



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2024 – 06:16 AM EST

PDB ID : 4QCC
Title : Structure of a cube-shaped, highly porous protein cage designed by fusing symmetric oligomeric domains
Authors : Lai, Y.-T.; Yeates, T.O.
Deposited on : 2014-05-10
Resolution : 7.08 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

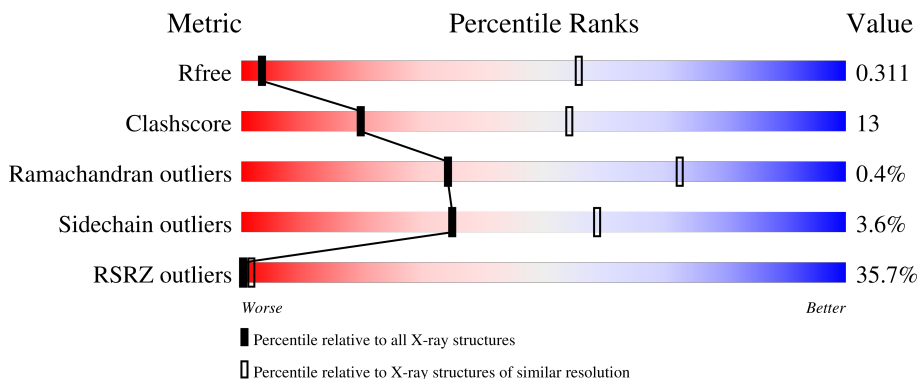
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.08 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	1004 (10.00-3.90)
Clashscore	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
Sidechain outliers	138945	1002 (10.00-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

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	291	
1	B	291	

2 Entry composition i

There is only 1 type of molecule in this entry. The entry contains 3954 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 2-dehydro-3-deoxy-6-phosphogalactonate aldolase, peptidyl-prolyl cis-trans isomerase chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	270	1977	1251	335	384	7	0	1	0
1	B	270	1977	1251	335	384	7	0	1	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	204	GLN	-	linker	UNP U6NBA4
A	205	LYS	-	linker	UNP U6NBA4
A	206	GLN	-	linker	UNP U6NBA4
A	207	LYS	-	linker	UNP U6NBA4
A	208	GLU	-	linker	UNP U6NBA4
A	209	GLN	-	linker	UNP U6NBA4
A	210	ARG	-	linker	UNP U6NBA4
A	211	GLN	-	linker	UNP U6NBA4
A	284	LEU	-	expression tag	UNP U6NBA4
A	285	GLU	-	expression tag	UNP U6NBA4
A	286	HIS	-	expression tag	UNP U6NBA4
A	287	HIS	-	expression tag	UNP U6NBA4
A	288	HIS	-	expression tag	UNP U6NBA4
A	289	HIS	-	expression tag	UNP U6NBA4
A	290	HIS	-	expression tag	UNP U6NBA4
A	291	HIS	-	expression tag	UNP U6NBA4
B	204	GLN	-	linker	UNP U6NBA4
B	205	LYS	-	linker	UNP U6NBA4
B	206	GLN	-	linker	UNP U6NBA4
B	207	LYS	-	linker	UNP U6NBA4
B	208	GLU	-	linker	UNP U6NBA4
B	209	GLN	-	linker	UNP U6NBA4
B	210	ARG	-	linker	UNP U6NBA4
B	211	GLN	-	linker	UNP U6NBA4

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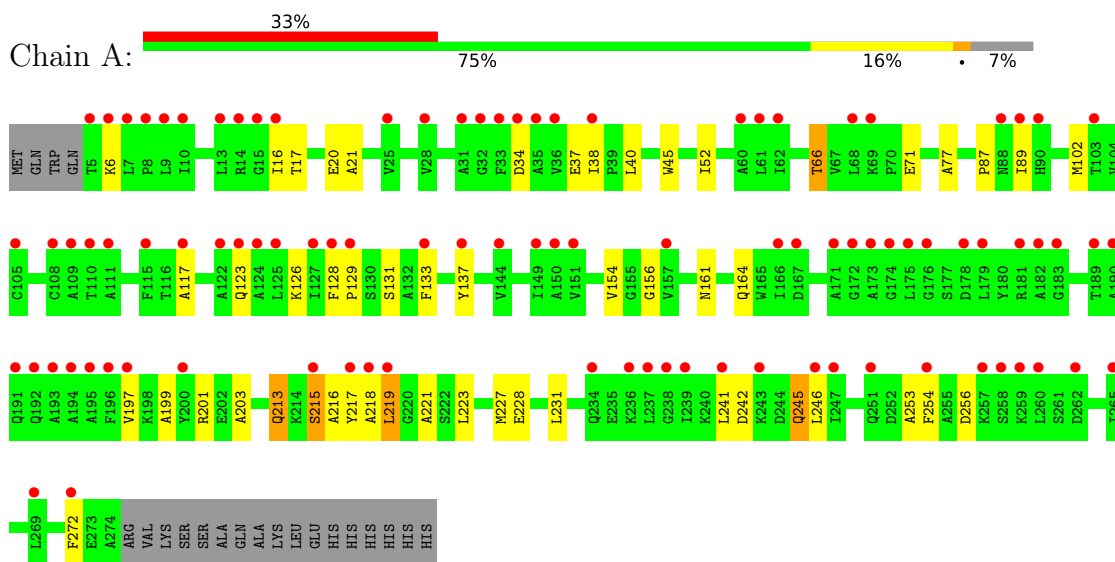
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Chain	Residue	Modelled	Actual	Comment	Reference
B	284	LEU	-	expression tag	UNP U6NBA4
B	285	GLU	-	expression tag	UNP U6NBA4
B	286	HIS	-	expression tag	UNP U6NBA4
B	287	HIS	-	expression tag	UNP U6NBA4
B	288	HIS	-	expression tag	UNP U6NBA4
B	289	HIS	-	expression tag	UNP U6NBA4
B	290	HIS	-	expression tag	UNP U6NBA4
B	291	HIS	-	expression tag	UNP U6NBA4

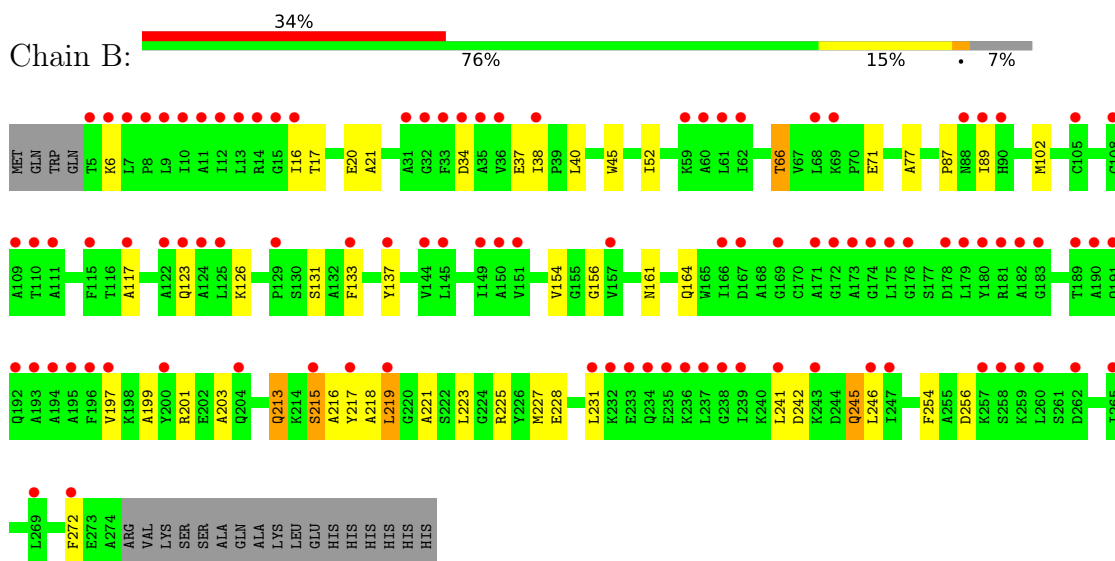
3 Residue-property plots i

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: 2-dehydro-3-deoxy-6-phosphogalactonate aldolase, peptidyl-prolyl cis-trans isomerase chimera



- Molecule 1: 2-dehydro-3-deoxy-6-phosphogalactonate aldolase, peptidyl-prolyl cis-trans isomerase chimera



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 3	Depositor
Cell constants a, b, c, α , β , γ	272.68Å 272.68Å 272.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.41 – 7.08 96.41 – 7.08	Depositor EDS
% Data completeness (in resolution range)	94.7 (96.41-7.08) 94.7 (96.41-7.08)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.55 (at 7.43Å)	Xtrriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.283 , 0.317 0.274 , 0.311	Depositor DCC
R_{free} test set	127 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	410.5	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 467.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.437 for k,h,-l	Xtrriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	3954	wwPDB-VP
Average B, all atoms (Å ²)	292.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.33% 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	0.42	0/2009	0.58	0/2729
1	B	0.42	0/2009	0.58	0/2729
All	All	0.42	0/4018	0.58	0/5458

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 [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	1977	0	1963	69	0
1	B	1977	0	1963	68	0
All	All	3954	0	3926	100	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 13.

All (100) 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:216:ALA:HB2	1:B:241:LEU:HD22	1.17	1.10
1:A:241:LEU:HD22	1:B:216:ALA:HB2	1.35	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ALA:HB2	1:B:241:LEU:CD2	1.90	1.01
1:A:216:ALA:CB	1:B:241:LEU:HD22	2.02	0.88
1:B:21:ALA:HB1	1:B:52:ILE:HD11	1.56	0.87
1:A:77:ALA:HA	1:A:102:MET:CE	2.05	0.87
1:B:77:ALA:HA	1:B:102:MET:CE	2.06	0.86
1:A:21:ALA:HB1	1:A:52:ILE:HD11	1.56	0.86
1:B:77:ALA:HA	1:B:102:MET:HE1	1.58	0.85
1:A:241:LEU:CD2	1:B:216:ALA:HB2	2.07	0.84
1:A:245:GLN:HB3	1:B:217:TYR:HD2	1.47	0.80
1:A:77:ALA:HA	1:A:102:MET:HE1	1.62	0.80
1:A:217:TYR:HD2	1:B:245:GLN:HB3	1.46	0.80
1:A:215:SER:HB3	1:B:272:PHE:CD1	2.22	0.75
1:A:241:LEU:HD13	1:B:216:ALA:HA	1.68	0.75
1:A:241:LEU:HD22	1:B:216:ALA:CB	2.15	0.74
1:A:227:MET:HE1	1:A:246:LEU:HG	1.71	0.71
1:A:216:ALA:HA	1:B:241:LEU:HD13	1.74	0.70
1:A:216:ALA:HB2	1:B:241:LEU:CG	2.23	0.68
1:B:197:VAL:HG12	1:B:201:ARG:HD2	1.77	0.67
1:B:227:MET:HE1	1:B:246:LEU:HG	1.77	0.67
1:A:131:SER:OG	1:A:156:GLY:HA3	1.95	0.67
1:A:197:VAL:HG12	1:A:201:ARG:HD2	1.77	0.67
1:B:131:SER:OG	1:B:156:GLY:HA3	1.95	0.66
1:B:77:ALA:CA	1:B:102:MET:HE1	2.25	0.65
1:A:245:GLN:HB3	1:B:217:TYR:CD2	2.30	0.65
1:A:242:ASP:HB2	1:B:213:GLN:HG3	1.77	0.65
1:A:241:LEU:HB3	1:B:216:ALA:CB	2.30	0.62
1:A:217:TYR:CD2	1:B:245:GLN:HB3	2.34	0.61
1:A:77:ALA:HB2	1:A:102:MET:HE3	1.83	0.61
1:A:227:MET:CE	1:A:246:LEU:HD11	2.32	0.60
1:B:161:ASN:O	1:B:164:GLN:HG2	2.02	0.60
1:B:227:MET:CE	1:B:246:LEU:HD11	2.32	0.59
1:A:161:ASN:O	1:A:164:GLN:HG2	2.02	0.59
1:A:272:PHE:CD1	1:B:215:SER:HB3	2.38	0.58
1:B:16:ILE:HG13	1:B:20:GLU:HG3	1.85	0.58
1:A:16:ILE:HG13	1:A:20:GLU:HG3	1.85	0.58
1:A:218:ALA:O	1:A:221:ALA:N	2.37	0.57
1:B:218:ALA:O	1:B:221:ALA:N	2.37	0.57
1:A:77:ALA:CB	1:A:102:MET:HE3	2.34	0.57
1:A:77:ALA:CA	1:A:102:MET:CE	2.82	0.57
1:A:256:ASP:OD1	1:B:228:GLU:OE2	2.21	0.57
1:A:216:ALA:CB	1:B:241:LEU:HD13	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:LEU:CG	1:B:216:ALA:HB2	2.35	0.57
1:A:216:ALA:CA	1:B:241:LEU:HD13	2.36	0.56
1:B:77:ALA:CA	1:B:102:MET:CE	2.82	0.56
1:B:197:VAL:CG1	1:B:201:ARG:HD2	2.36	0.56
1:A:242:ASP:HB2	1:B:213:GLN:CG	2.36	0.55
1:A:241:LEU:CB	1:B:216:ALA:HB2	2.37	0.55
1:A:197:VAL:CG1	1:A:201:ARG:HD2	2.36	0.55
1:B:133:PHE:HB3	1:B:137:TYR:CG	2.42	0.55
1:A:213:GLN:HG3	1:B:242:ASP:HB2	1.88	0.54
1:A:216:ALA:CB	1:B:241:LEU:HB3	2.37	0.54
1:B:89:ILE:HD12	1:B:117:ALA:HB2	1.90	0.54
1:B:38:ILE:HD11	1:B:52:ILE:CD1	2.38	0.54
1:B:227:MET:HE1	1:B:246:LEU:CG	2.37	0.54
1:A:89:ILE:HD12	1:A:117:ALA:HB2	1.89	0.54
1:A:38:ILE:HD11	1:A:52:ILE:CD1	2.38	0.54
1:A:133:PHE:HB3	1:A:137:TYR:CG	2.42	0.53
1:A:241:LEU:HB3	1:B:216:ALA:HB1	1.89	0.53
1:A:227:MET:HE1	1:A:246:LEU:CG	2.36	0.53
1:A:77:ALA:CA	1:A:102:MET:HE1	2.38	0.53
1:B:66:THR:HA	1:B:87:PRO:HD3	1.91	0.53
1:A:66:THR:HA	1:A:87:PRO:HD3	1.91	0.52
1:A:213:GLN:CG	1:B:242:ASP:HB2	2.40	0.52
1:A:254:PHE:HZ	1:B:231:LEU:HD22	1.74	0.51
1:A:253:ALA:O	1:B:225:ARG:NH1	2.44	0.51
1:A:216:ALA:HB1	1:B:241:LEU:HB3	1.93	0.51
1:A:199:ALA:O	1:A:203:ALA:CB	2.59	0.50
1:B:199:ALA:O	1:B:203:ALA:CB	2.59	0.50
1:B:227:MET:HE2	1:B:246:LEU:HD11	1.93	0.50
1:A:254:PHE:CZ	1:B:231:LEU:HD22	2.49	0.48
1:B:227:MET:CE	1:B:246:LEU:HG	2.43	0.48
1:A:216:ALA:HB2	1:B:241:LEU:CB	2.43	0.47
1:A:241:LEU:HD13	1:B:216:ALA:CA	2.39	0.47
1:A:231:LEU:HD22	1:B:254:PHE:HZ	1.79	0.47
1:B:71:GLU:H	1:B:71:GLU:CD	2.19	0.47
1:A:227:MET:HE2	1:A:246:LEU:HD11	1.97	0.46
1:A:71:GLU:H	1:A:71:GLU:CD	2.18	0.46
1:A:126:LYS:HE3	1:A:154:VAL:HG11	1.99	0.45
1:B:126:LYS:HE3	1:B:154:VAL:HG11	1.99	0.44
1:A:228:GLU:OE2	1:B:256:ASP:OD1	2.36	0.44
1:A:227:MET:CE	1:A:246:LEU:CD1	2.96	0.44
1:A:227:MET:CE	1:A:246:LEU:HG	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:THR:OG1	1:B:20:GLU:HG2	2.18	0.44
1:B:227:MET:CE	1:B:246:LEU:CG	2.96	0.44
1:A:227:MET:CE	1:A:246:LEU:CG	2.95	0.43
1:A:241:LEU:HB3	1:B:216:ALA:HB2	1.94	0.43
1:A:17:THR:OG1	1:A:20:GLU:HG2	2.18	0.43
1:B:216:ALA:O	1:B:219:LEU:HB2	2.19	0.43
1:A:216:ALA:O	1:A:219:LEU:HB2	2.19	0.42
1:B:77:ALA:CB	1:B:102:MET:HE3	2.50	0.42
1:B:227:MET:CE	1:B:246:LEU:CD1	2.96	0.41
1:A:40:LEU:HD22	1:A:45:TRP:CD2	2.56	0.41
1:B:40:LEU:HD22	1:B:45:TRP:CD2	2.56	0.41
1:A:128:PHE:HA	1:A:129:PRO:HA	1.94	0.41
1:A:6:LYS:HB2	1:A:34:ASP:OD2	2.21	0.41
1:A:241:LEU:HD22	1:B:216:ALA:CA	2.50	0.41
1:B:6:LYS:HB2	1:B:34:ASP:OD2	2.21	0.41
1:B:77:ALA:HB2	1:B:102:MET:HE3	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	268/291 (92%)	263 (98%)	4 (2%)	1 (0%)	34	72
1	B	268/291 (92%)	263 (98%)	4 (2%)	1 (0%)	34	72
All	All	536/582 (92%)	526 (98%)	8 (2%)	2 (0%)	34	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	LEU
1	B	219	LEU

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	195/222 (88%)	188 (96%)	7 (4%)	35	59
1	B	195/222 (88%)	188 (96%)	7 (4%)	35	59
All	All	390/444 (88%)	376 (96%)	14 (4%)	35	59

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	66	THR
1	A	123	GLN
1	A	213	GLN
1	A	215	SER
1	A	223	LEU
1	A	245	GLN
1	B	37	GLU
1	B	66	THR
1	B	123	GLN
1	B	213	GLN
1	B	215	SER
1	B	223	LEU
1	B	245	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	GLN
1	A	251	GLN
1	A	263	GLN
1	A	270	GLN
1	B	245	GLN
1	B	251	GLN
1	B	263	GLN
1	B	270	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 [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	270/291 (92%)	1.69	95 (35%) 0 2	120, 289, 414, 440	1 (0%)
1	B	270/291 (92%)	1.72	98 (36%) 0 1	118, 285, 406, 443	1 (0%)
All	All	540/582 (92%)	1.70	193 (35%) 0 1	118, 286, 414, 443	2 (0%)

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	259	LYS	11.6
1	B	258	SER	9.9
1	A	259	LYS	9.9
1	A	258	SER	9.8
1	B	260	LEU	6.2
1	A	260	LEU	5.8
1	B	192	GLN	5.4
1	A	34	ASP	5.2
1	A	192	GLN	5.1
1	B	34	ASP	5.0
1	A	123	GLN	4.7
1	B	109	ALA	4.7
1	A	109	ALA	4.6
1	A	8	PRO	4.6
1	B	7	LEU	4.6
1	B	123	GLN	4.5
1	A	150	ALA	4.5
1	B	175	LEU	4.5
1	A	193	ALA	4.4
1	A	179	LEU	4.4
1	B	171	ALA	4.4
1	B	5	THR	4.3
1	B	182	ALA	4.3
1	B	33	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	7	LEU	4.3
1	B	179	LEU	4.3
1	B	8	PRO	4.2
1	B	124	ALA	4.2
1	A	9	LEU	4.2
1	B	9	LEU	4.2
1	B	196	PHE	4.1
1	A	171	ALA	4.1
1	B	13	LEU	4.1
1	A	33	PHE	4.0
1	A	124	ALA	4.0
1	A	238	GLY	4.0
1	A	175	LEU	4.0
1	A	5	THR	4.0
1	B	193	ALA	3.9
1	A	36	VAL	3.9
1	A	196	PHE	3.9
1	A	219	LEU	3.9
1	B	14	ARG	3.8
1	A	149	ILE	3.8
1	A	262	ASP	3.8
1	B	237	LEU	3.8
1	A	110	THR	3.7
1	B	110	THR	3.7
1	B	36	VAL	3.7
1	A	13	LEU	3.7
1	B	241	LEU	3.6
1	B	272	PHE	3.6
1	B	234	GLN	3.6
1	B	183	GLY	3.5
1	A	125	LEU	3.5
1	B	236	LYS	3.5
1	B	191	GLN	3.5
1	B	6	LYS	3.4
1	A	191	GLN	3.4
1	A	272	PHE	3.4
1	A	35	ALA	3.4
1	A	237	LEU	3.4
1	B	68	LEU	3.4
1	B	265	ILE	3.3
1	A	241	LEU	3.3
1	B	167	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	60	ALA	3.3
1	A	265	ILE	3.2
1	B	149	ILE	3.2
1	A	14	ARG	3.2
1	A	6	LYS	3.2
1	B	35	ALA	3.2
1	B	60	ALA	3.2
1	B	125	LEU	3.2
1	A	182	ALA	3.2
1	A	173	ALA	3.2
1	B	111	ALA	3.2
1	B	243	LYS	3.2
1	A	61	LEU	3.1
1	B	166	ILE	3.1
1	B	197	VAL	3.1
1	B	150	ALA	3.1
1	A	178	ASP	3.1
1	B	61	LEU	3.1
1	A	194	ALA	3.1
1	A	68	LEU	3.1
1	A	243	LYS	3.1
1	B	16	ILE	3.0
1	A	215	SER	3.0
1	A	69	LYS	3.0
1	A	197	VAL	3.0
1	B	219	LEU	3.0
1	B	88	ASN	3.0
1	B	269	LEU	3.0
1	A	167	ASP	3.0
1	B	129	PRO	3.0
1	A	129	PRO	3.0
1	B	174	GLY	3.0
1	A	247	ILE	3.0
1	B	178	ASP	3.0
1	B	173	ALA	3.0
1	B	90	HIS	2.9
1	B	195	ALA	2.9
1	A	234	GLN	2.9
1	B	69	LYS	2.9
1	B	238	GLY	2.9
1	B	31	ALA	2.9
1	B	262	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	89	ILE	2.9
1	B	32	GLY	2.9
1	B	194	ALA	2.9
1	A	195	ALA	2.8
1	A	16	ILE	2.8
1	A	15	GLY	2.8
1	B	115	PHE	2.8
1	A	111	ALA	2.8
1	A	189	THR	2.8
1	B	15	GLY	2.8
1	A	239	ILE	2.8
1	B	239	ILE	2.8
1	B	172	GLY	2.8
1	A	174	GLY	2.8
1	A	166	ILE	2.8
1	A	172	GLY	2.7
1	A	31	ALA	2.7
1	A	217	TYR	2.7
1	B	200	TYR	2.6
1	A	176	GLY	2.6
1	A	218	ALA	2.6
1	A	236	LYS	2.6
1	B	122	ALA	2.6
1	A	200	TYR	2.6
1	B	157	VAL	2.6
1	B	233	GLU	2.6
1	A	144	VAL	2.6
1	B	144	VAL	2.6
1	A	183	GLY	2.6
1	A	90	HIS	2.5
1	A	32	GLY	2.5
1	B	38	ILE	2.5
1	B	247	ILE	2.5
1	A	151	VAL	2.5
1	B	176	GLY	2.5
1	B	215	SER	2.5
1	B	151	VAL	2.5
1	B	189	THR	2.4
1	A	137	TYR	2.4
1	B	169	GLY	2.4
1	A	117	ALA	2.4
1	B	246	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	235	GLU	2.4
1	A	115	PHE	2.4
1	A	62	ILE	2.4
1	A	190	ALA	2.4
1	B	117	ALA	2.3
1	A	246	LEU	2.3
1	A	257	LYS	2.3
1	B	137	TYR	2.3
1	A	133	PHE	2.3
1	A	251	GLN	2.3
1	B	217	TYR	2.3
1	A	38	ILE	2.3
1	A	88	ASN	2.3
1	B	133	PHE	2.3
1	A	122	ALA	2.3
1	A	269	LEU	2.3
1	B	12	ILE	2.3
1	B	62	ILE	2.3
1	A	108	CYS	2.2
1	B	231	LEU	2.2
1	B	10	ILE	2.2
1	B	232	LYS	2.2
1	B	181	ARG	2.2
1	A	28	VAL	2.2
1	A	105	CYS	2.2
1	A	128	PHE	2.2
1	A	254	PHE	2.2
1	B	108	CYS	2.2
1	B	59	LYS	2.2
1	A	25	VAL	2.1
1	A	181	ARG	2.1
1	A	157	VAL	2.1
1	A	127	ILE	2.1
1	A	10	ILE	2.1
1	B	180	TYR	2.1
1	B	190	ALA	2.1
1	B	11	ALA	2.1
1	A	89	ILE	2.1
1	A	103	THR	2.1
1	B	257	LYS	2.0
1	B	105	CYS	2.0
1	B	204	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	145	LEU	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.