Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:54 PM GMT

PDB ID	:	3VDX
Title	:	Structure of a 16 nm protein cage designed by fusing symmetric oligomeric domains
Authors	:	Lai, Y.-T.; Cascio, D.; Yeates, T.O.
Deposited on	:	2012-01-06
Resolution	:	3.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

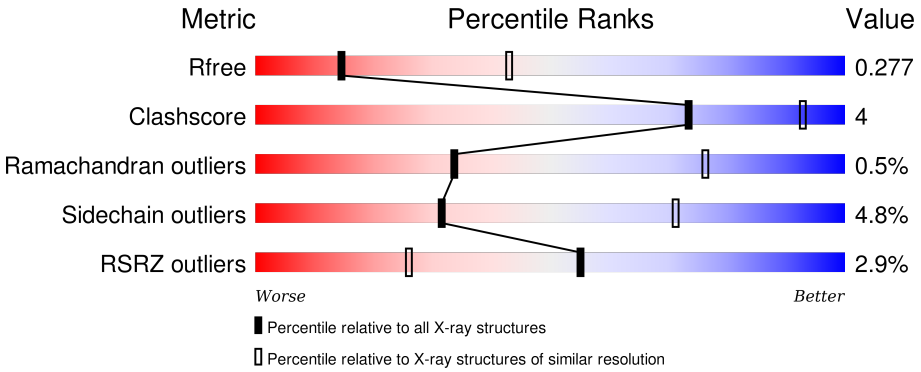
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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. 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	456	3% 81% 14%
1	B	456	4% 83% 11%
1	C	456	% 85% 11%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10149 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 Designed 16nm tetrahedral protein cage containing Non-haem bromoperoxidase BPO-A2 and Matrix protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3383	2161	569	645	8			
1	B	438	Total	C	N	O	S	0	0	0
			3383	2161	569	645	8			
1	C	438	Total	C	N	O	S	0	0	0
			3383	2161	569	645	8			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	VAL	GLN	CONFLICT	UNP P29715
A	118	ALA	LYS	CONFLICT	UNP P29715
A	278	ALA	-	LINKER	UNP P29715
A	279	LEU	-	LINKER	UNP P29715
A	280	GLU	-	LINKER	UNP P29715
A	281	ALA	-	LINKER	UNP P29715
A	282	GLN	-	LINKER	UNP P29715
A	283	LYS	-	LINKER	UNP P29715
A	284	GLN	-	LINKER	UNP P29715
A	285	LYS	-	LINKER	UNP P29715
A	448	LEU	-	EXPRESSION TAG	UNP P03485
A	449	GLU	-	EXPRESSION TAG	UNP P03485
A	450	HIS	-	EXPRESSION TAG	UNP P03485
A	451	HIS	-	EXPRESSION TAG	UNP P03485
A	452	HIS	-	EXPRESSION TAG	UNP P03485
A	453	HIS	-	EXPRESSION TAG	UNP P03485
A	454	HIS	-	EXPRESSION TAG	UNP P03485
A	455	HIS	-	EXPRESSION TAG	UNP P03485
B	24	VAL	GLN	CONFLICT	UNP P29715
B	118	ALA	LYS	CONFLICT	UNP P29715
B	278	ALA	-	LINKER	UNP P29715
B	279	LEU	-	LINKER	UNP P29715

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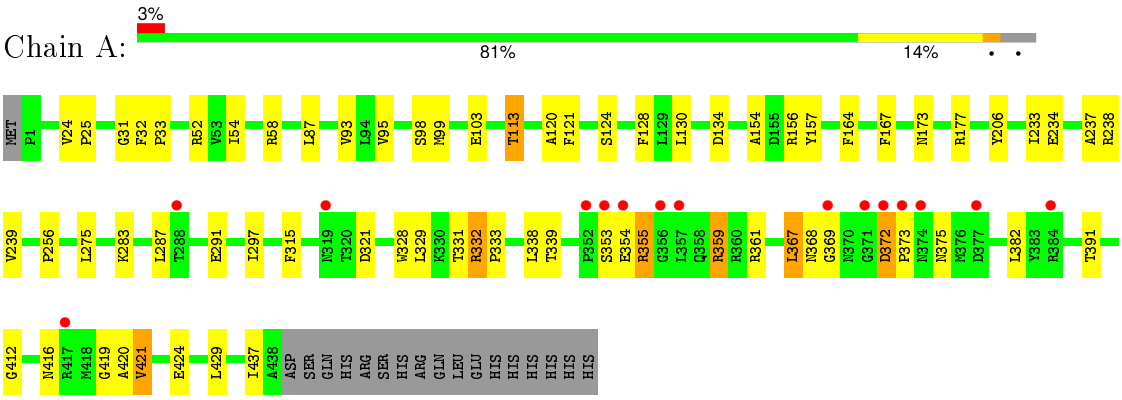
Chain	Residue	Modelled	Actual	Comment	Reference
B	280	GLU	-	LINKER	UNP P29715
B	281	ALA	-	LINKER	UNP P29715
B	282	GLN	-	LINKER	UNP P29715
B	283	LYS	-	LINKER	UNP P29715
B	284	GLN	-	LINKER	UNP P29715
B	285	LYS	-	LINKER	UNP P29715
B	448	LEU	-	EXPRESSION TAG	UNP P03485
B	449	GLU	-	EXPRESSION TAG	UNP P03485
B	450	HIS	-	EXPRESSION TAG	UNP P03485
B	451	HIS	-	EXPRESSION TAG	UNP P03485
B	452	HIS	-	EXPRESSION TAG	UNP P03485
B	453	HIS	-	EXPRESSION TAG	UNP P03485
B	454	HIS	-	EXPRESSION TAG	UNP P03485
B	455	HIS	-	EXPRESSION TAG	UNP P03485
C	24	VAL	GLN	CONFLICT	UNP P29715
C	118	ALA	LYS	CONFLICT	UNP P29715
C	278	ALA	-	LINKER	UNP P29715
C	279	LEU	-	LINKER	UNP P29715
C	280	GLU	-	LINKER	UNP P29715
C	281	ALA	-	LINKER	UNP P29715
C	282	GLN	-	LINKER	UNP P29715
C	283	LYS	-	LINKER	UNP P29715
C	284	GLN	-	LINKER	UNP P29715
C	285	LYS	-	LINKER	UNP P29715
C	448	LEU	-	EXPRESSION TAG	UNP P03485
C	449	GLU	-	EXPRESSION TAG	UNP P03485
C	450	HIS	-	EXPRESSION TAG	UNP P03485
C	451	HIS	-	EXPRESSION TAG	UNP P03485
C	452	HIS	-	EXPRESSION TAG	UNP P03485
C	453	HIS	-	EXPRESSION TAG	UNP P03485
C	454	HIS	-	EXPRESSION TAG	UNP P03485
C	455	HIS	-	EXPRESSION TAG	UNP P03485

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.

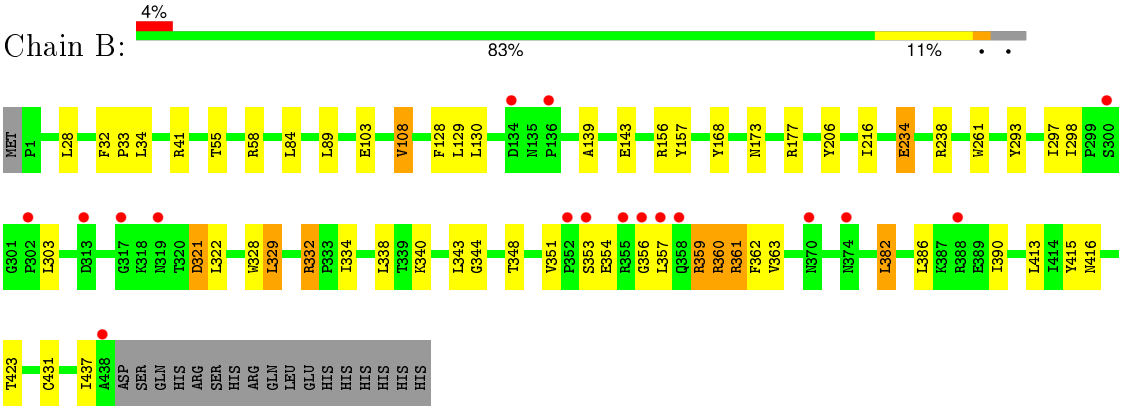
• Molecule 1: Designed 16nm tetrahedral protein cage containing Non-haem bromoperoxidase BPO-A2 and Matrix protein 1

Chain A:



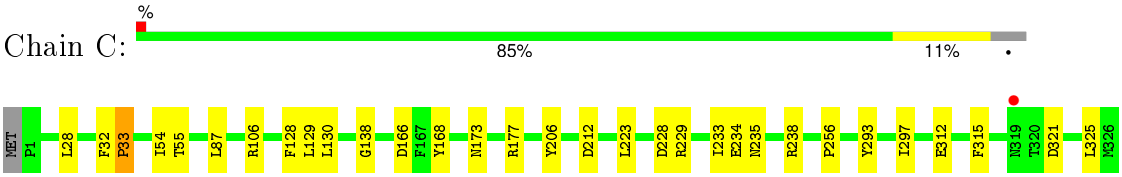
• Molecule 1: Designed 16nm tetrahedral protein cage containing Non-haem bromoperoxidase BPO-A2 and Matrix protein 1

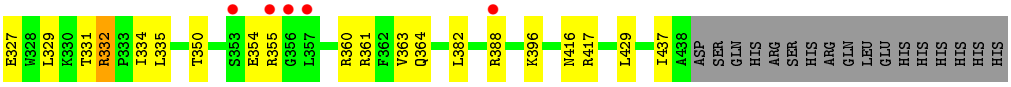
Chain B:



• Molecule 1: Designed 16nm tetrahedral protein cage containing Non-haem bromoperoxidase BPO-A2 and Matrix protein 1

Chain C:




E327
W328
L329
K330
T331
R332
P333
I334
L335
T350
S353
E354
R355
G356
L357
R360
R361
F362
V363
Q364
L382
R388
K396
N416
R417
L429
I437
A438
ASP
SER
GLN
HIS
ARG
SER
HIS
ARG
GLN
LEU
GLU
HIS
HIS
HIS
HIS
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HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	122.59Å 127.71Å 204.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.73 – 3.00 19.73 – 3.00	Depositor EDS
% Data completeness (in resolution range)	68.6 (19.73-3.00) 68.6 (19.73-3.00)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 2.98Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.229 , 0.281 0.220 , 0.277	Depositor DCC
R_{free} test set	1133 reflections (5.12%)	DCC
Wilson B-factor (Å^2)	41.4	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 18.4	EDS
Estimated twinning fraction	0.029 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 22135 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	10149	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.21	0/3460	0.38	0/4709
1	B	0.22	0/3460	0.39	0/4709
1	C	0.21	0/3460	0.37	0/4709
All	All	0.21	0/10380	0.38	0/14127

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	3383	0	3322	34	0
1	B	3383	0	3322	30	0
1	C	3383	0	3322	19	0
All	All	10149	0	9966	82	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 4.

All (82) 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:B:354:GLU:HG3	1:B:356:GLY:H	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:TRP:O	1:B:332:ARG:NH1	2.29	0.65
1:B:322:LEU:HD13	1:B:351:VAL:HG11	1.79	0.65
1:C:130:LEU:HB2	1:C:206:TYR:HB2	1.80	0.63
1:A:297:ILE:HD11	1:A:437:ILE:HB	1.80	0.62
1:C:168:TYR:O	1:C:173:ASN:ND2	2.31	0.61
1:A:130:LEU:HB2	1:A:206:TYR:HB2	1.84	0.59
1:A:353:SER:O	1:A:355:ARG:NH2	2.30	0.59
1:C:332:ARG:HG2	1:C:335:LEU:HD12	1.84	0.58
1:A:354:GLU:OE1	1:A:359:ARG:NH2	2.37	0.58
1:A:173:ASN:HB3	1:A:177:ARG:HB2	1.86	0.57
1:A:328:TRP:O	1:A:332:ARG:NH1	2.37	0.56
1:B:344:GLY:O	1:B:348:THR:OG1	2.22	0.56
1:C:138:GLY:O	1:C:235:ASN:ND2	2.39	0.55
1:B:329:LEU:HD11	1:B:343:LEU:HD12	1.88	0.55
1:B:297:ILE:HD12	1:B:437:ILE:HD12	1.87	0.55
1:B:321:ASP:N	1:B:321:ASP:OD1	2.41	0.54
1:B:130:LEU:HB2	1:B:206:TYR:HB2	1.88	0.54
1:A:372:ASP:HB3	1:A:375:ASN:HB3	1.90	0.53
1:A:412:GLY:O	1:A:416:ASN:ND2	2.35	0.53
1:B:303:LEU:HD12	1:B:334:ILE:HD12	1.90	0.53
1:B:293:TYR:HD2	1:B:431:CYS:HB3	1.74	0.53
1:A:291:GLU:HB2	1:A:315:PHE:HE2	1.75	0.52
1:C:327:GLU:OE1	1:C:360:ARG:NH2	2.43	0.52
1:C:293:TYR:OH	1:C:396:LYS:NZ	2.36	0.51
1:B:359:ARG:NH2	1:B:415:TYR:O	2.44	0.51
1:A:121:PHE:HB3	1:A:124:SER:HB3	1.93	0.50
1:C:54:ILE:HD13	1:C:87:LEU:HD23	1.94	0.49
1:B:168:TYR:O	1:B:173:ASN:ND2	2.45	0.49
1:A:419:GLY:HA2	1:A:420:ALA:HB3	1.94	0.48
1:C:315:PHE:CE1	1:C:350:THR:HG21	2.48	0.48
1:A:367:LEU:HD23	1:A:412:GLY:HA2	1.95	0.47
1:A:233:ILE:HG13	1:A:237:ALA:HB3	1.96	0.47
1:A:372:ASP:CB	1:A:375:ASN:HB3	2.45	0.47
1:B:298:ILE:HD11	1:B:343:LEU:HD11	1.96	0.47
1:B:41:ARG:NH1	1:B:261:TRP:O	2.48	0.47
1:A:154:ALA:O	1:B:41:ARG:NH2	2.34	0.47
1:B:108:VAL:HG11	1:B:216:ILE:HG12	1.97	0.47
1:A:93:VAL:HG11	1:A:275:LEU:HD21	1.97	0.46
1:A:283:LYS:NZ	1:A:424:GLU:OE1	2.32	0.46
1:C:233:ILE:HG12	1:C:238:ARG:HG2	1.97	0.46
1:B:173:ASN:HB3	1:B:177:ARG:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:PHE:HA	1:C:33:PRO:HA	1.75	0.46
1:B:234:GLU:HA	1:B:238:ARG:HG3	1.97	0.46
1:A:32:PHE:HB2	1:A:99:MET:SD	2.56	0.46
1:C:364:GLN:NE2	1:C:416:ASN:OD1	2.42	0.45
1:A:58:ARG:NE	1:A:103:GLU:OE2	2.41	0.45
1:A:368:ASN:N	1:A:368:ASN:OD1	2.49	0.45
1:B:382:LEU:HD22	1:B:386:LEU:HG	1.98	0.45
1:C:173:ASN:HB3	1:C:177:ARG:HB2	1.99	0.45
1:B:156:ARG:NH2	1:B:157:TYR:OH	2.50	0.45
1:B:361:ARG:HD2	1:B:362:PHE:N	2.32	0.45
1:A:25:PRO:HA	1:A:52:ARG:HB3	1.99	0.44
1:A:95:VAL:HG22	1:A:120:ALA:HB3	1.99	0.44
1:A:32:PHE:HA	1:A:33:PRO:HA	1.76	0.44
1:B:351:VAL:HG22	1:B:353:SER:H	1.81	0.44
1:B:84:LEU:HD23	1:B:89:LEU:HD12	1.98	0.44
1:B:58:ARG:NE	1:B:103:GLU:OE2	2.45	0.44
1:B:332:ARG:HB3	1:B:340:LYS:NZ	2.33	0.43
1:B:129:LEU:O	1:B:139:ALA:N	2.43	0.43
1:C:28:LEU:HB2	1:C:55:THR:HG22	2.00	0.43
1:A:372:ASP:OD1	1:A:373:PRO:HD2	2.19	0.43
1:A:54:ILE:HD13	1:A:87:LEU:HD23	2.01	0.42
1:B:357:LEU:HA	1:B:357:LEU:HD23	1.87	0.42
1:C:166:ASP:HA	1:C:229:ARG:HD2	2.02	0.42
1:C:106:ARG:NE	1:C:212:ASP:OD2	2.52	0.42
1:C:321:ASP:HB2	1:C:355:ARG:NH2	2.34	0.42
1:B:32:PHE:HA	1:B:33:PRO:HA	1.75	0.42
1:A:420:ALA:HA	1:A:421:VAL:HA	1.70	0.42
1:B:28:LEU:HB2	1:B:55:THR:HG22	2.02	0.41
1:A:156:ARG:NH2	1:A:157:TYR:OH	2.53	0.41
1:A:332:ARG:HG3	1:A:333:PRO:HD2	2.01	0.41
1:A:164:PHE:HA	1:A:167:PHE:HB3	2.02	0.41
1:C:297:ILE:HD12	1:C:437:ILE:HB	2.02	0.41
1:A:321:ASP:OD1	1:A:321:ASP:N	2.54	0.41
1:A:31:GLY:HA3	1:A:98:SER:HB3	2.03	0.41
1:A:234:GLU:HA	1:A:238:ARG:HG3	2.03	0.41
1:A:113:THR:O	1:A:113:THR:OG1	2.27	0.41
1:C:315:PHE:HE1	1:C:350:THR:HG21	1.84	0.40
1:A:24:VAL:HA	1:A:25:PRO:HD3	1.93	0.40
1:C:234:GLU:HA	1:C:238:ARG:HG3	2.02	0.40
1:B:143:GLU:N	1:B:143:GLU:OE1	2.49	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	436/456 (96%)	412 (94%)	22 (5%)	2 (0%)	34	76
1	B	436/456 (96%)	396 (91%)	37 (8%)	3 (1%)	26	70
1	C	436/456 (96%)	411 (94%)	23 (5%)	2 (0%)	34	76
All	All	1308/1368 (96%)	1219 (93%)	82 (6%)	7 (0%)	34	76

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	369	GLY
1	B	416	ASN
1	A	256	PRO
1	B	34	LEU
1	B	360	ARG
1	C	256	PRO
1	C	33	PRO

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	352/370 (95%)	333 (95%)	19 (5%)	27	66
1	B	352/370 (95%)	337 (96%)	15 (4%)	35	75
1	C	352/370 (95%)	335 (95%)	17 (5%)	31	71
All	All	1056/1110 (95%)	1005 (95%)	51 (5%)	31	71

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	THR
1	A	128	PHE
1	A	134	ASP
1	A	239	VAL
1	A	287	LEU
1	A	329	LEU
1	A	331	THR
1	A	332	ARG
1	A	338	LEU
1	A	339	THR
1	A	355	ARG
1	A	359	ARG
1	A	361	ARG
1	A	367	LEU
1	A	372	ASP
1	A	382	LEU
1	A	391	THR
1	A	421	VAL
1	A	429	LEU
1	B	108	VAL
1	B	128	PHE
1	B	234	GLU
1	B	321	ASP
1	B	329	LEU
1	B	332	ARG
1	B	338	LEU
1	B	359	ARG
1	B	360	ARG
1	B	361	ARG
1	B	363	VAL
1	B	382	LEU
1	B	390	ILE
1	B	413	LEU
1	B	423	THR
1	C	128	PHE
1	C	129	LEU
1	C	223	LEU
1	C	228	ASP
1	C	312	GLU
1	C	325	LEU
1	C	329	LEU
1	C	331	THR

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Mol	Chain	Res	Type
1	C	332	ARG
1	C	334	ILE
1	C	354	GLU
1	C	361	ARG
1	C	363	VAL
1	C	382	LEU
1	C	388	ARG
1	C	417	ARG
1	C	429	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates 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	438/456 (96%)	-0.25	15 (3%) 49 21	25, 48, 96, 136	0
1	B	438/456 (96%)	-0.23	17 (3%) 43 18	29, 53, 98, 143	0
1	C	438/456 (96%)	-0.47	6 (1%) 78 51	24, 43, 76, 127	0
All	All	1314/1368 (96%)	-0.32	38 (2%) 55 26	24, 47, 95, 143	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	373	PRO	6.2
1	A	352	PRO	5.1
1	A	356	GLY	4.8
1	B	356	GLY	4.8
1	B	357	LEU	4.5
1	A	372	ASP	3.9
1	A	417	ARG	3.8
1	C	353	SER	3.7
1	B	352	PRO	3.6
1	B	319	ASN	3.4
1	A	371	GLY	3.1
1	C	319	ASN	3.0
1	B	374	ASN	2.9
1	C	356	GLY	2.8
1	B	438	ALA	2.8
1	A	353	SER	2.7
1	A	357	LEU	2.7
1	C	357	LEU	2.7
1	B	317	GLY	2.6
1	A	377	ASP	2.6
1	B	355	ARG	2.6
1	A	384	ARG	2.5
1	A	319	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	369	GLY	2.4
1	A	374	ASN	2.4
1	C	355	ARG	2.4
1	B	300	SER	2.4
1	B	302	PRO	2.4
1	B	370	ASN	2.3
1	B	134	ASP	2.3
1	B	358	GLN	2.3
1	B	313	ASP	2.3
1	A	288	THR	2.3
1	A	354	GLU	2.2
1	B	353	SER	2.1
1	B	136	PRO	2.1
1	C	388	ARG	2.0
1	B	388	ARG	2.0

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.