LEU:HD11	1:A:270:VAL:HG13	2.00	0.43
1:B:394:LYS:HA	1:B:397:ALA:HB3	2.00	0.43
1:B:32:VAL:O	1:B:33:ASN:O	2.36	0.43
1:B:78:GLN:O	1:B:79:ILE:C	2.56	0.43
1:B:175:ASN:HA	1:B:232:GLY:O	2.18	0.43
1:A:246:ALA:HB1	1:A:256:VAL:HG11	2.01	0.43
1:B:139:SER:O	1:B:140:GLU:C	2.56	0.43
1:A:160:LEU:HD23	1:A:397:ALA:HA	2.01	0.43
1:A:51:LEU:C	1:A:53:ALA:H	2.21	0.42
1:A:78:GLN:O	1:A:79:ILE:C	2.57	0.42
1:B:85:GLN:O	1:B:86:LYS:C	2.57	0.42
1:B:216:ALA:HB1	1:B:225:ALA:HA	2.01	0.42
1:B:42:VAL:HG21	1:B:71:MET:HE2	2.01	0.42
1:A:100:ILE:HD12	1:A:101:ALA:N	2.35	0.42
1:B:174:LEU:HD21	1:B:270:VAL:CG1	2.49	0.42
1:A:137:ILE:HD12	1:A:137:ILE:C	2.40	0.42
1:A:78:GLN:HG3	1:A:82:GLN:HE21	1.85	0.42
1:A:251:LYS:HA	1:A:273:LEU:HD11	2.01	0.42
1:A:77:ASP:O	1:A:81:LEU:HB3	2.20	0.42
1:B:188:THR:O	1:B:189:SER:C	2.59	0.42
1:A:234:GLY:HA2	2:C:1:ASN:HD22	1.84	0.41
1:A:175:ASN:OD1	1:A:176:LEU:N	2.53	0.41
1:B:154:PRO:HD2	1:B:155:GLN:HE22	1.85	0.41
1:B:128:TYR:HA	1:B:131:GLN:HB2	2.02	0.41
1:B:87:MET:CE	1:B:141:VAL:HG13	2.49	0.41
1:B:131:GLN:O	1:B:134:LYS:HB3	2.20	0.41
1:A:158:GLU:HG3	1:B:103:ILE:HD11	2.03	0.41
2:C:9:ILE:O	2:C:9:ILE:HG22	2.21	0.41
1:B:401:LEU:C	1:B:403:ASN:N	2.73	0.41
2:C:7:TRP:C	2:C:9:ILE:N	2.75	0.40
1:A:239:LEU:HD13	1:A:247:LEU:HD12	2.03	0.40
1:A:114:MET:O	1:A:115:ARG:C	2.59	0.40
1:A:120:TYR:O	1:A:120:TYR:CG	2.74	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	278/299 (93%)	228 (82%)	40 (14%)	10 (4%)	5	47
1	B	278/299 (93%)	224 (81%)	42 (15%)	12 (4%)	4	40
2	C	8/12 (67%)	3 (38%)	3 (38%)	2 (25%)	0	1
All	All	564/610 (92%)	455 (81%)	85 (15%)	24 (4%)	4	40

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	LEU
1	A	168	ASN
1	B	33	ASN
1	B	168	ASN
2	C	8	ASP
1	A	52	ASN
1	A	108	ASN
1	A	140	GLU
1	A	144	ASN
1	A	415	GLN
1	B	34	ASN
2	C	5	LYS
1	B	144	ASN
1	B	167	GLN
1	B	170	ALA
1	B	252	LYS
1	A	148	ARG
1	A	404	ARG
1	B	140	GLU
1	B	189	SER
1	A	129	ARG
1	B	92	SER
1	B	411	ALA
1	B	32	VAL

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	238/249 (96%)	219 (92%)	19 (8%)	17	61
1	B	238/249 (96%)	214 (90%)	24 (10%)	11	46
2	C	10/12 (83%)	8 (80%)	2 (20%)	2	10
All	All	486/510 (95%)	441 (91%)	45 (9%)	13	52

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	36	VAL
1	A	45	LEU
1	A	63	ASP
1	A	80	ILE
1	A	81	LEU
1	A	93	ASP
1	A	103	ILE
1	A	110	THR
1	A	140	GLU
1	A	147	ARG
1	A	152	ILE
1	A	176	LEU
1	A	236	ILE
1	A	261	SER
1	A	401	LEU
1	A	407	SER
1	A	422	TYR
1	A	425	ILE
1	B	32	VAL
1	B	63	ASP
1	B	75	ILE
1	B	81	LEU
1	B	85	GLN
1	B	92	SER
1	B	93	ASP
1	B	151	THR

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Mol	Chain	Res	Type
1	B	155	GLN
1	B	164	VAL
1	B	174	LEU
1	B	176	LEU
1	B	190	ASP
1	B	219	HIS
1	B	222	ASP
1	B	231	MET
1	B	245	GLN
1	B	261	SER
1	B	268	LEU
1	B	400	MET
1	B	417	GLN
1	B	418	ARG
1	B	423	VAL
1	B	425	ILE
2	C	2	PHE
2	C	6	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	59	GLN
1	A	107	ASN
1	A	143	ASN
1	A	144	ASN
1	A	162	GLN
1	A	198	GLN
1	A	205	GLN
1	A	208	ASN
1	A	266	HIS
1	A	271	ASN
1	A	403	ASN
1	B	95	GLN
1	B	106	GLN
1	B	130	ASN
1	B	143	ASN
1	B	155	GLN
1	B	162	GLN
1	B	208	ASN
1	B	245	GLN

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Mol	Chain	Res	Type
1	B	271	ASN
1	B	393	GLN
1	B	403	ASN
2	C	1	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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	284/299 (94%)	0.00	2 (0%) 84 52	79, 178, 261, 265	0
1	B	284/299 (94%)	-0.07	0 100 100	53, 163, 239, 265	0
2	C	10/12 (83%)	0.62	0 100 100	121, 163, 231, 237	0
All	All	578/610 (94%)	-0.02	2 (0%) 91 73	53, 170, 256, 265	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	391	ALA	2.8
1	A	212	PHE	2.2

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.