Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2021 – 09:14 PM EST

PDB ID	:	3QK7
Title	:	Crystal structure of putative Transcriptional regulator from Yersinia pestis biovar Microtus str. 91001
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Deposited on	:	2011-01-31
Resolution	:	2.70 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:

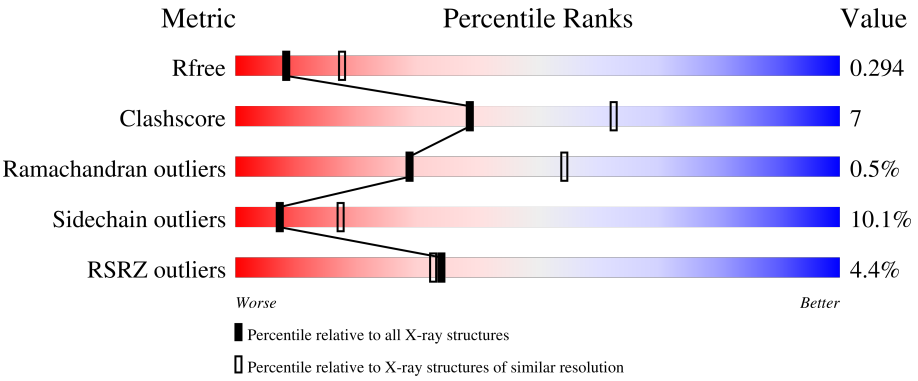
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	294	6% 79% 13% • 5%
1	B	294	2% 75% 16% • 5%
1	C	294	4% 74% 16% • •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6567 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 Transcriptional regulators.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	Se	0	0	0
			2157	1372	372	406	2	5			
1	B	280	Total	C	N	O	S	Se	0	0	0
			2157	1372	372	406	2	5			
1	C	281	Total	C	N	O	S	Se	0	0	0
			2168	1378	376	407	2	5			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP Q74V61
A	2	SER	-	expression tag	UNP Q74V61
A	3	LEU	-	expression tag	UNP Q74V61
A	287	GLU	-	expression tag	UNP Q74V61
A	288	GLY	-	expression tag	UNP Q74V61
A	289	HIS	-	expression tag	UNP Q74V61
A	290	HIS	-	expression tag	UNP Q74V61
A	291	HIS	-	expression tag	UNP Q74V61
A	292	HIS	-	expression tag	UNP Q74V61
A	293	HIS	-	expression tag	UNP Q74V61
A	294	HIS	-	expression tag	UNP Q74V61
B	1	MSE	-	expression tag	UNP Q74V61
B	2	SER	-	expression tag	UNP Q74V61
B	3	LEU	-	expression tag	UNP Q74V61
B	287	GLU	-	expression tag	UNP Q74V61
B	288	GLY	-	expression tag	UNP Q74V61
B	289	HIS	-	expression tag	UNP Q74V61
B	290	HIS	-	expression tag	UNP Q74V61
B	291	HIS	-	expression tag	UNP Q74V61
B	292	HIS	-	expression tag	UNP Q74V61
B	293	HIS	-	expression tag	UNP Q74V61
B	294	HIS	-	expression tag	UNP Q74V61
C	1	MSE	-	expression tag	UNP Q74V61

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2	SER	-	expression tag	UNP Q74V61
C	3	LEU	-	expression tag	UNP Q74V61
C	287	GLU	-	expression tag	UNP Q74V61
C	288	GLY	-	expression tag	UNP Q74V61
C	289	HIS	-	expression tag	UNP Q74V61
C	290	HIS	-	expression tag	UNP Q74V61
C	291	HIS	-	expression tag	UNP Q74V61
C	292	HIS	-	expression tag	UNP Q74V61
C	293	HIS	-	expression tag	UNP Q74V61
C	294	HIS	-	expression tag	UNP Q74V61

- Molecule 2 is water.

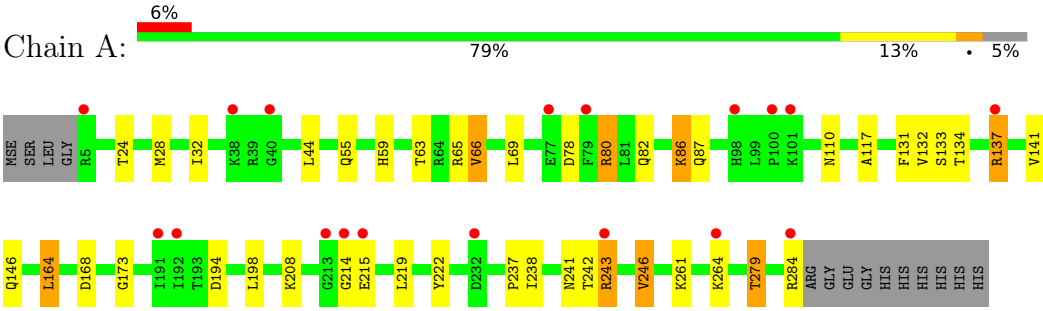
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	25	Total O 25 25	0	0
2	B	32	Total O 32 32	0	0
2	C	28	Total O 28 28	0	0

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.

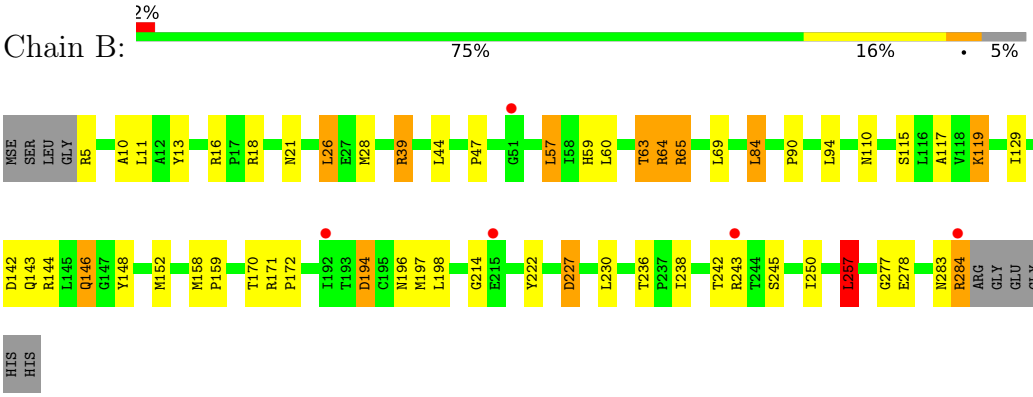
• Molecule 1: Transcriptional regulators

Chain A:



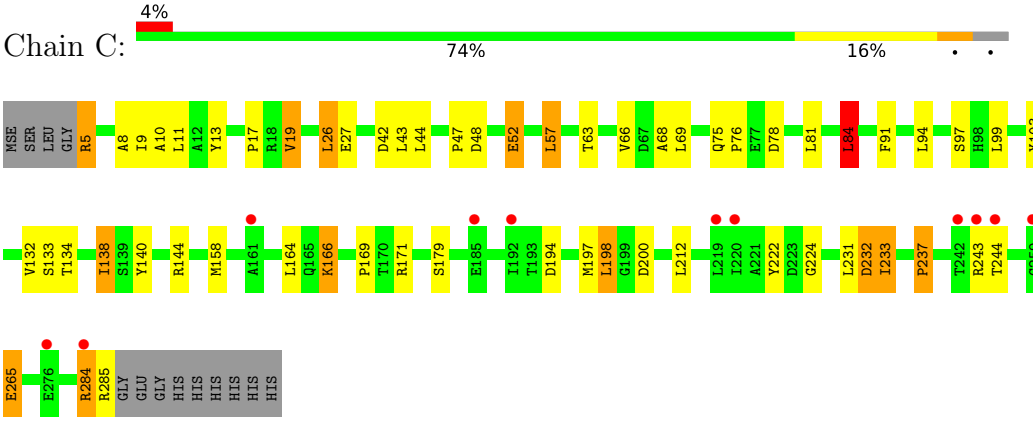
• Molecule 1: Transcriptional regulators

Chain B:



• Molecule 1: Transcriptional regulators

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	96.70Å 96.70Å 256.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.74 – 2.70 19.63 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.5 (19.74-2.70) 97.5 (19.63-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.04 (at 2.71Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.234 , 0.299 0.231 , 0.294	Depositor DCC
R_{free} test set	1574 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	80.0	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 52.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.57$, $< L^2 > = 0.42$	Xtriage
Estimated twinning fraction	0.000 for -h,k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6567	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.46	0/2195	0.63	0/2975
1	B	0.51	0/2195	0.67	1/2975 (0.0%)
1	C	0.49	0/2206	0.68	2/2989 (0.1%)
All	All	0.49	0/6596	0.66	3/8939 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	57	LEU	CA-CB-CG	5.59	128.16	115.30
1	B	257	LEU	CA-CB-CG	5.20	127.26	115.30
1	C	84	LEU	CA-CB-CG	5.06	126.94	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	2157	0	2177	21	0
1	B	2157	0	2177	41	0
1	C	2168	0	2190	42	0
2	A	25	0	0	0	0
2	B	32	0	0	0	0
2	C	28	0	0	1	0
All	All	6567	0	6544	97	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 7.

All (97) 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:C:284:ARG:HH21	1:C:284:ARG:HG3	1.29	0.97
1:A:63:THR:HG23	1:A:65:ARG:HG2	1.52	0.92
1:B:64:ARG:HH11	1:B:64:ARG:HG2	1.35	0.89
1:A:142:ASP:O	1:A:146:GLN:HG2	1.80	0.82
1:B:142:ASP:O	1:B:146:GLN:HG2	1.78	0.82
1:A:219:LEU:O	1:A:279:THR:HG22	1.87	0.74
1:B:39:ARG:HH11	1:B:39:ARG:HG3	1.53	0.74
1:C:284:ARG:CG	1:C:284:ARG:HH21	2.01	0.72
1:A:63:THR:CG2	1:A:65:ARG:HG2	2.20	0.71
1:A:28:MSE:O	1:A:32:ILE:HG12	1.91	0.71
1:C:232:ASP:HA	2:C:302:HOH:O	1.93	0.69
1:A:134:THR:HG23	1:A:194:ASP:OD1	1.95	0.67
1:A:110:ASN:HB3	1:A:144:ARG:HG3	1.77	0.66
1:C:261:LYS:HG2	1:C:265:GLU:HG2	1.78	0.66
1:B:117:ALA:HB2	1:B:238:ILE:HD11	1.79	0.64
1:B:110:ASN:HD22	1:B:143:GLN:NE2	1.97	0.62
1:B:65:ARG:HD3	1:C:42:ASP:OD2	2.01	0.61
1:B:63:THR:HG22	1:B:65:ARG:HB2	1.84	0.60
1:C:134:THR:N	1:C:194:ASP:OD2	2.35	0.60
1:C:138:ILE:HD11	1:C:140:TYR:CE2	2.36	0.60
1:B:21:ASN:HB3	1:C:26:LEU:CD1	2.32	0.60
1:C:284:ARG:HG3	1:C:284:ARG:NH2	2.09	0.60
1:B:63:THR:CG2	1:B:65:ARG:HB2	2.32	0.59
1:C:138:ILE:HD11	1:C:140:TYR:HE2	1.68	0.58
1:C:5:ARG:N	1:C:5:ARG:HH11	2.01	0.58
1:C:5:ARG:O	1:C:5:ARG:HD2	2.05	0.57
1:C:134:THR:HB	1:C:194:ASP:OD2	2.05	0.57
1:B:26:LEU:HG	1:C:26:LEU:HG	1.85	0.57
1:B:148:TYR:O	1:B:152:MSE:HB2	2.04	0.56
1:C:134:THR:CB	1:C:194:ASP:OD2	2.53	0.56
1:C:75:GLN:HB2	1:C:76:PRO:HD2	1.86	0.56
1:C:171:ARG:HD3	1:C:200:ASP:OD2	2.07	0.55
1:B:110:ASN:HD22	1:B:143:GLN:HE22	1.53	0.55
1:C:284:ARG:CG	1:C:284:ARG:NH2	2.66	0.55
1:B:39:ARG:HG3	1:B:39:ARG:NH1	2.20	0.55
1:A:59:HIS:O	1:A:63:THR:HG22	2.06	0.55
1:C:10:ALA:HB2	1:C:66:VAL:HG11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LEU:HD21	1:A:164:LEU:HD21	1.90	0.53
1:B:230:LEU:CD1	1:C:171:ARG:HB3	2.39	0.52
1:C:133:SER:HB3	1:C:166:LYS:HE2	1.91	0.52
1:A:24:THR:HG23	1:A:243:ARG:HD2	1.92	0.51
1:C:169:PRO:HA	1:C:198:LEU:HD13	1.93	0.51
1:A:219:LEU:O	1:A:279:THR:CG2	2.56	0.50
1:A:132:VAL:HG12	1:A:198:LEU:HD13	1.93	0.50
1:C:212:LEU:HD21	1:C:233:ILE:HG21	1.93	0.50
1:B:134:THR:HB	1:B:194:ASP:OD2	2.13	0.49
1:B:90:PRO:HB3	1:B:257:LEU:CD1	2.43	0.49
1:B:21:ASN:HB3	1:C:26:LEU:HD13	1.95	0.49
1:C:99:LEU:HD12	1:C:103:TYR:CD2	2.48	0.49
1:C:48:ASP:OD2	1:C:52:GLU:HA	2.13	0.49
1:C:5:ARG:HD2	1:C:5:ARG:N	2.28	0.48
1:A:131:PHE:HE2	1:A:133:SER:HB2	1.78	0.48
1:C:132:VAL:O	1:C:194:ASP:HB2	2.14	0.48
1:C:17:PRO:HB2	1:C:19:VAL:HG23	1.96	0.48
1:A:44:LEU:HD12	1:A:66:VAL:HG23	1.96	0.48
1:B:13:TYR:CZ	1:B:47:PRO:HB3	2.49	0.48
1:B:59:HIS:O	1:B:63:THR:HB	2.13	0.47
1:B:170:THR:HB	1:B:172:PRO:HD2	1.94	0.47
1:A:117:ALA:HB2	1:A:238:ILE:HD11	1.96	0.47
1:C:11:LEU:HB2	1:C:43:LEU:HD11	1.96	0.47
1:B:134:THR:CB	1:B:194:ASP:OD2	2.63	0.47
1:B:227:ASP:N	1:B:227:ASP:OD1	2.47	0.47
1:A:78:ASP:OD1	1:A:80:ARG:HG2	2.15	0.46
1:B:110:ASN:HB3	1:B:144:ARG:HG3	1.97	0.46
1:C:5:ARG:O	1:C:5:ARG:CD	2.64	0.46
1:C:110:ASN:HB3	1:C:144:ARG:HG3	1.98	0.46
1:A:24:THR:HG23	1:A:243:ARG:CD	2.45	0.45
1:B:64:ARG:HH11	1:B:64:ARG:CG	2.18	0.45
1:B:57:LEU:O	1:B:57:LEU:HD12	2.16	0.45
1:B:230:LEU:HD13	1:C:171:ARG:HB3	1.99	0.44
1:B:28:MSE:HE2	1:B:250:ILE:HD11	1.99	0.44
1:C:224:GLY:CA	1:C:237:PRO:HB3	2.48	0.44
1:C:78:ASP:HB3	1:C:81:LEU:HD12	1.99	0.44
1:B:115:SER:O	1:B:119:LYS:HG2	2.17	0.43
1:B:158:MSE:HA	1:B:159:PRO:HD3	1.90	0.43
1:B:146:GLN:H	1:B:146:GLN:HG2	1.70	0.43
1:B:242:THR:HG23	1:B:245:SER:HB2	1.99	0.43
1:B:171:ARG:HD3	1:B:197:MSE:HE1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LEU:HD11	1:B:84:LEU:HD11	2.00	0.42
1:C:99:LEU:HD12	1:C:103:TYR:CG	2.55	0.42
1:A:82:GLN:O	1:A:86:LYS:HB2	2.20	0.42
1:C:198:LEU:HD12	1:C:198:LEU:HA	1.94	0.42
1:B:129:ILE:HD12	1:B:152:MSE:SE	2.69	0.42
1:B:236:THR:HA	1:B:277:GLY:HA3	2.00	0.41
1:C:84:LEU:HD13	1:C:91:PHE:CD2	2.55	0.41
1:A:242:THR:O	1:A:246:VAL:HG13	2.21	0.41
1:B:132:VAL:HG12	1:B:198:LEU:HD13	2.02	0.41
1:C:8:ALA:HB1	1:C:44:LEU:HD23	2.01	0.41
1:B:158:MSE:HE3	1:B:158:MSE:HB2	1.85	0.41
1:B:283:ASN:O	1:B:284:ARG:HG3	2.20	0.41
1:B:10:ALA:HA	1:B:44:LEU:O	2.20	0.41
1:B:64:ARG:HG2	1:B:64:ARG:NH1	2.13	0.41
1:A:168:ASP:O	1:A:173:GLY:HA3	2.21	0.41
1:C:75:GLN:HB2	1:C:76:PRO:CD	2.50	0.41
1:C:13:TYR:CZ	1:C:47:PRO:HB3	2.56	0.41
1:A:137:ARG:NH2	1:B:214:GLY:H	2.18	0.40
1:C:9:ILE:HD12	1:C:68:ALA:HB3	2.03	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	278/294 (95%)	263 (95%)	12 (4%)	3 (1%)	14 34
1	B	278/294 (95%)	266 (96%)	12 (4%)	0	100 100
1	C	279/294 (95%)	268 (96%)	10 (4%)	1 (0%)	34 60
All	All	835/882 (95%)	797 (95%)	34 (4%)	4 (0%)	29 54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	LYS
1	C	237	PRO
1	A	237	PRO
1	A	214	GLY

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	230/235 (98%)	212 (92%)	18 (8%)	12 29
1	B	230/235 (98%)	206 (90%)	24 (10%)	7 16
1	C	231/235 (98%)	203 (88%)	28 (12%)	5 11
All	All	691/705 (98%)	621 (90%)	70 (10%)	7 17

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	66	VAL
1	A	69	LEU
1	A	80	ARG
1	A	86	LYS
1	A	87	GLN
1	A	137	ARG
1	A	141	VAL
1	A	164	LEU
1	A	208	LYS
1	A	215	GLU
1	A	222	TYR
1	A	241	ASN
1	A	243	ARG
1	A	246	VAL
1	A	261	LYS
1	A	279	THR
1	A	284	ARG
1	B	5	ARG

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Mol	Chain	Res	Type
1	B	11	LEU
1	B	16	ARG
1	B	18	ARG
1	B	26	LEU
1	B	39	ARG
1	B	57	LEU
1	B	60	LEU
1	B	63	THR
1	B	64	ARG
1	B	65	ARG
1	B	69	LEU
1	B	84	LEU
1	B	94	LEU
1	B	119	LYS
1	B	146	GLN
1	B	194	ASP
1	B	196	ASN
1	B	222	TYR
1	B	227	ASP
1	B	243	ARG
1	B	257	LEU
1	B	278	GLU
1	B	284	ARG
1	C	5	ARG
1	C	19	VAL
1	C	26	LEU
1	C	27	GLU
1	C	52	GLU
1	C	57	LEU
1	C	63	THR
1	C	69	LEU
1	C	84	LEU
1	C	94	LEU
1	C	97	SER
1	C	119	LYS
1	C	138	ILE
1	C	158	MSE
1	C	164	LEU
1	C	166	LYS
1	C	179	SER
1	C	197	MSE
1	C	198	LEU

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Mol	Chain	Res	Type
1	C	222	TYR
1	C	231	LEU
1	C	232	ASP
1	C	233	ILE
1	C	243	ARG
1	C	244	THR
1	C	265	GLU
1	C	284	ARG
1	C	285	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	249	GLN
1	B	73	HIS
1	B	143	GLN
1	B	196	ASN
1	C	150	GLN

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 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

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, 95^{th} 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	275/294 (93%)	0.25	18 (6%)	18	17	47, 73, 99, 114	0
1	B	275/294 (93%)	0.05	5 (1%)	68	70	40, 60, 84, 100	0
1	C	276/294 (93%)	0.15	13 (4%)	31	30	42, 65, 91, 100	0
All	All	826/882 (93%)	0.15	36 (4%)	34	33	40, 67, 95, 114	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	284	ARG	3.9
1	B	284	ARG	3.8
1	C	243	ARG	3.2
1	C	242	THR	3.1
1	A	98	HIS	3.0
1	A	79	PHE	3.0
1	A	192	ILE	3.0
1	C	192	ILE	2.7
1	A	215	GLU	2.7
1	A	101	LYS	2.7
1	A	213	GLY	2.6
1	C	260	GLY	2.6
1	A	100	PRO	2.6
1	B	51	GLY	2.6
1	A	40	GLY	2.5
1	C	185	GLU	2.5
1	B	192	ILE	2.5
1	A	5	ARG	2.5
1	C	259	GLY	2.5
1	A	137	ARG	2.4
1	A	232	ASP	2.4
1	A	284	ARG	2.4
1	A	243	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	38	LYS	2.3
1	A	264	LYS	2.3
1	C	264	LYS	2.3
1	A	214	GLY	2.3
1	B	215	GLU	2.2
1	C	219	LEU	2.2
1	C	161	ALA	2.2
1	C	244	THR	2.2
1	C	220	ILE	2.2
1	A	77	GLU	2.1
1	A	191	ILE	2.1
1	C	276	GLU	2.1
1	B	243	ARG	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.