



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:45 am GMT

PDB ID : 2QZV
Title : Draft Crystal Structure of the Vault Shell at 9 Angstroms Resolution
Authors : Anderson, D.H.; Kickhoefer, V.A.; Sievers, S.A.; Rome, L.H.; Eisenberg, D.
Deposited on : 2007-08-17
Resolution : 9.00 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

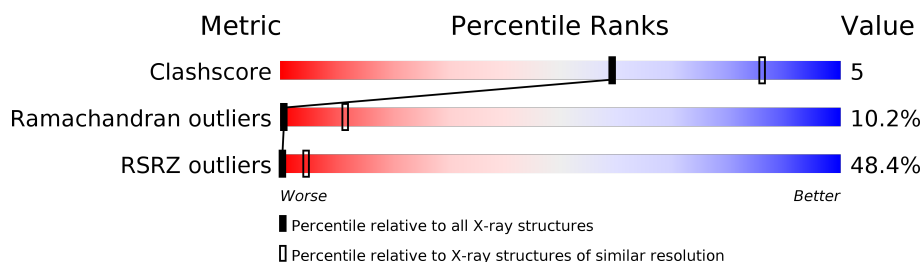
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 9.00 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))
Clashscore	112137	1036 (11.50-3.80)
Ramachandran outliers	110173	1004 (11.50-3.76)
RSRZ outliers	101464	1004 (11.50-3.72)

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 $\leq 5\%$. 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	873	<div> <div>48%</div> <div> <div>71%</div> <div>14%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	873	<div> <div>35%</div> <div> <div>72%</div> <div>13%</div> <div>•</div> <div>14%</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7404 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 Major vault protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	749	Total	C	N	O	0	0	0
			3702	2204	749	749			
1	B	749	Total	C	N	O	0	0	0
			3702	2204	749	749			

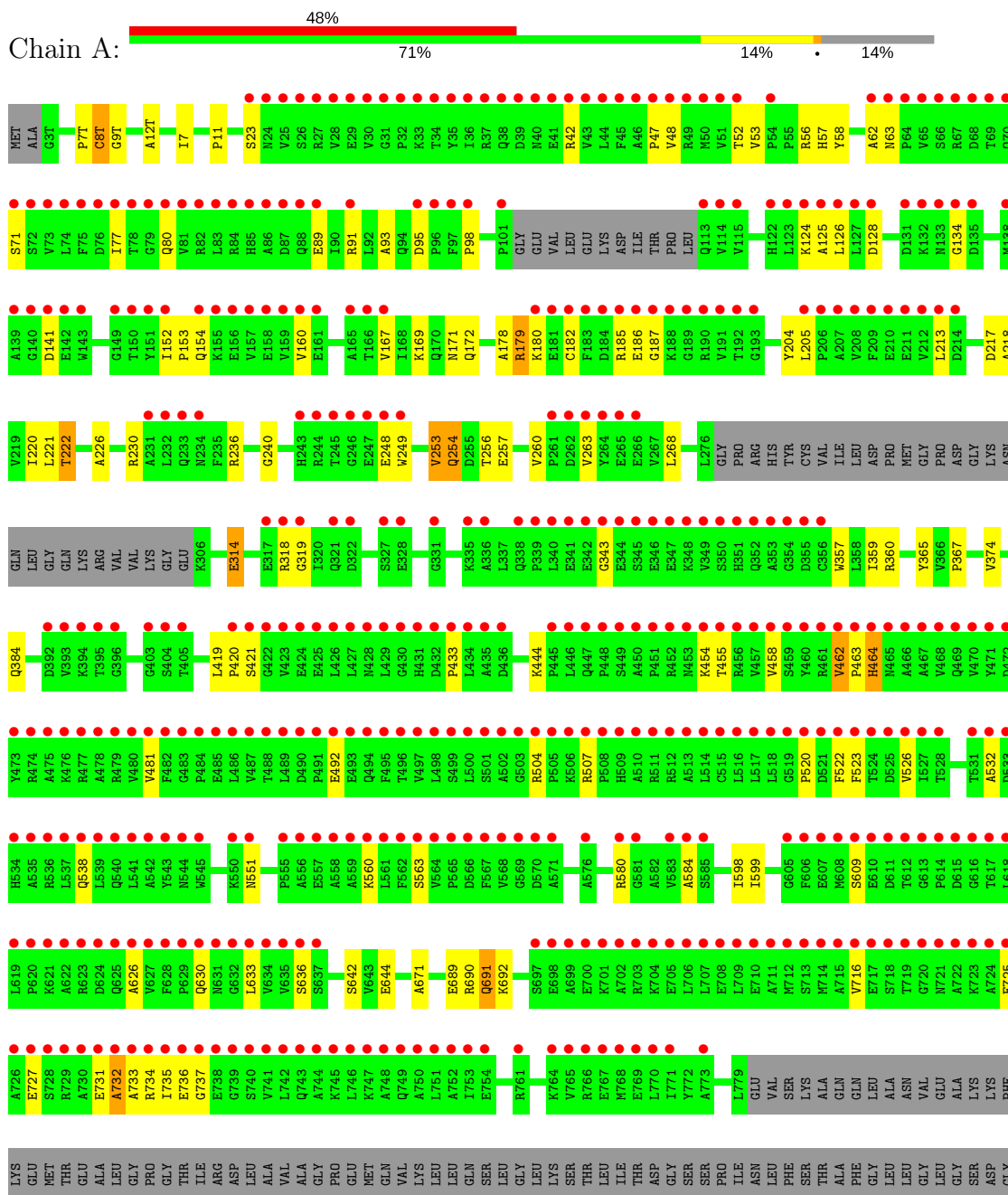
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1T	MET	-	EXPRESSION TAG	UNP Q62667
A	2T	ALA	-	EXPRESSION TAG	UNP Q62667
A	3T	GLY	-	EXPRESSION TAG	UNP Q62667
A	4T	CYS	-	EXPRESSION TAG	UNP Q62667
A	5T	GLY	-	EXPRESSION TAG	UNP Q62667
A	6T	CYS	-	EXPRESSION TAG	UNP Q62667
A	7T	PRO	-	EXPRESSION TAG	UNP Q62667
A	8T	CYS	-	EXPRESSION TAG	UNP Q62667
A	9T	GLY	-	EXPRESSION TAG	UNP Q62667
A	10T	CYS	-	EXPRESSION TAG	UNP Q62667
A	11T	GLY	-	EXPRESSION TAG	UNP Q62667
A	12T	ALA	-	EXPRESSION TAG	UNP Q62667
B	1T	MET	-	EXPRESSION TAG	UNP Q62667
B	2T	ALA	-	EXPRESSION TAG	UNP Q62667
B	3T	GLY	-	EXPRESSION TAG	UNP Q62667
B	4T	CYS	-	EXPRESSION TAG	UNP Q62667
B	5T	GLY	-	EXPRESSION TAG	UNP Q62667
B	6T	CYS	-	EXPRESSION TAG	UNP Q62667
B	7T	PRO	-	EXPRESSION TAG	UNP Q62667
B	8T	CYS	-	EXPRESSION TAG	UNP Q62667
B	9T	GLY	-	EXPRESSION TAG	UNP Q62667
B	10T	CYS	-	EXPRESSION TAG	UNP Q62667
B	11T	GLY	-	EXPRESSION TAG	UNP Q62667
B	12T	ALA	-	EXPRESSION TAG	UNP Q62667

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 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.

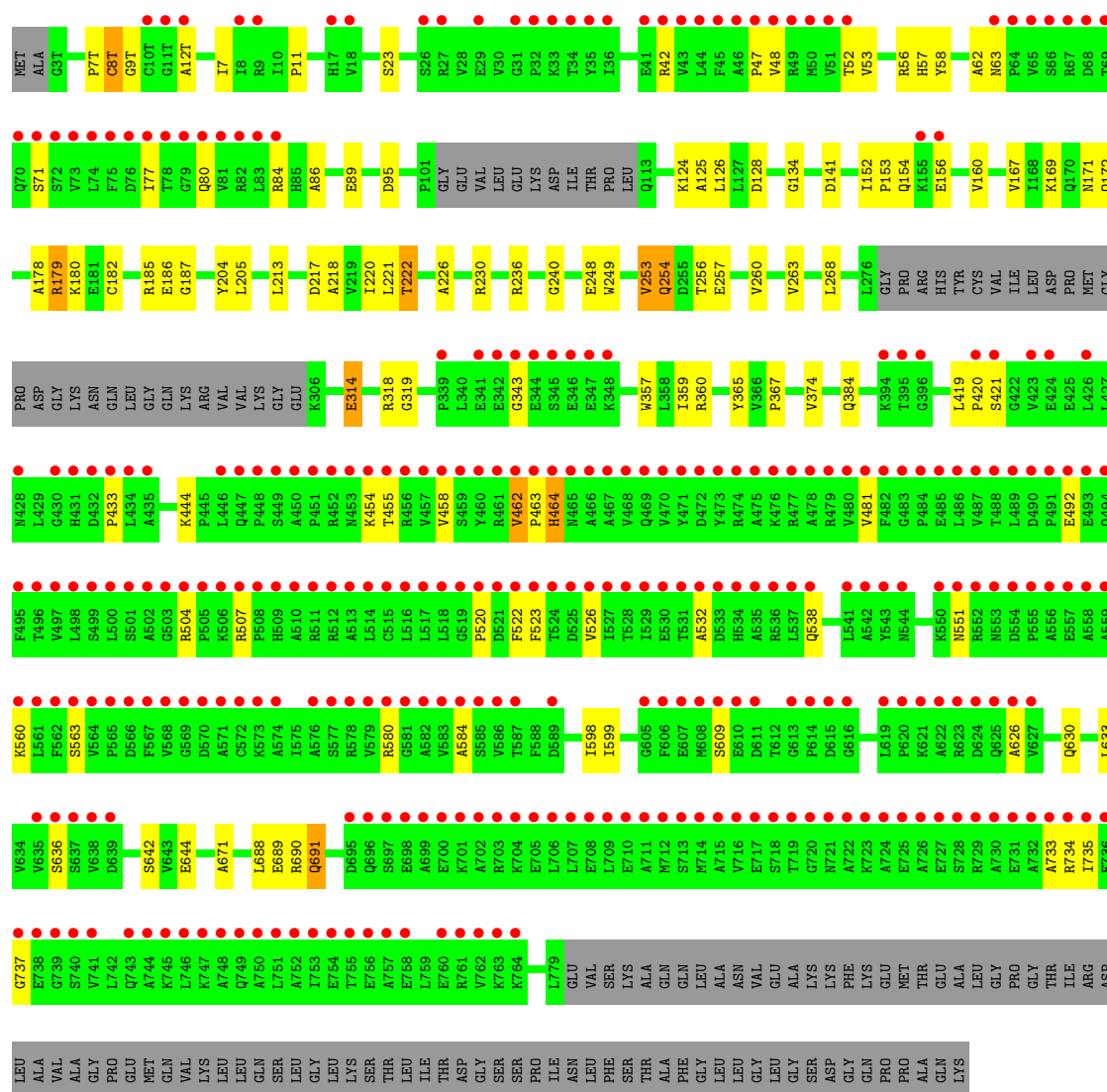
• Molecule 1: Major vault protein



GLN
PRO
PRO
ALA
GLN
LYS

• Molecule 1: Major vault protein

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	631.45Å 464.72Å 584.57Å 90.00° 123.84° 90.00°	Depositor
Resolution (Å)	200.00 – 9.00 188.73 – 9.00	Depositor EDS
% Data completeness (in resolution range)	98.0 (200.00-9.00) 91.2 (188.73-9.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.22	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 8.44Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.615 , (Not available) 0.563 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	-1.2	Xtriage
Anisotropy	4.910	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	-0.27 , 1880.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.69	EDS
Total number of atoms	7404	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.46% 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	0.31	0/3699	0.70	4/5148 (0.1%)
1	B	0.31	0/3699	0.69	5/5148 (0.1%)
All	All	0.31	0/7398	0.69	9/10296 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	THR	N-CA-C	5.51	125.87	111.00
1	B	222	THR	N-CA-C	5.50	125.86	111.00
1	B	8(T)	CYS	N-CA-C	5.29	125.27	111.00
1	A	8(T)	CYS	N-CA-C	5.28	125.25	111.00
1	A	220	ILE	C-N-CA	5.20	134.71	121.70
1	B	220	ILE	C-N-CA	5.19	134.68	121.70
1	A	9(T)	GLY	N-CA-C	-5.17	100.17	113.10
1	B	9(T)	GLY	N-CA-C	-5.17	100.18	113.10
1	B	220	ILE	CA-C-N	-5.01	106.18	117.20

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	3702	0	1718	33	0
1	B	3702	0	1718	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7404	0	3436	58	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 5.

All (58) 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:98:PRO:CB	1:B:156:GLU:CB	2.42	0.98
1:A:692:LYS:CB	1:B:688:LEU:HA	2.32	0.58
1:A:56:ARG:O	1:A:58:TYR:N	2.36	0.58
1:B:56:ARG:O	1:B:58:TYR:N	2.36	0.58
1:A:172:GLN:HA	1:A:217:ASP:HA	1.86	0.57
1:B:172:GLN:HA	1:B:217:ASP:HA	1.86	0.57
1:B:63:ASN:CB	1:B:77:ILE:HA	2.35	0.56
1:A:63:ASN:CB	1:A:77:ILE:HA	2.35	0.56
1:A:91:ARG:O	1:B:84:ARG:HA	2.06	0.54
1:B:185:ARG:O	1:B:187:GLY:N	2.42	0.53
1:A:185:ARG:O	1:A:187:GLY:N	2.42	0.52
1:A:626:ALA:O	1:A:636:SER:HA	2.10	0.52
1:A:630:GLN:N	1:A:633:LEU:O	2.42	0.51
1:B:630:GLN:N	1:B:633:LEU:O	2.42	0.51
1:A:167:VAL:H	1:A:204:TYR:HA	1.76	0.51
1:A:731:GLU:O	1:A:732:ALA:HB2	2.11	0.50
1:B:626:ALA:O	1:B:636:SER:HA	2.10	0.50
1:B:167:VAL:H	1:B:204:TYR:HA	1.76	0.50
1:B:253:VAL:O	1:B:254:GLN:CB	2.59	0.50
1:B:462:VAL:O	1:B:464:HIS:N	2.45	0.50
1:A:462:VAL:O	1:A:464:HIS:N	2.45	0.49
1:A:253:VAL:O	1:A:254:GLN:CB	2.59	0.49
1:A:230:ARG:HA	1:A:248:GLU:CB	2.43	0.48
1:B:230:ARG:HA	1:B:248:GLU:CB	2.43	0.48
1:B:124:LYS:HA	1:B:141:ASP:O	2.15	0.47
1:B:419:LEU:O	1:B:421:SER:N	2.48	0.47
1:B:52:THR:O	1:B:62:ALA:HA	2.15	0.47
1:A:236:ARG:HA	1:A:240:GLY:O	2.15	0.46
1:B:580:ARG:HA	1:B:584:ALA:HB3	1.97	0.46
1:A:734:ARG:CB	1:B:733:ALA:HA	2.46	0.46
1:A:580:ARG:HA	1:A:584:ALA:HB3	1.97	0.46
1:A:52:THR:O	1:A:62:ALA:HA	2.15	0.46
1:A:124:LYS:HA	1:A:141:ASP:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:LEU:O	1:A:421:SER:N	2.48	0.46
1:B:236:ARG:HA	1:B:240:GLY:O	2.15	0.46
1:A:314:GLU:HA	1:A:319:GLY:O	2.16	0.46
1:B:152:ILE:O	1:B:154:GLN:N	2.49	0.45
1:B:12(T):ALA:HA	1:B:7:ILE:O	2.17	0.45
1:A:171:ASN:O	1:A:218:ALA:N	2.50	0.45
1:B:314:GLU:HA	1:B:319:GLY:O	2.16	0.45
1:B:690:ARG:O	1:B:691:GLN:C	2.55	0.45
1:A:12(T):ALA:HA	1:A:7:ILE:O	2.17	0.45
1:B:171:ASN:O	1:B:218:ALA:N	2.50	0.45
1:B:532:ALA:CB	1:B:551:ASN:HA	2.47	0.45
1:A:178:ALA:O	1:A:179:ARG:CB	2.65	0.45
1:B:178:ALA:O	1:B:179:ARG:CB	2.65	0.45
1:A:152:ILE:O	1:A:154:GLN:N	2.49	0.44
1:A:690:ARG:O	1:A:691:GLN:C	2.55	0.44
1:A:532:ALA:CB	1:A:551:ASN:HA	2.47	0.44
1:B:222:THR:O	1:B:257:GLU:N	2.51	0.43
1:A:98:PRO:CB	1:B:156:GLU:CA	2.96	0.43
1:A:222:THR:O	1:A:257:GLU:N	2.51	0.43
1:A:256:THR:O	1:A:257:GLU:C	2.57	0.43
1:B:256:THR:O	1:B:257:GLU:C	2.57	0.43
1:A:226:ALA:HB2	1:A:253:VAL:HA	2.02	0.42
1:A:737:GLY:HA3	1:B:737:GLY:O	2.20	0.41
1:B:226:ALA:HB2	1:B:253:VAL:HA	2.02	0.41
1:A:93:ALA:HB3	1:B:86:ALA:HA	2.03	0.41

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	743/873 (85%)	524 (70%)	141 (19%)	78 (10%)	0 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	743/873 (85%)	528 (71%)	142 (19%)	73 (10%)	1	13
All	All	1486/1746 (85%)	1052 (71%)	283 (19%)	151 (10%)	1	11

All (151) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8(T)	CYS
1	A	57	HIS
1	A	71	SER
1	A	160	VAL
1	A	179	ARG
1	A	186	GLU
1	A	205	LEU
1	A	213	LEU
1	A	221	LEU
1	A	260	VAL
1	A	268	LEU
1	A	314	GLU
1	A	360	ARG
1	A	454	LYS
1	A	492	GLU
1	A	507	ARG
1	A	563	SER
1	A	598	ILE
1	A	599	ILE
1	A	671	ALA
1	A	689	GLU
1	A	727	GLU
1	A	732	ALA
1	B	8(T)	CYS
1	B	57	HIS
1	B	71	SER
1	B	160	VAL
1	B	179	ARG
1	B	186	GLU
1	B	205	LEU
1	B	213	LEU
1	B	221	LEU
1	B	260	VAL
1	B	268	LEU
1	B	314	GLU
1	B	360	ARG

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Mol	Chain	Res	Type
1	B	454	LYS
1	B	492	GLU
1	B	507	ARG
1	B	563	SER
1	B	598	ILE
1	B	599	ILE
1	B	671	ALA
1	B	689	GLU
1	B	735	ILE
1	A	80	GLN
1	A	126	LEU
1	A	169	LYS
1	A	253	VAL
1	A	254	GLN
1	A	367	PRO
1	A	560	LYS
1	A	609	SER
1	A	691	GLN
1	A	725	GLU
1	B	80	GLN
1	B	126	LEU
1	B	169	LYS
1	B	253	VAL
1	B	254	GLN
1	B	367	PRO
1	B	560	LYS
1	B	609	SER
1	B	691	GLN
1	A	11	PRO
1	A	42	ARG
1	A	48	VAL
1	A	125	ALA
1	A	153	PRO
1	A	180	LYS
1	A	182	CYS
1	A	365	TYR
1	A	384	GLN
1	A	433	PRO
1	A	463	PRO
1	A	464	HIS
1	A	520	PRO
1	A	523	PHE

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Mol	Chain	Res	Type
1	A	526	VAL
1	A	538	GLN
1	A	642	SER
1	A	644	GLU
1	B	11	PRO
1	B	42	ARG
1	B	48	VAL
1	B	125	ALA
1	B	153	PRO
1	B	180	LYS
1	B	182	CYS
1	B	365	TYR
1	B	384	GLN
1	B	433	PRO
1	B	463	PRO
1	B	464	HIS
1	B	520	PRO
1	B	523	PHE
1	B	526	VAL
1	B	538	GLN
1	B	642	SER
1	B	644	GLU
1	B	734	ARG
1	A	23	SER
1	A	89	GLU
1	A	128	ASP
1	A	318	ARG
1	A	359	ILE
1	A	522	PHE
1	A	733	ALA
1	B	23	SER
1	B	89	GLU
1	B	128	ASP
1	B	359	ILE
1	B	522	PHE
1	A	134	GLY
1	A	249	TRP
1	A	357	TRP
1	A	455	THR
1	A	504	ARG
1	A	716	VAL
1	A	736	GLU

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Mol	Chain	Res	Type
1	B	134	GLY
1	B	249	TRP
1	B	318	ARG
1	B	357	TRP
1	B	455	THR
1	B	504	ARG
1	A	7(T)	PRO
1	A	95	ASP
1	A	420	PRO
1	A	462	VAL
1	A	735	ILE
1	B	7(T)	PRO
1	B	95	ASP
1	B	420	PRO
1	B	462	VAL
1	A	481	VAL
1	B	481	VAL
1	A	47	PRO
1	A	53	VAL
1	A	458	VAL
1	B	47	PRO
1	B	53	VAL
1	B	458	VAL
1	A	263	VAL
1	A	343	GLY
1	A	374	VAL
1	A	444	LYS
1	B	263	VAL
1	B	374	VAL
1	B	444	LYS
1	B	343	GLY

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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, 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	749/873 (85%)	3.56	421 (56%) 0 4	50, 50, 50, 50	0
1	B	749/873 (85%)	2.59	304 (40%) 0 5	50, 50, 50, 50	0
All	All	1498/1746 (85%)	3.07	725 (48%) 0 4	50, 50, 50, 50	0

All (725) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	ASP	20.5
1	A	732	ALA	19.7
1	B	731	GLU	19.6
1	A	520	PRO	18.8
1	B	730	ALA	18.3
1	A	731	GLU	17.6
1	A	734	ARG	16.6
1	A	472	ASP	16.6
1	A	519	GLY	16.4
1	A	730	ALA	15.9
1	B	729	ARG	15.8
1	A	476	LYS	15.6
1	B	727	GLU	15.2
1	A	70	GLN	15.0
1	B	732	ALA	14.9
1	B	46	ALA	14.8
1	B	720	GLY	14.7
1	A	72	SER	14.4
1	A	66	SER	14.2
1	A	67	ARG	14.0
1	B	474	ARG	13.2
1	B	565	PRO	13.1
1	B	70	GLN	12.9
1	B	465	ASN	12.8

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Mol	Chain	Res	Type	RSRZ
1	A	515	CYS	12.8
1	B	49	ARG	12.7
1	A	719	THR	12.7
1	A	49	ARG	12.6
1	A	491	PRO	12.5
1	A	727	GLU	12.4
1	A	516	LEU	12.3
1	B	722	ALA	12.2
1	B	726	ALA	12.2
1	A	453	ASN	12.2
1	A	535	ALA	12.1
1	B	68	ASP	12.0
1	A	474	ARG	11.8
1	B	728	SER	11.8
1	A	456	ARG	11.7
1	B	723	LYS	11.6
1	B	466	ALA	11.6
1	B	491	PRO	11.6
1	B	725	GLU	11.6
1	A	728	SER	11.5
1	A	48	VAL	11.5
1	B	472	ASP	11.5
1	B	463	PRO	11.5
1	B	476	LYS	11.4
1	B	494	GLN	11.3
1	B	475	ALA	11.2
1	B	721	ASN	11.2
1	A	76	ASP	11.2
1	A	729	ARG	11.1
1	B	733	ALA	11.1
1	A	64	PRO	11.1
1	A	494	GLN	11.1
1	B	492	GLU	10.9
1	A	469	GLN	10.8
1	A	455	THR	10.8
1	A	720	GLY	10.8
1	B	473	TYR	10.8
1	B	48	VAL	10.8
1	B	493	GLU	10.7
1	A	71	SER	10.7
1	B	520	PRO	10.7
1	A	47	PRO	10.7

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Mol	Chain	Res	Type	RSRZ
1	A	141	ASP	10.7
1	B	519	GLY	10.6
1	A	69	THR	10.5
1	A	447	GLN	10.5
1	A	718	SER	10.5
1	B	718	SER	10.5
1	B	47	PRO	10.5
1	B	521	ASP	10.5
1	A	73	VAL	10.5
1	A	563	SER	10.4
1	B	455	THR	10.4
1	A	721	ASN	10.4
1	B	471	TYR	10.3
1	A	567	PHE	10.2
1	A	65	VAL	10.2
1	A	505	PRO	10.2
1	A	715	ALA	10.2
1	A	733	ALA	10.1
1	B	467	ALA	10.0
1	B	724	ALA	10.0
1	A	521	ASP	9.9
1	A	450	ALA	9.9
1	B	44	LEU	9.9
1	A	449	SER	9.8
1	A	518	LEU	9.8
1	A	477	ARG	9.8
1	A	712	MET	9.7
1	B	462	VAL	9.7
1	A	724	ALA	9.7
1	B	456	ARG	9.6
1	A	722	ALA	9.6
1	B	719	THR	9.6
1	A	615	ASP	9.6
1	A	448	PRO	9.5
1	A	46	ALA	9.5
1	A	717	GLU	9.5
1	A	50	MET	9.4
1	B	566	ASP	9.4
1	B	460	TYR	9.4
1	A	710	GLU	9.4
1	B	71	SER	9.3
1	A	475	ALA	9.3

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Mol	Chain	Res	Type	RSRZ
1	A	611	ASP	9.3
1	A	623	ARG	9.3
1	B	564	VAL	9.3
1	A	501	SER	9.3
1	A	467	ALA	9.2
1	A	74	LEU	9.2
1	B	72	SER	9.1
1	A	614	PRO	9.1
1	A	504	ARG	9.0
1	A	713	SER	9.0
1	B	623	ARG	8.9
1	B	609	SER	8.9
1	A	75	PHE	8.9
1	B	50	MET	8.9
1	B	43	VAL	8.9
1	A	460	TYR	8.9
1	A	726	ALA	8.8
1	A	502	ALA	8.8
1	A	622	ALA	8.8
1	A	470	VAL	8.8
1	A	506	LYS	8.8
1	A	711	ALA	8.8
1	A	714	MET	8.7
1	A	492	GLU	8.7
1	A	566	ASP	8.7
1	B	453	ASN	8.7
1	B	567	PHE	8.6
1	B	69	THR	8.6
1	A	565	PRO	8.6
1	B	563	SER	8.5
1	A	723	LYS	8.5
1	A	610	GLU	8.5
1	A	513	ALA	8.5
1	A	465	ASN	8.4
1	A	473	TYR	8.4
1	A	462	VAL	8.4
1	A	140	GLY	8.4
1	A	569	GLY	8.4
1	B	754	GLU	8.3
1	A	725	GLU	8.3
1	A	43	VAL	8.3
1	A	466	ALA	8.3

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Mol	Chain	Res	Type	RSRZ
1	A	499	SER	8.3
1	B	622	ALA	8.3
1	A	471	TYR	8.2
1	B	45	PHE	8.2
1	A	503	GLY	8.2
1	A	564	VAL	8.2
1	B	569	GLY	8.2
1	A	716	VAL	8.1
1	B	461	ARG	8.1
1	B	562	PHE	8.1
1	A	341	GLU	8.1
1	A	493	GLU	8.1
1	B	454	LYS	8.0
1	B	67	ARG	8.0
1	A	708	GLU	8.0
1	B	469	GLN	7.9
1	A	459	SER	7.9
1	B	395	THR	7.8
1	A	210	GLU	7.8
1	B	755	THR	7.8
1	B	717	GLU	7.8
1	A	735	ILE	7.8
1	B	468	VAL	7.8
1	A	483	GLY	7.7
1	A	490	ASP	7.7
1	A	451	PRO	7.7
1	B	496	THR	7.6
1	B	568	VAL	7.6
1	A	81	VAL	7.6
1	A	617	THR	7.5
1	B	753	ILE	7.5
1	B	470	VAL	7.5
1	A	621	LYS	7.4
1	A	484	PRO	7.4
1	A	517	LEU	7.4
1	B	490	ASP	7.4
1	A	45	PHE	7.4
1	A	142	GLU	7.4
1	B	51	VAL	7.4
1	A	496	THR	7.3
1	A	124	LYS	7.3
1	B	394	LYS	7.3

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Mol	Chain	Res	Type	RSRZ
1	A	78	THR	7.3
1	B	710	GLU	7.3
1	A	432	ASP	7.3
1	A	461	ARG	7.2
1	A	468	VAL	7.2
1	B	457	VAL	7.2
1	A	51	VAL	7.2
1	A	458	VAL	7.2
1	A	433	PRO	7.2
1	A	522	PHE	7.2
1	A	156	GLU	7.2
1	B	535	ALA	7.1
1	B	712	MET	7.1
1	B	749	GLN	7.0
1	A	44	LEU	7.0
1	A	464	HIS	7.0
1	B	477	ARG	7.0
1	A	507	ARG	7.0
1	B	713	SER	7.0
1	A	537	LEU	7.0
1	A	616	GLY	6.9
1	A	745	LYS	6.9
1	A	512	ARG	6.9
1	B	505	PRO	6.9
1	B	716	VAL	6.9
1	A	709	LEU	6.8
1	B	734	ARG	6.8
1	A	125	ALA	6.8
1	B	715	ALA	6.8
1	A	63	ASN	6.8
1	B	499	SER	6.7
1	A	342	GLU	6.7
1	A	562	PHE	6.7
1	B	515	CYS	6.7
1	B	459	SER	6.7
1	B	450	ALA	6.7
1	B	711	ALA	6.7
1	A	613	GLY	6.6
1	A	344	GLU	6.6
1	B	432	ASP	6.6
1	A	431	HIS	6.6
1	B	522	PHE	6.6

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Mol	Chain	Res	Type	RSRZ
1	A	608	MET	6.6
1	B	750	ALA	6.6
1	A	209	PHE	6.6
1	B	610	GLU	6.5
1	A	485	GLU	6.5
1	A	536	ARG	6.5
1	B	517	LEU	6.5
1	B	518	LEU	6.5
1	A	317	GLU	6.5
1	A	511	ARG	6.5
1	B	66	SER	6.5
1	B	607	GLU	6.5
1	B	464	HIS	6.4
1	A	514	LEU	6.4
1	B	714	MET	6.4
1	A	83	LEU	6.4
1	A	609	SER	6.4
1	A	736	GLU	6.4
1	A	80	GLN	6.4
1	A	245	THR	6.4
1	B	752	ALA	6.4
1	B	497	VAL	6.4
1	B	516	LEU	6.3
1	B	624	ASP	6.3
1	A	246	GLY	6.3
1	A	612	THR	6.3
1	B	748	ALA	6.2
1	A	343	GLY	6.2
1	B	708	GLU	6.2
1	B	65	VAL	6.2
1	B	554	ASP	6.2
1	A	345	SER	6.2
1	A	31	GLY	6.1
1	A	347	GLU	6.1
1	B	452	ARG	6.1
1	B	553	ASN	6.1
1	A	247	GLU	6.1
1	A	424	GLU	6.0
1	A	159	VAL	6.0
1	A	79	GLY	6.0
1	B	625	GLN	6.0
1	A	77	ILE	6.0

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Mol	Chain	Res	Type	RSRZ
1	B	608	MET	5.9
1	B	42	ARG	5.9
1	A	34	THR	5.9
1	A	155	LYS	5.9
1	A	454	LYS	5.9
1	B	506	LYS	5.9
1	B	433	PRO	5.8
1	B	495	PHE	5.8
1	A	620	PRO	5.8
1	B	561	LEU	5.8
1	B	557	GLU	5.8
1	B	558	ALA	5.8
1	A	486	LEU	5.8
1	A	463	PRO	5.8
1	A	41	GLU	5.8
1	B	451	PRO	5.8
1	B	555	PRO	5.8
1	A	705	GLU	5.8
1	B	483	GLY	5.7
1	B	560	LYS	5.7
1	B	458	VAL	5.7
1	A	607	GLU	5.7
1	A	339	PRO	5.7
1	B	449	SER	5.7
1	A	208	VAL	5.7
1	B	757	ALA	5.7
1	A	395	THR	5.7
1	A	42	ARG	5.6
1	A	744	ALA	5.6
1	B	448	PRO	5.6
1	B	34	THR	5.6
1	B	705	GLU	5.6
1	A	428	ASN	5.6
1	A	206	PRO	5.6
1	A	560	LYS	5.5
1	A	740	SER	5.5
1	A	500	LEU	5.5
1	A	568	VAL	5.5
1	A	427	LEU	5.5
1	A	452	ARG	5.5
1	A	707	LEU	5.5
1	A	629	PRO	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	30	VAL	5.4
1	A	498	LEU	5.4
1	B	484	PRO	5.4
1	B	523	PHE	5.4
1	B	584	ALA	5.4
1	A	211	GLU	5.4
1	B	636	SER	5.3
1	A	457	VAL	5.3
1	B	507	ARG	5.3
1	A	523	PHE	5.3
1	A	625	GLN	5.3
1	B	552	ARG	5.3
1	A	33	LYS	5.3
1	A	82	ARG	5.3
1	B	747	LYS	5.3
1	A	214	ASP	5.3
1	B	745	LYS	5.3
1	A	207	ALA	5.3
1	B	74	LEU	5.3
1	A	32	PRO	5.3
1	B	637	SER	5.3
1	B	611	ASP	5.3
1	B	537	LEU	5.2
1	B	52	THR	5.2
1	B	501	SER	5.2
1	A	126	LEU	5.2
1	A	624	ASP	5.2
1	A	636	SER	5.2
1	B	737	GLY	5.2
1	A	478	ALA	5.2
1	B	621	LYS	5.2
1	A	423	VAL	5.2
1	A	212	VAL	5.1
1	A	706	LEU	5.1
1	B	498	LEU	5.1
1	A	113	GLN	5.1
1	A	618	LEU	5.1
1	B	556	ALA	5.1
1	A	425	GLU	5.1
1	B	82	ARG	5.1
1	B	64	PRO	5.1
1	B	756	GLU	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	635	VAL	5.0
1	A	750	ALA	5.0
1	A	479	ARG	5.0
1	B	504	ARG	5.0
1	A	746	LEU	5.0
1	A	743	GLN	5.0
1	B	479	ARG	5.0
1	B	709	LEU	5.0
1	B	701	LYS	4.9
1	A	248	GLU	4.9
1	A	394	LYS	4.9
1	A	346	GLU	4.9
1	B	503	GLY	4.9
1	A	426	LEU	4.8
1	B	81	VAL	4.8
1	B	620	PRO	4.8
1	B	570	ASP	4.8
1	A	52	THR	4.8
1	B	735	ILE	4.8
1	A	26	SER	4.8
1	B	78	THR	4.8
1	A	37	ARG	4.8
1	A	154	GLN	4.7
1	B	580	ARG	4.7
1	B	343	GLY	4.7
1	A	133	ASN	4.7
1	A	213	LEU	4.7
1	A	495	PHE	4.7
1	A	430	GLY	4.7
1	A	703	ARG	4.7
1	A	747	LYS	4.7
1	A	158	GLU	4.6
1	A	244	ARG	4.6
1	A	626	ALA	4.6
1	B	751	LEU	4.6
1	B	33	LYS	4.6
1	B	73	VAL	4.6
1	B	63	ASN	4.6
1	B	536	ARG	4.6
1	B	80	GLN	4.6
1	B	342	GLU	4.6
1	A	584	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	76	ASP	4.6
1	A	482	PHE	4.6
1	A	528	THR	4.5
1	B	551	ASN	4.5
1	A	488	THR	4.5
1	A	497	VAL	4.5
1	B	500	LEU	4.5
1	B	345	SER	4.5
1	A	338	GLN	4.5
1	A	540	GLN	4.5
1	B	582	ALA	4.5
1	B	396	GLY	4.5
1	A	627	VAL	4.5
1	B	615	ASP	4.5
1	A	421	SER	4.5
1	A	739	GLY	4.4
1	A	748	ALA	4.4
1	B	32	PRO	4.4
1	A	160	VAL	4.4
1	A	481	VAL	4.4
1	A	243	HIS	4.4
1	B	581	GLY	4.4
1	A	704	LYS	4.4
1	A	123	LEU	4.4
1	B	702	ALA	4.4
1	B	79	GLY	4.4
1	A	166	THR	4.4
1	A	188	LYS	4.4
1	A	738	GLU	4.4
1	A	348	LYS	4.3
1	B	703	ARG	4.4
1	A	737	GLY	4.3
1	B	514	LEU	4.3
1	B	704	LYS	4.3
1	A	749	GLN	4.3
1	A	637	SER	4.3
1	A	538	GLN	4.3
1	B	344	GLU	4.3
1	B	513	ALA	4.3
1	A	265	GLU	4.3
1	A	544	ASN	4.3
1	B	576	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	481	VAL	4.3
1	B	534	HIS	4.3
1	B	485	GLU	4.3
1	B	707	LEU	4.3
1	A	38	GLN	4.2
1	A	702	ALA	4.2
1	B	585	SER	4.2
1	B	743	GLN	4.2
1	A	161	GLU	4.2
1	B	480	VAL	4.2
1	B	502	ALA	4.2
1	B	559	ALA	4.2
1	B	736	GLU	4.2
1	B	431	HIS	4.2
1	A	510	ALA	4.2
1	B	746	LEU	4.2
1	A	84	ARG	4.2
1	A	542	ALA	4.2
1	A	534	HIS	4.2
1	B	488	THR	4.1
1	B	700	GLU	4.1
1	B	525	ASP	4.1
1	B	583	VAL	4.1
1	A	630	GLN	4.1
1	A	134	GLY	4.1
1	B	83	LEU	4.1
1	A	585	SER	4.1
1	A	29	GLU	4.1
1	A	446	LEU	4.1
1	B	447	GLN	4.1
1	A	619	LEU	4.1
1	B	706	LEU	4.0
1	A	543	TYR	4.0
1	B	697	SER	4.0
1	B	744	ALA	4.0
1	A	487	VAL	4.0
1	A	36	ILE	4.0
1	A	434	LEU	4.0
1	A	186	GLU	4.0
1	A	114	VAL	4.0
1	A	570	ASP	4.0
1	B	424	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	340	LEU	4.0
1	A	187	GLY	3.9
1	B	36	ILE	3.9
1	A	634	VAL	3.9
1	A	701	LYS	3.9
1	A	742	LEU	3.9
1	A	143	TRP	3.9
1	A	351	HIS	3.9
1	A	396	GLY	3.9
1	B	528	THR	3.8
1	B	698	GLU	3.8
1	B	532	ALA	3.8
1	B	533	ASP	3.8
1	A	741	VAL	3.8
1	B	512	ARG	3.8
1	A	98	PRO	3.8
1	A	35	TYR	3.8
1	B	478	ALA	3.8
1	B	578	ARG	3.8
1	A	631	ASN	3.8
1	B	27	ARG	3.7
1	B	347	GLU	3.7
1	A	189	GLY	3.7
1	B	11(T)	GLY	3.7
1	B	626	ALA	3.7
1	B	524	THR	3.7
1	B	577	SER	3.7
1	B	758	GLU	3.7
1	B	482	PHE	3.7
1	B	572	CYS	3.7
1	B	423	VAL	3.6
1	B	538	GLN	3.6
1	B	434	LEU	3.6
1	B	508	PRO	3.6
1	A	559	ALA	3.6
1	A	700	GLU	3.6
1	B	699	ALA	3.6
1	A	533	ASP	3.6
1	B	587	THR	3.6
1	A	420	PRO	3.5
1	A	139	ALA	3.5
1	A	541	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	35	TYR	3.5
1	B	740	SER	3.5
1	B	738	GLU	3.5
1	A	349	VAL	3.5
1	B	526	VAL	3.4
1	A	132	LYS	3.4
1	A	480	VAL	3.4
1	A	628	PHE	3.4
1	B	638	VAL	3.4
1	A	232	LEU	3.4
1	A	150	THR	3.4
1	A	115	VAL	3.4
1	B	579	VAL	3.4
1	A	350	SER	3.4
1	A	266	GLU	3.4
1	A	767	GLU	3.4
1	B	571	ALA	3.4
1	B	761	ARG	3.3
1	B	487	VAL	3.3
1	B	486	LEU	3.3
1	A	185	ARG	3.3
1	A	184	ASP	3.3
1	A	24	ASN	3.3
1	A	233	GLN	3.3
1	A	88	GLN	3.3
1	A	770	LEU	3.3
1	B	511	ARG	3.3
1	A	352	GLN	3.2
1	A	752	ALA	3.2
1	A	422	GLY	3.2
1	A	205	LEU	3.2
1	A	157	VAL	3.2
1	A	321	GLN	3.2
1	B	605	GLY	3.1
1	A	191	VAL	3.1
1	A	262	ASP	3.1
1	A	580	ARG	3.1
1	A	527	ILE	3.1
1	A	128	ASP	3.1
1	B	614	PRO	3.1
1	A	525	ASP	3.1
1	A	558	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	489	LEU	3.1
1	A	545	TRP	3.1
1	A	190	ARG	3.1
1	B	31	GLY	3.0
1	B	9	ARG	3.0
1	A	606	PHE	3.0
1	A	429	LEU	3.0
1	B	606	PHE	3.0
1	B	430	GLY	3.0
1	A	583	VAL	3.0
1	A	435	ALA	3.0
1	B	741	VAL	3.0
1	B	760	GLU	3.0
1	A	556	ALA	3.0
1	A	561	LEU	3.0
1	A	182	CYS	3.0
1	B	156	GLU	3.0
1	A	403	GLY	2.9
1	B	542	ALA	2.9
1	A	263	VAL	2.9
1	A	62	ALA	2.9
1	A	85	HIS	2.9
1	B	544	ASN	2.9
1	B	639	ASP	2.9
1	A	632	GLY	2.9
1	A	27	ARG	2.9
1	B	550	LYS	2.8
1	A	539	LEU	2.8
1	A	769	GLU	2.8
1	A	526	VAL	2.8
1	A	40	ASN	2.8
1	B	421	SER	2.8
1	B	29	GLU	2.8
1	A	551	ASN	2.8
1	A	508	PRO	2.8
1	B	12(T)	ALA	2.8
1	B	10(T)	CYS	2.8
1	B	531	THR	2.8
1	A	555	PRO	2.8
1	B	696	GLN	2.8
1	A	335	LYS	2.8
1	A	355	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	336	ALA	2.8
1	A	354	GLY	2.8
1	B	739	GLY	2.8
1	B	586	VAL	2.8
1	A	766	ARG	2.8
1	B	616	GLY	2.8
1	B	527	ILE	2.8
1	A	751	LEU	2.7
1	A	25	VAL	2.7
1	B	26	SER	2.7
1	A	699	ALA	2.7
1	A	393	VAL	2.7
1	A	509	HIS	2.7
1	A	445	PRO	2.7
1	A	28	VAL	2.7
1	A	768	MET	2.7
1	A	264	TYR	2.7
1	A	697	SER	2.7
1	A	331	GLY	2.7
1	B	341	GLU	2.7
1	A	698	GLU	2.7
1	B	627	VAL	2.7
1	B	613	GLY	2.7
1	A	489	LEU	2.7
1	A	135	ASP	2.6
1	A	557	GLU	2.6
1	A	249	TRP	2.6
1	A	771	ILE	2.6
1	A	96	PRO	2.6
1	A	605	GLY	2.6
1	A	765	VAL	2.6
1	A	576	ALA	2.6
1	A	39	ASP	2.6
1	B	84	ARG	2.6
1	A	353	ALA	2.6
1	B	573	LYS	2.5
1	B	510	ALA	2.5
1	A	183	PHE	2.5
1	A	192	THR	2.5
1	A	524	THR	2.5
1	A	87	ASP	2.5
1	A	773	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	571	ALA	2.5
1	B	589	ASP	2.5
1	A	122	HIS	2.5
1	A	167	VAL	2.5
1	B	420	PRO	2.5
1	B	529	ILE	2.5
1	A	86	ALA	2.5
1	A	89	GLU	2.5
1	B	446	LEU	2.5
1	B	346	GLU	2.5
1	A	261	PRO	2.5
1	B	77	ILE	2.4
1	A	193	GLY	2.4
1	A	356	CYS	2.4
1	B	428	ASN	2.4
1	B	75	PHE	2.4
1	A	149	GLY	2.4
1	B	574	ALA	2.4
1	A	764	LYS	2.4
1	A	151	TYR	2.4
1	A	327	SER	2.4
1	A	127	LEU	2.4
1	B	17	HIS	2.4
1	B	18	VAL	2.4
1	B	695	ASP	2.3
1	A	633	LEU	2.3
1	A	318	ARG	2.3
1	A	404	SER	2.3
1	A	581	GLY	2.3
1	A	319	GLY	2.3
1	B	509	HIS	2.3
1	A	101	PRO	2.3
1	A	91	ARG	2.3
1	A	181	GLU	2.2
1	A	392	ASP	2.2
1	A	54	PRO	2.2
1	A	753	ILE	2.2
1	A	531	THR	2.2
1	A	405	THR	2.2
1	A	138	MET	2.2
1	B	635	VAL	2.2
1	A	23	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	165	ALA	2.2
1	B	435	ALA	2.2
1	A	95	ASP	2.2
1	A	436	ASP	2.2
1	B	619	LEU	2.2
1	B	764	LYS	2.2
1	A	322	ASP	2.2
1	A	532	ALA	2.1
1	A	152	ILE	2.1
1	B	426	LEU	2.1
1	B	41	GLU	2.1
1	A	550	LYS	2.1
1	B	543	TYR	2.1
1	B	348	LYS	2.1
1	A	131	ASP	2.1
1	A	761	ARG	2.1
1	A	754	GLU	2.1
1	B	155	LYS	2.1
1	B	339	PRO	2.1
1	B	762	VAL	2.1
1	A	328	GLU	2.1
1	B	8	ILE	2.1
1	B	530	GLU	2.1
1	B	541	LEU	2.0
1	A	97	PHE	2.0
1	A	180	LYS	2.0
1	B	763	LYS	2.0
1	A	234	ASN	2.0
1	A	231	ALA	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 [i](#)

There are no such residues in this entry.