WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2023 – 11:05 AM EDT

PDB ID : 1Q87
Title : Crystal structure of the C-domain of the T.vaginalis Inr binding protein, IBP39 (tetragonal form)
Authors : Schumacher, M.A.; Johnson, P.J.
Deposited on : 2003-08-20
Resolution : 2.32 Å(reported)

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	:	2.35
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)	:	2.35
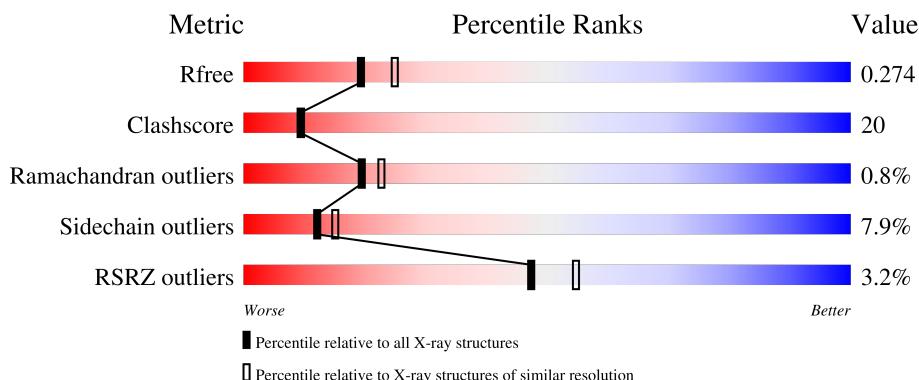
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
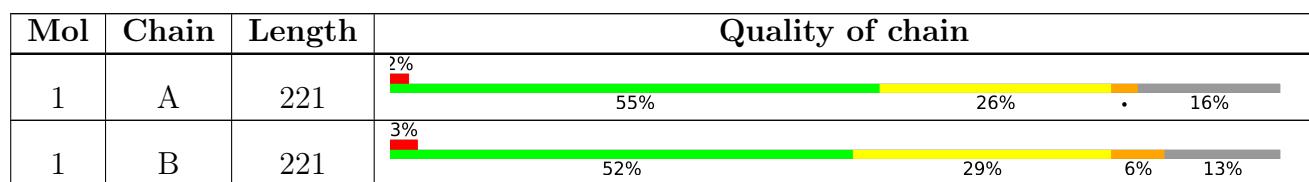
The reported resolution of this entry is 2.32 Å.

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	Percentile Ranks	Value
Rfree		0.274
Clashscore		20
Ramachandran outliers		0.8%
Sidechain outliers		7.9%
RSRZ outliers		3.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	221	2% 55% 26% • 16%
1	B	221	3% 52% 29% 6% 13%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 3115 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 39 kDa initiator binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	0	0
			1494	963	239	282	10			
1	B	193	Total	C	N	O	S	0	0	0
			1560	1005	249	296	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	342	HIS	-	expression tag	UNP Q95VR4
A	343	HIS	-	expression tag	UNP Q95VR4
A	344	HIS	-	expression tag	UNP Q95VR4
A	345	HIS	-	expression tag	UNP Q95VR4
A	346	HIS	-	expression tag	UNP Q95VR4
A	347	HIS	-	expression tag	UNP Q95VR4
B	342	HIS	-	expression tag	UNP Q95VR4
B	343	HIS	-	expression tag	UNP Q95VR4
B	344	HIS	-	expression tag	UNP Q95VR4
B	345	HIS	-	expression tag	UNP Q95VR4
B	346	HIS	-	expression tag	UNP Q95VR4
B	347	HIS	-	expression tag	UNP Q95VR4
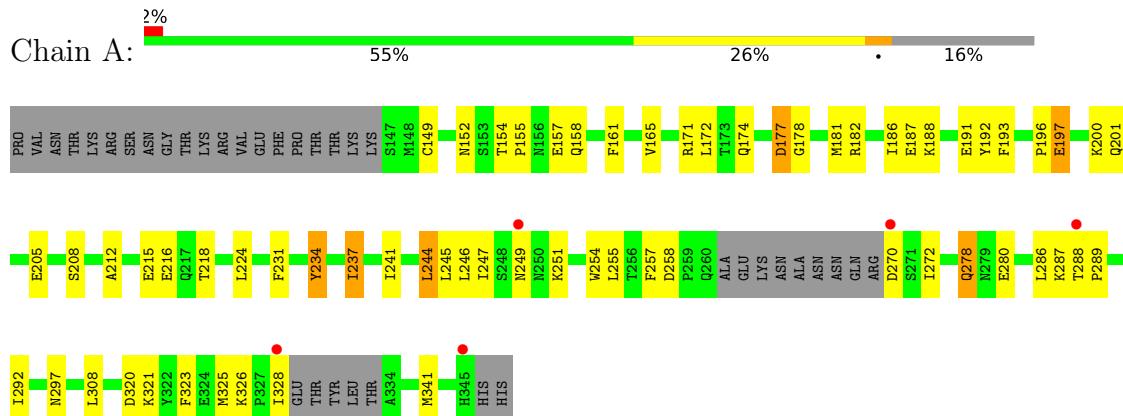
- Molecule 2 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	34	Total	O	0	0
			34	34		
2	B	27	Total	O	0	0
			27	27		
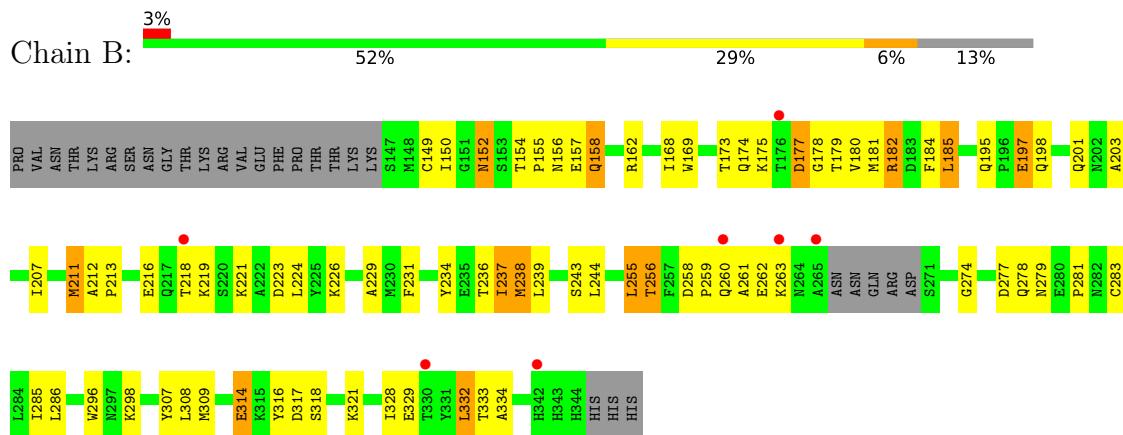
3 Residue-property plots ⓘ

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: 39 kDa initiator binding protein

• Molecule 1: 39 kDa initiator binding protein

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	76.42Å　76.42Å　157.62Å 90.00°　90.00°　90.00°	Depositor
Resolution (Å)	65.00　–　2.32 68.76　–　2.32	Depositor EDS
% Data completeness (in resolution range)	91.0 (65.00-2.32) 91.1 (68.76-2.32)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.32Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.215　,　0.274 0.217　,　0.274	Depositor DCC
R_{free} test set	1891 reflections (9.89%)	wwPDB-VP
Wilson B-factor (Å^2)	61.2	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 63.5	EDS
L-test for twinning[2]	$< |L| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3115	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.63	0/1531	0.73	0/2070
1	B	0.57	0/1599	0.69	0/2164
All	All	0.60	0/3130	0.71	0/4234

There are no bond length outliers.

There are no bond angle outliers.

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	1494	0	1453	42	0
1	B	1560	0	1523	77	0
2	A	34	0	0	4	0
2	B	27	0	0	3	0
All	All	3115	0	2976	119	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 20.

All (119) 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:177:ASP:CG	1:A:178:GLY:H	1.74	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ASP:H	1:B:321:LYS:HD2	1.48	0.78
1:B:177:ASP:OD1	1:B:178:GLY:N	2.19	0.76
1:B:203:ALA:O	1:B:207:ILE:HG12	1.86	0.75
1:B:332:LEU:HD13	1:B:334:ALA:H	1.52	0.73
1:A:191:GLU:HG2	2:A:367:HOH:O	1.89	0.72
1:B:197:GLU:H	1:B:197:GLU:CD	1.91	0.72
1:A:287:LYS:HD2	1:A:292:ILE:HD11	1.72	0.72
1:A:321:LYS:HE3	2:A:352:HOH:O	1.89	0.72
1:A:177:ASP:CG	1:A:178:GLY:N	2.44	0.70
1:B:226:LYS:NZ	1:B:278:GLN:HE22	1.89	0.70
1:B:332:LEU:CD1	1:B:334:ALA:H	2.03	0.70
1:B:180:VAL:HG13	1:B:184:PHE:HB3	1.74	0.69
1:B:286:LEU:HD22	1:B:328:ILE:HD11	1.76	0.67
1:B:317:ASP:HB2	1:B:321:LYS:HD2	1.80	0.64
1:B:169:TRP:CE3	1:B:221:LYS:HA	2.34	0.63
1:B:212:ALA:HB1	1:B:213:PRO:HA	1.79	0.62
1:B:229:ALA:HB3	1:B:281:PRO:HB2	1.81	0.62
1:B:185:LEU:HD22	1:B:211:MET:HE1	1.80	0.62
1:B:317:ASP:H	1:B:321:LYS:CD	2.13	0.60
1:A:215:GLU:H	1:A:215:GLU:CD	2.04	0.60
1:B:213:PRO:HD3	1:B:259:PRO:HG2	1.84	0.59
1:A:287:LYS:HA	1:A:292:ILE:HD13	1.84	0.59
1:B:195:GLN:HB2	1:B:198:GLN:HB2	1.85	0.58
1:B:328:ILE:CG2	1:B:329:GLU:N	2.66	0.57
1:B:234:TYR:HA	1:B:237:ILE:HB	1.85	0.57
1:B:181:MET:O	1:B:184:PHE:N	2.38	0.56
1:A:171:ARG:HH21	1:A:192:TYR:HE2	1.54	0.56
1:A:244:LEU:HD13	1:A:255:LEU:HD22	1.87	0.56
1:B:263:LYS:HE2	1:B:263:LYS:H	1.71	0.56
1:B:149:CYS:SG	1:B:158:GLN:HG2	2.46	0.55
1:B:231:PHE:HB2	1:B:237:ILE:HD11	1.87	0.55
1:A:201:GLN:O	1:A:205:GLU:HG3	2.06	0.55
1:A:272:ILE:HD13	1:A:328:ILE:HG21	1.90	0.54
1:A:241:ILE:O	1:A:245:LEU:HB2	2.08	0.54
1:B:237:ILE:CG2	1:B:238:MET:N	2.71	0.54
1:B:243:SER:HA	2:B:372:HOH:O	2.08	0.53
1:B:180:VAL:HG13	1:B:181:MET:N	2.23	0.53
1:B:169:TRP:CZ2	1:B:173:THR:HG21	2.44	0.52
1:A:172:LEU:HD22	1:A:188:LYS:HB3	1.92	0.52
1:B:175:LYS:HE3	1:B:177:ASP:O	2.10	0.51
1:B:277:ASP:HB2	1:B:285:ILE:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:ALA:CB	1:B:281:PRO:HB2	2.41	0.51
1:A:254:TRP:CZ3	1:A:286:LEU:HD21	2.47	0.50
1:B:258:ASP:O	1:B:261:ALA:HB2	2.11	0.50
1:B:262:GLU:HB3	1:B:263:LYS:HE2	1.94	0.50
1:B:155:PRO:HA	1:B:158:GLN:NE2	2.26	0.50
1:A:182:ARG:HD2	1:A:216:GLU:O	2.12	0.50
1:A:155:PRO:HA	1:A:158:GLN:HE21	1.76	0.50
1:A:174:GLN:HG3	2:A:371:HOH:O	2.12	0.50
1:B:328:ILE:HG23	1:B:329:GLU:N	2.26	0.49
1:B:231:PHE:HB3	1:B:237:ILE:HD13	1.95	0.49
1:A:288:THR:HB	1:A:289:PRO:HD2	1.95	0.49
1:A:191:GLU:HG3	1:A:200:LYS:HE3	1.94	0.49
1:B:283:CYS:HB2	1:B:296:TRP:CD1	2.49	0.48
1:B:279:ASN:O	1:B:281:PRO:HD3	2.14	0.48
1:B:236:THR:HG22	1:B:239:LEU:HD12	1.95	0.47
1:A:341:MET:CE	1:A:341:MET:HA	2.44	0.47
1:B:218:THR:HG22	1:B:219:LYS:N	2.28	0.47
1:B:317:ASP:N	1:B:321:LYS:HD2	2.24	0.47
1:B:226:LYS:CD	1:B:278:GLN:HE22	2.27	0.47
1:B:219:LYS:HG3	1:B:223:ASP:OD2	2.14	0.47
1:A:154:THR:OG1	1:A:157:GLU:HG3	2.15	0.47
1:A:297:ASN:HA	1:A:308:LEU:HD23	1.97	0.46
1:B:180:VAL:CG1	1:B:181:MET:N	2.77	0.46
1:B:152:ASN:HD22	1:B:152:ASN:HA	1.56	0.46
1:B:332:LEU:HD13	1:B:333:THR:N	2.30	0.46
1:A:212:ALA:CB	1:A:258:ASP:HB2	2.46	0.46
1:B:154:THR:OG1	1:B:157:GLU:HG3	2.17	0.45
1:B:286:LEU:HD22	1:B:328:ILE:CD1	2.44	0.45
1:B:317:ASP:H	1:B:321:LYS:HZ2	1.64	0.45
1:B:182:ARG:HD2	1:B:216:GLU:O	2.16	0.44
1:A:181:MET:HA	1:A:181:MET:HE2	1.99	0.44
1:B:317:ASP:N	1:B:321:LYS:HZ2	2.16	0.44
1:A:245:LEU:HA	1:A:245:LEU:HD12	1.76	0.44
1:A:197:GLU:H	1:A:197:GLU:CD	2.20	0.44
1:B:155:PRO:HA	1:B:158:GLN:HE21	1.82	0.44
1:A:231:PHE:C	1:A:237:ILE:HD12	2.38	0.44
1:A:247:ILE:HD11	1:A:320:ASP:OD1	2.18	0.43
1:B:174:GLN:HA	1:B:174:GLN:OE1	2.19	0.43
1:B:180:VAL:CG1	1:B:184:PHE:HB3	2.45	0.43
1:B:307:TYR:CZ	1:B:318:SER:HA	2.53	0.43
1:B:317:ASP:CB	1:B:321:LYS:HD2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:PRO:HD2	1:A:197:GLU:OE2	2.19	0.43
1:A:149:CYS:O	1:A:280:GLU:HA	2.19	0.43
1:A:161:PHE:O	1:A:165:VAL:HG23	2.19	0.43
1:A:325:MET:C	1:A:326:LYS:HG2	2.38	0.43
1:B:278:GLN:HB2	2:B:357:HOH:O	2.19	0.43
1:B:150:ILE:O	1:B:150:ILE:HG13	2.17	0.42
1:B:263:LYS:HE2	1:B:263:LYS:N	2.33	0.42
1:B:274:GLY:HA2	1:B:285:ILE:O	2.19	0.42
1:B:298:LYS:HD3	1:B:309:MET:HE2	2.02	0.42
1:B:260:GLN:HA	1:B:263:LYS:HG2	2.00	0.42
1:B:226:LYS:HZ2	1:B:278:GLN:HE22	1.61	0.42
1:B:309:MET:HA	1:B:314:GLU:O	2.20	0.42
1:A:288:THR:HB	1:A:289:PRO:CD	2.49	0.42
1:B:198:GLN:OE1	1:B:238:MET:HG2	2.19	0.42
1:A:245:LEU:O	1:A:249:ASN:ND2	2.53	0.41
1:B:237:ILE:HG23	1:B:238:MET:N	2.34	0.41
1:B:328:ILE:HG23	1:B:329:GLU:HG2	2.01	0.41
1:A:244:LEU:HD13	1:A:255:LEU:CD2	2.49	0.41
1:B:156:ASN:ND2	2:B:349:HOH:O	2.53	0.41
1:B:231:PHE:HB2	1:B:237:ILE:CD1	2.49	0.41
1:A:257:PHE:HA	2:A:368:HOH:O	2.20	0.41
1:A:186:ILE:HD13	1:A:208:SER:HA	2.03	0.41
1:B:255:LEU:HD22	1:B:256:THR:N	2.35	0.41
1:A:193:PHE:CE1	1:A:234:TYR:HB2	2.55	0.41
1:A:278:GLN:HA	1:A:278:GLN:OE1	2.21	0.41
1:B:168:ILE:HD11	1:B:234:TYR:CD2	2.56	0.41
1:B:185:LEU:HD23	1:B:185:LEU:O	2.21	0.41
1:B:179:THR:HB	1:B:218:THR:CG2	2.51	0.41
1:B:332:LEU:HD11	1:B:334:ALA:HB3	2.02	0.41
1:B:277:ASP:HB2	1:B:285:ILE:CD1	2.50	0.40
1:A:272:ILE:CD1	1:A:328:ILE:HG21	2.50	0.40
1:B:283:CYS:HB2	1:B:296:TRP:NE1	2.36	0.40
1:A:181:MET:CE	1:A:218:THR:HG22	2.52	0.40
1:A:323:PHE:HE1	1:A:328:ILE:HD11	1.86	0.40
1:B:152:ASN:CG	1:B:309:MET:HE3	2.41	0.40
1:B:308:LEU:HB2	1:B:316:TYR:HB2	2.03	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	179/221 (81%)	174 (97%)	4 (2%)	1 (1%)	25	30
1	B	189/221 (86%)	181 (96%)	6 (3%)	2 (1%)	14	15
All	All	368/442 (83%)	355 (96%)	10 (3%)	3 (1%)	19	23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	177	ASP
1	A	177	ASP
1	B	182	ARG

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	161/198 (81%)	150 (93%)	11 (7%)	16	20
1	B	168/198 (85%)	153 (91%)	15 (9%)	9	11
All	All	329/396 (83%)	303 (92%)	26 (8%)	12	15

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	187	GLU
1	A	197	GLU

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Mol	Chain	Res	Type
1	A	224	LEU
1	A	234	TYR
1	A	237	ILE
1	A	244	LEU
1	A	246	LEU
1	A	251	LYS
1	A	270	ASP
1	A	278	GLN
1	B	152	ASN
1	B	158	GLN
1	B	162	ARG
1	B	185	LEU
1	B	197	GLU
1	B	201	GLN
1	B	211	MET
1	B	224	LEU
1	B	237	ILE
1	B	238	MET
1	B	244	LEU
1	B	255	LEU
1	B	256	THR
1	B	314	GLU
1	B	332	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	156	ASN
1	A	158	GLN
1	A	253	HIS
1	A	260	GLN
1	B	152	ASN
1	B	158	GLN
1	B	217	GLN
1	B	249	ASN
1	B	278	GLN

5.3.3 RNA (i)

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 ⓘ

There are no monosaccharides 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	185/221 (83%)	0.36	5 (2%) 54	62	41, 58, 92, 115	0
1	B	193/221 (87%)	0.41	7 (3%) 42	49	41, 66, 104, 134	0
All	All	378/442 (85%)	0.39	12 (3%) 47	55	41, 62, 99, 134	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	176	THR	4.2
1	A	270	ASP	3.6
1	B	265	ALA	3.4
1	A	288	THR	2.8
1	A	345	HIS	2.8
1	A	249	ASN	2.8
1	B	263	LYS	2.6
1	B	260	GLN	2.4
1	B	342	HIS	2.3
1	B	218	THR	2.1
1	A	328	ILE	2.1
1	B	330	THR	2.1

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 monosaccharides 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.