



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:31 AM EDT

PDB ID : 2PV3 / pdb_00002pv3
Title : Crystallographic Structure of SurA fragment lacking the second peptidyl-prolyl isomerase domain complexed with peptide NFTLKFWDFRK
Authors : Xu, X.; McKay, D.B.
Deposited on : 2007-05-09
Resolution : 3.39 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:

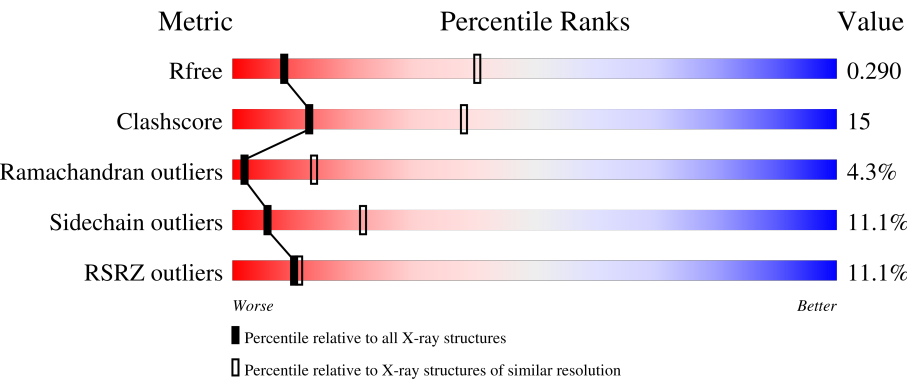
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	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 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 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			

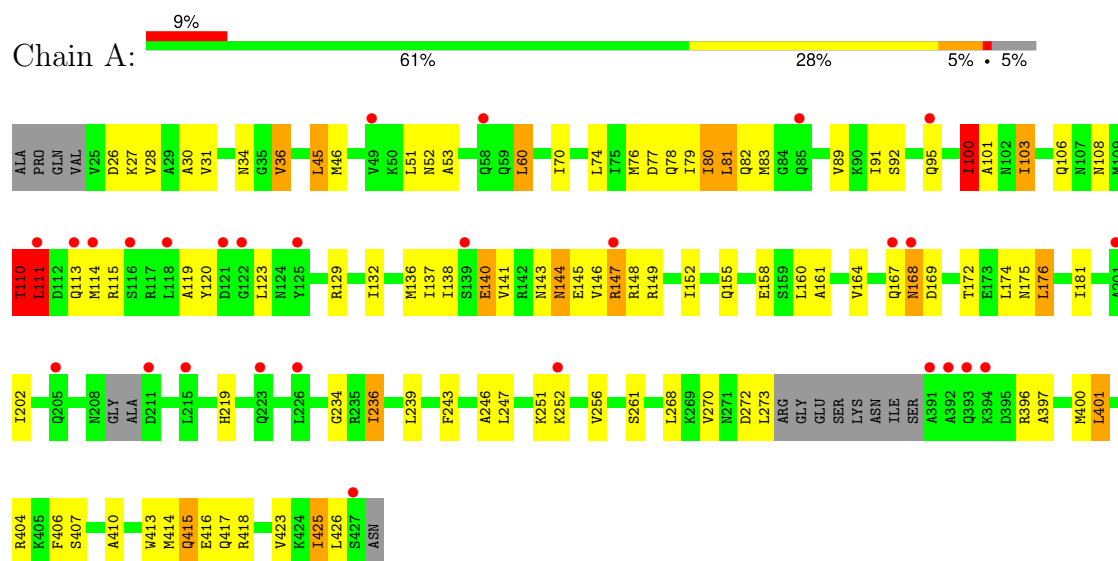
- Molecule 2 is a protein called C-peptide.

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

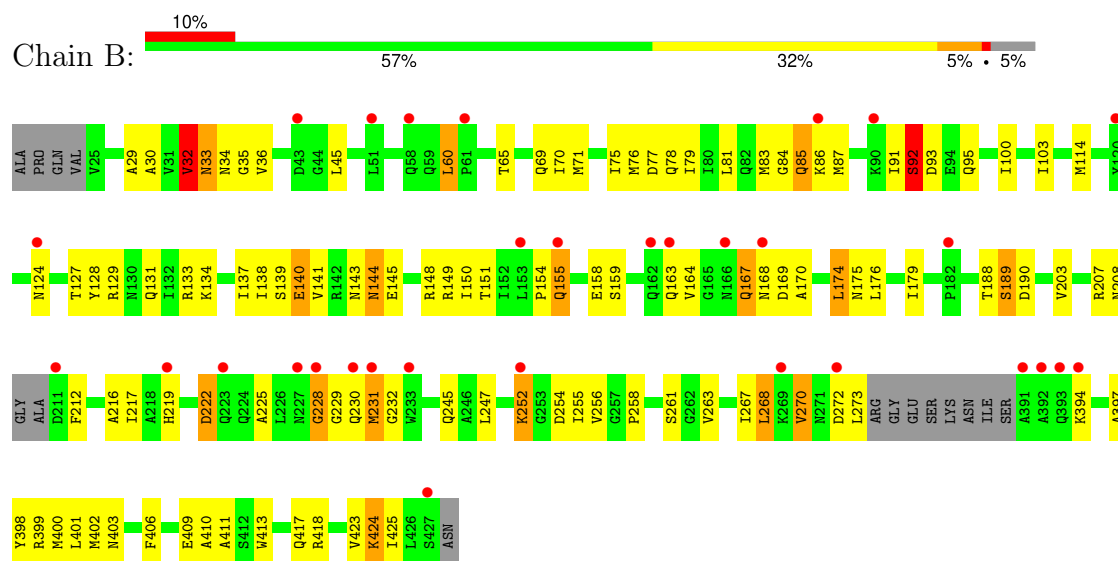
3 Residue-property plots [i](#)

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.

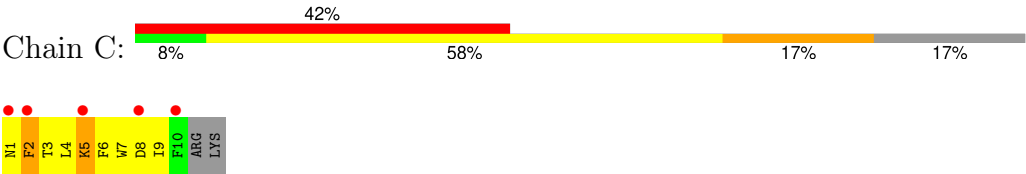
• Molecule 1: Chaperone surA



• 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 50.00 – 3.39	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.00-3.39) 98.2 (50.00-3.39)	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 0.275 , 0.290	Depositor DCC
R_{free} test set	1690 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	123.9	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 238.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.008 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	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.

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	0.65	1/2238 (0.0%)	0.90	4/3013 (0.1%)
1	B	0.70	2/2238 (0.1%)	0.94	3/3013 (0.1%)
2	C	0.82	0/99	0.87	0/133
All	All	0.68	3/4575 (0.1%)	0.92	7/6159 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	228	GLY	N-CA	10.69	1.60	1.45
1	B	228	GLY	CA-C	6.55	1.60	1.51
1	A	100	ILE	CA-CB	5.04	1.60	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	VAL	N-CA-C	5.67	118.31	108.90
1	A	272	ASP	N-CA-C	5.57	115.90	108.38
1	A	30	ALA	N-CA-C	5.51	116.52	108.14
1	B	36	VAL	N-CA-C	5.24	117.39	108.86
1	B	228	GLY	N-CA-C	5.13	122.91	115.32
1	B	222	ASP	N-CA-C	5.05	116.63	110.41
1	A	110	THR	N-CA-C	5.00	115.90	108.60

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	2217	0	2231	75	0
1	B	2217	0	2231	61	0
2	C	95	0	91	6	0
All	All	4529	0	4553	138	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 15.

All (138) 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: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:B:29:ALA:HB1	1:B:71:MET:HE1	1.69	0.73
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:B:267:ILE:C	1:B:268:LEU:HD23	2.23	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:401:LEU:O	1:B:402:MET:C	2.44	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:A:155:GLN:H	1:B:95:GLN:NE2	2.00	0.59
2:C:7:TRP:C	2:C:9:ILE:H	2.12	0.58
1:B:33:ASN:O	1:B:35:GLY:N	2.38	0.57
1:B:91:ILE:O	1:B:92:SER:C	2.46	0.57
1:A:45:LEU:HD11	1:A:70:ILE:HG12	1.85	0.57
1:B:229:GLY:O	1:B:230:GLN:C	2.46	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:46:MET:HA	1:A:70:ILE:HD13	1.87	0.56
1:A:91:ILE:CD1	1:A:136:MET:HB3	2.35	0.56
1:B:32:VAL:C	1:B:33:ASN:O	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ARG:O	1:B:137:ILE:HG12	2.05	0.55
1:A:45:LEU:C	1:A:45:LEU:HD12	2.32	0.55
1:A:174:LEU:HD21	1:A:247:LEU:HD13	1.87	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:124:ASN:O	1:B:127:THR:OG1	2.16	0.54
1:B:203:VAL:HG21	1:B:258:PRO:HD3	1.90	0.54
1:B:174:LEU:HD21	1:B:270:VAL:HG13	1.90	0.53
1:A:110:THR:OG1	1:A:111:LEU:N	2.41	0.53
1:A:406:PHE:CD2	1:A:406:PHE:C	2.87	0.53
1:A:161:ALA:HA	1:A:164:VAL:HG12	1.89	0.52
1:A:119:ALA:HA	1:A:123:LEU:O	2.10	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:228:GLY:C	1:B:230:GLN:H	2.18	0.52
1:B:150:ILE:HD11	1:B:406:PHE:HA	1.92	0.51
1:A:76:MET:HE1	1:A:418:ARG:HB2	1.92	0.51
1:A:413:TRP:CG	1:A:413:TRP:O	2.63	0.51
2:C:2:PHE:O	2:C:3:THR:C	2.54	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:143:ASN:O	1:B:144:ASN:C	2.53	0.50
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:425:ILE:H	1:A:425:ILE:HD12	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:A:396:ARG:HG3	1:A:400:MET:HE3	1.93	0.49
1:B:155:GLN:NE2	1:B:155:GLN:N	2.61	0.49
1:B:267:ILE:C	1:B:268:LEU:CD2	2.86	0.48
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:53:ALA:CB	1:A:60:LEU:HD11	2.44	0.48
1:A:243:PHE:CD1	1:A:268:LEU:HD11	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:SER:O	1:B:140:GLU:C	2.56	0.47
1:A:51:LEU:C	1:A:53:ALA:H	2.21	0.47
1:B:410:ALA:O	1:B:413:TRP:N	2.48	0.47
1:A:78:GLN:O	1:A:79:ILE:C	2.57	0.47
1:B:78:GLN:O	1:B:79:ILE:C	2.56	0.47
1:B:85:GLN:O	1:B:86:LYS:C	2.57	0.47
1:A:80:ILE:CD1	1:A:138:ILE:HG23	2.41	0.47
1:A:137:ILE:C	1:A:137:ILE:HD12	2.40	0.46
1:B:188:THR:O	1:B:189:SER:C	2.59	0.46
1:B:30:ALA:HB1	1:B:424:LYS:O	2.14	0.46
1:B:179:ILE:HD13	1:B:212:PHE:CZ	2.50	0.46
1:A:28:VAL:HG12	1:A:426:LEU:HD12	1.97	0.45
1:B:401:LEU:C	1:B:403:ASN:N	2.73	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:B:398:TYR:O	1:B:399:ARG:C	2.61	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:B:228:GLY:C	1:B:230:GLN:N	2.74	0.44
1:A:80:ILE:HD11	1:A:138:ILE:CA	2.48	0.44
1:A:147:ARG:C	1:A:149:ARG:H	2.26	0.44
1:B:65:THR:O	1:B:69:GLN:HG2	2.17	0.44
1:B:272:ASP:C	1:B:273:LEU:HD12	2.42	0.44
1:A:28:VAL:CG1	1:A:426:LEU:HD12	2.48	0.44
1:A:239:LEU:CD1	1:A:247:LEU:HD12	2.48	0.44
1:B:83:MET:O	1:B:84:GLY:C	2.60	0.44
1:A:114:MET:O	1:A:115:ARG:C	2.59	0.43
1:A:174:LEU:HD11	1:A:270:VAL:HG13	2.00	0.43
1:A:143:ASN:C	1:A:145:GLU:N	2.76	0.43
1:A:83:MET:HE1	1:A:417:GLN:OE1	2.18	0.43
1:A:143:ASN:O	1:A:144:ASN:C	2.60	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:207:ARG:C	1:B:208:ASN:HD22	2.27	0.43
1:A:246:ALA:HB1	1:A:256:VAL:HG11	2.01	0.43
1:B:175:ASN:HA	1:B:232:GLY:O	2.18	0.43
1:A:414:MET:C	1:A:416:GLU:N	2.77	0.43
1:A:160:LEU:HD23	1:A:397:ALA:HA	2.01	0.43
1:A:114:MET:HE3	1:A:114:MET:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:ALA:HB1	1:B:225:ALA:HA	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: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:414:MET:O	1:A:415:GLN:C	2.63	0.42
1:A:77:ASP:O	1:A:81:LEU:HB3	2.20	0.42
1:A:175:ASN:OD1	1:A:176:LEU:N	2.53	0.41
1:A:234:GLY:HA2	2:C:1:ASN:HD22	1.84	0.41
1:B:114:MET:HE2	1:B:114:MET:HB3	1.99	0.41
2:C:4:LEU:O	2:C:5:LYS:C	2.63	0.41
1:B:76:MET:O	1:B:77:ASP:C	2.62	0.41
1:B:128:TYR:HA	1:B:131:GLN:HB2	2.02	0.41
1:B:154:PRO:HD2	1:B:155:GLN:HE22	1.85	0.41
1:A:167:GLN:O	1:A:168:ASN:C	2.61	0.41
1:B:87:MET:CE	1:B:141:VAL:HG13	2.49	0.41
1:A:158:GLU:HG3	1:B:103:ILE:HD11	2.03	0.41
1:B:131:GLN:O	1:B:134:LYS:HB3	2.20	0.41
2:C:9:ILE:HG22	2:C:9:ILE:O	2.21	0.41
1:B:158:GLU:O	1:B:159:SER:C	2.64	0.40
1:A:239:LEU:HD13	1:A:247:LEU:HD12	2.03	0.40
1:A:76:MET:O	1:A:77:ASP:C	2.64	0.40
1:A:120:TYR:O	1:A:120:TYR:CG	2.74	0.40
1:A:26:ASP:O	1:A:27:LYS:C	2.65	0.40
1:A:251:LYS:O	1:A:252:LYS:C	2.63	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	278/299 (93%)	228 (82%)	40 (14%)	10 (4%)	2 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	278/299 (93%)	224 (81%)	42 (15%)	12 (4%)	2	13
2	C	8/12 (67%)	3 (38%)	3 (38%)	2 (25%)	0	0
All	All	564/610 (92%)	455 (81%)	85 (15%)	24 (4%)	2	13

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%)	216 (91%)	22 (9%)	8	29
1	B	238/249 (96%)	208 (87%)	30 (13%)	4	18
2	C	10/12 (83%)	8 (80%)	2 (20%)	1	4
All	All	486/510 (95%)	432 (89%)	54 (11%)	6	21

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	VAL
1	A	34	ASN
1	A	36	VAL
1	A	45	LEU
1	A	60	LEU
1	A	80	ILE
1	A	81	LEU
1	A	100	ILE
1	A	103	ILE
1	A	110	THR
1	A	111	LEU
1	A	132	ILE
1	A	140	GLU
1	A	147	ARG
1	A	152	ILE
1	A	176	LEU
1	A	219	HIS
1	A	236	ILE
1	A	261	SER
1	A	401	LEU
1	A	407	SER
1	A	425	ILE
1	B	32	VAL
1	B	60	LEU
1	B	75	ILE
1	B	81	LEU
1	B	85	GLN
1	B	92	SER
1	B	93	ASP
1	B	138	ILE
1	B	151	THR
1	B	155	GLN
1	B	163	GLN
1	B	164	VAL

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Mol	Chain	Res	Type
1	B	174	LEU
1	B	176	LEU
1	B	190	ASP
1	B	217	ILE
1	B	219	HIS
1	B	222	ASP
1	B	231	MET
1	B	245	GLN
1	B	261	SER
1	B	263	VAL
1	B	268	LEU
1	B	270	VAL
1	B	400	MET
1	B	417	GLN
1	B	418	ARG
1	B	423	VAL
1	B	424	LYS
1	B	425	ILE
2	C	2	PHE
2	C	6	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	107	ASN
1	A	124	ASN
1	A	131	GLN
1	A	143	ASN
1	A	144	ASN
1	A	162	GLN
1	A	198	GLN
1	A	224	GLN
1	A	266	HIS
1	A	403	ASN
1	B	33	ASN
1	B	95	GLN
1	B	124	ASN
1	B	130	ASN
1	B	155	GLN
1	B	162	GLN
1	B	168	ASN

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Mol	Chain	Res	Type
1	B	198	GLN
1	B	205	GLN
1	B	208	ASN
1	B	230	GLN
1	B	245	GLN
1	B	271	ASN
1	B	393	GLN
1	B	403	ASN
2	C	1	ASN

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	284/299 (94%)	0.76	28 (9%) 13 12	79, 178, 261, 265	0
1	B	284/299 (94%)	0.74	31 (10%) 10 11	53, 163, 239, 265	0
2	C	10/12 (83%)	1.89	5 (50%) 0 0	121, 163, 231, 237	0
All	All	578/610 (94%)	0.77	64 (11%) 10 11	53, 170, 256, 265	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	391	ALA	11.7
1	B	391	ALA	6.4
1	B	230	GLN	5.9
1	B	252	LYS	4.5
1	A	58	GLN	4.3
1	A	122	GLY	4.3
1	A	394	LYS	4.1
2	C	10	PHE	4.0
1	A	226	LEU	3.9
1	A	215	LEU	3.9
1	A	85	GLN	3.8
1	B	153	LEU	3.6
1	A	118	LEU	3.6
1	A	111	LEU	3.6
1	A	427	SER	3.5
1	A	392	ALA	3.4
1	B	393	GLN	3.3
1	B	269	LYS	3.3
1	A	114	MET	3.2
1	B	394	LYS	3.2
1	A	205	GLN	3.2
1	B	427	SER	3.2
1	B	392	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	252	LYS	3.1
1	B	163	GLN	3.1
1	B	182	PRO	3.1
2	C	1	ASN	3.1
1	A	223	GLN	3.0
1	A	139	SER	3.0
2	C	2	PHE	3.0
1	B	168	ASN	3.0
1	B	120	TYR	2.9
1	B	166	ASN	2.9
2	C	5	LYS	2.9
1	B	90	LYS	2.7
1	A	121	ASP	2.7
1	B	155	GLN	2.7
1	A	393	GLN	2.6
1	B	227	ASN	2.6
1	A	167	GLN	2.6
1	B	223	GLN	2.6
1	B	272	ASP	2.6
1	A	147	ARG	2.5
1	B	58	GLN	2.5
1	A	113	GLN	2.5
1	B	86	LYS	2.5
1	B	219	HIS	2.5
1	B	231	MET	2.4
1	A	168	ASN	2.4
1	B	43	ASP	2.4
1	B	228	GLY	2.3
1	A	49	VAL	2.3
1	B	211	ASP	2.3
1	A	125	TYR	2.2
1	A	201	ALA	2.2
1	B	233	TRP	2.2
1	B	162	GLN	2.2
1	B	51	LEU	2.2
1	B	124	ASN	2.2
1	A	211	ASP	2.2
2	C	8	ASP	2.1
1	A	116	SER	2.1
1	A	95	GLN	2.1
1	B	61	PRO	2.1

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.