Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:30 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 (i) symbol.

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

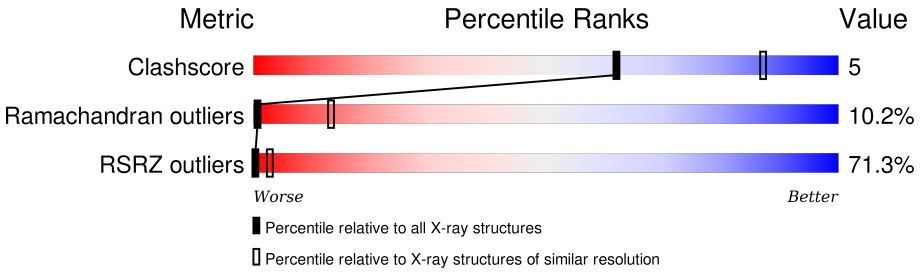
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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	102246	1064 (11.50-3.70)
Ramachandran outliers	100387	1036 (11.50-3.66)
RSRZ outliers	91569	1014 (11.50-3.66)

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	873	71% 71% 14% • 14%
1	B	873	51% 72% 13% • 14%

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:

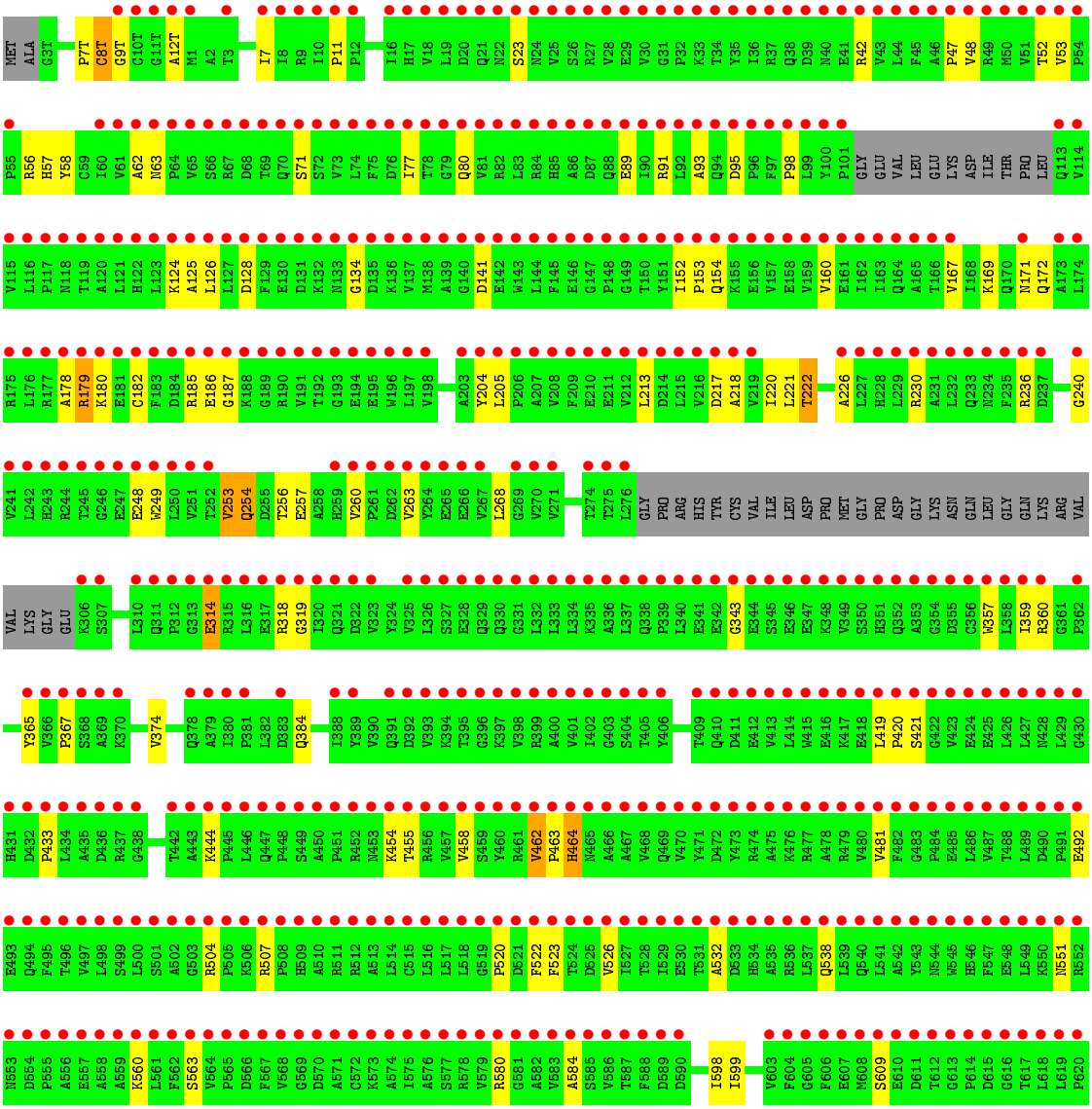
Chain	Residue	Modelled	Actual	Comment	Reference
A	1T	MET	-	EXPRESSION TAG	UNP Q62667
A	2T	ALA	-	EXPRESSION TAG	UNP Q62667
A	3T	GLY	-	EXPRESSION TAG	UNP Q62667
A	4T	CYS	-	EXPRESSION TAG	UNP Q62667
A	5T	GLY	-	EXPRESSION TAG	UNP Q62667
A	6T	CYS	-	EXPRESSION TAG	UNP Q62667
A	7T	PRO	-	EXPRESSION TAG	UNP Q62667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

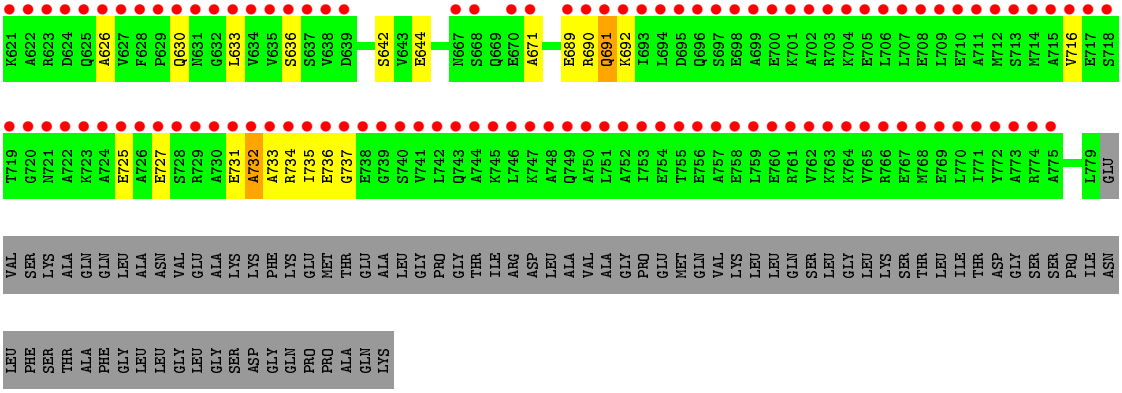
3 Residue-property plots (i)

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: Major vault protein

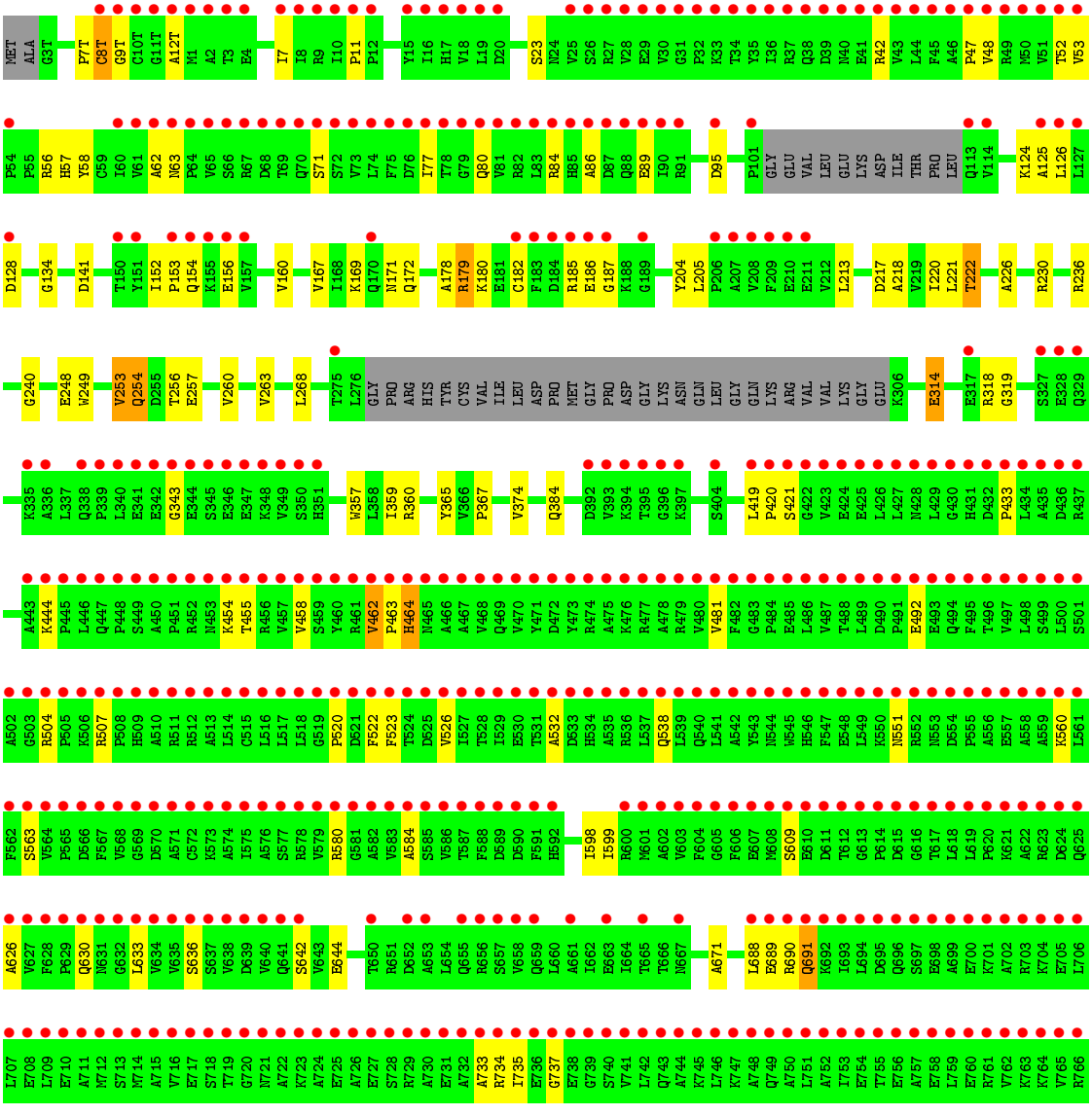
Chain A:

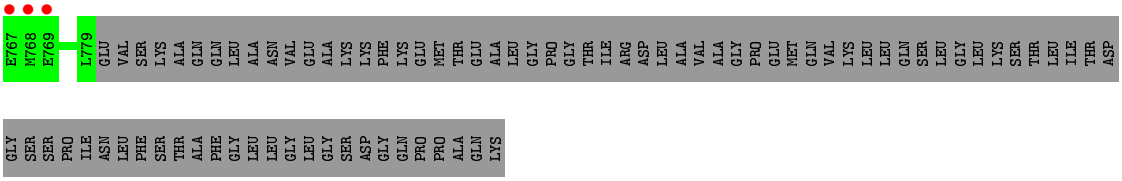




• Molecule 1: Major vault protein

Chain B:




E767
M768
E769
L779
GLU VAL SER LYS ALA GLN GLN LEU ALA ASN VAL GLU ALA LYS LYS PHE LYS GLU MET THR GLU ALA LEU GLY PRO GLY THR ILE ARG ASP LEU ALA VAL ALA GLY PRO GLU MET GLN VAL LYS LEU LEU GLN SER LEU GLY LEU LYS SER THR LEU ILE THR ASP
GLY SER SER PRO ILE ASN LEU PHE SER THR ALA PHE GLY LEU LEU GLY LEU GLY SER ASP GLY GLN PRO PRO ALA GLN LYS

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.09 (at 8.44Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.615 , (Not available) 0.626 , (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)	-0.38 , 1624.7	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Outliers	5 of 101681 reflections (0.005%)	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.*

[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	0.31	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(^{o})	Ideal(^{o})
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

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

Continued on next page...

Continued from previous page...

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:253:VAL:O	1:B:254:GLN:CB	2.59	0.50
1:B:167:VAL:H	1:B:204:TYR:HA	1.76	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

Continued on next page...

Continued from previous page...

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:B:314:GLU:HA	1:B:319:GLY:O	2.16	0.45
1:A:171:ASN:O	1:A:218:ALA:N	2.50	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 (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	743/873 (85%)	524 (70%)	141 (19%)	78 (10%)	1 12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	743/873 (85%)	528 (71%)	142 (19%)	73 (10%)	1 14
All	All	1486/1746 (85%)	1052 (71%)	283 (19%)	151 (10%)	1 13

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

5.3.3 RNA

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 carbohydrates 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, 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	749/873 (85%)	6.62	622 (83%) 0 2	50, 50, 50, 50	0
1	B	749/873 (85%)	4.87	446 (59%) 0 3	50, 50, 50, 50	0
All	All	1498/1746 (85%)	5.75	1068 (71%) 0 3	50, 50, 50, 50	0

All (1068) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	519	GLY	25.0
1	A	68	ASP	24.1
1	A	727	GLU	19.3
1	A	520	PRO	18.9
1	A	64	PRO	18.7
1	B	565	PRO	18.7
1	A	513	ALA	18.4
1	A	734	ARG	18.4
1	A	431	HIS	18.2
1	A	516	LEU	18.2
1	A	612	THR	18.0
1	A	66	SER	17.9
1	A	567	PHE	17.5
1	A	421	SER	17.3
1	B	730	ALA	17.3
1	B	726	ALA	17.2
1	A	535	ALA	17.1
1	A	519	GLY	17.1
1	B	722	ALA	17.0
1	B	731	GLU	16.8
1	A	569	GLY	16.7
1	B	718	SER	16.7
1	A	49	ARG	16.6
1	A	67	ARG	16.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	70	GLN	16.5
1	B	567	PHE	16.2
1	B	450	ALA	16.1
1	A	515	CYS	16.1
1	A	72	SER	16.0
1	A	336	ALA	15.9
1	B	720	GLY	15.7
1	A	420	PRO	15.7
1	B	496	THR	15.5
1	A	340	LEU	15.4
1	A	65	VAL	15.4
1	B	68	ASP	15.4
1	B	476	LYS	15.4
1	A	732	ALA	15.3
1	A	610	GLU	15.2
1	A	721	ASN	15.1
1	A	712	MET	15.1
1	A	715	ALA	15.1
1	A	63	ASN	14.9
1	B	520	PRO	14.8
1	B	516	LEU	14.7
1	B	49	ARG	14.7
1	A	76	ASP	14.6
1	B	725	GLU	14.6
1	B	465	ASN	14.6
1	A	565	PRO	14.6
1	B	732	ALA	14.5
1	A	722	ALA	14.5
1	A	449	SER	14.4
1	B	63	ASN	14.4
1	A	730	ALA	14.4
1	A	724	ALA	14.4
1	B	463	PRO	14.2
1	B	456	ARG	14.2
1	A	426	LEU	14.1
1	A	611	ASP	14.1
1	B	607	GLU	14.1
1	B	727	GLU	14.1
1	B	46	ALA	14.0
1	A	50	MET	14.0
1	A	425	GLU	13.9
1	A	456	ARG	13.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	723	LYS	13.9
1	A	726	ALA	13.9
1	A	621	LYS	13.9
1	B	494	GLN	13.8
1	A	51	VAL	13.8
1	B	466	ALA	13.8
1	B	568	VAL	13.8
1	A	347	GLU	13.7
1	B	571	ALA	13.7
1	B	557	GLU	13.6
1	A	346	GLU	13.6
1	B	455	THR	13.6
1	A	317	GLU	13.6
1	A	435	ALA	13.6
1	A	710	GLU	13.5
1	B	76	ASP	13.5
1	A	48	VAL	13.5
1	A	428	ASN	13.5
1	A	499	SER	13.5
1	A	728	SER	13.4
1	B	52	THR	13.4
1	A	566	ASP	13.4
1	B	609	SER	13.4
1	B	70	GLN	13.4
1	B	467	ALA	13.3
1	A	719	THR	13.3
1	B	729	ARG	13.3
1	B	521	ASP	13.2
1	A	502	ALA	13.2
1	A	617	THR	13.2
1	A	494	GLN	13.1
1	A	469	GLN	13.1
1	A	472	ASP	13.1
1	A	622	ALA	13.1
1	B	582	ALA	13.1
1	B	715	ALA	13.0
1	A	627	VAL	13.0
1	B	623	ARG	13.0
1	B	449	SER	13.0
1	A	339	PRO	12.9
1	A	623	ARG	12.9
1	B	566	ASP	12.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	470	VAL	12.8
1	B	719	THR	12.8
1	A	450	ALA	12.7
1	B	721	ASN	12.7
1	A	71	SER	12.7
1	B	578	ARG	12.7
1	A	455	THR	12.6
1	A	479	ARG	12.6
1	A	496	THR	12.6
1	A	52	THR	12.6
1	B	74	LEU	12.5
1	A	26	SER	12.5
1	B	622	ALA	12.5
1	B	714	MET	12.5
1	A	626	ALA	12.5
1	B	569	GLY	12.4
1	B	477	ARG	12.4
1	A	720	GLY	12.4
1	A	79	GLY	12.4
1	A	341	GLU	12.3
1	B	66	SER	12.3
1	A	521	ASP	12.3
1	A	78	THR	12.3
1	B	454	LYS	12.3
1	B	724	ALA	12.3
1	B	717	GLU	12.3
1	A	476	LYS	12.3
1	A	563	SER	12.2
1	A	77	ILE	12.2
1	B	51	VAL	12.2
1	B	65	VAL	12.2
1	A	353	ALA	12.1
1	A	47	PRO	12.1
1	A	731	GLU	12.1
1	B	625	GLN	12.1
1	A	568	VAL	12.0
1	B	637	SER	12.0
1	A	635	VAL	12.0
1	B	558	ALA	12.0
1	A	723	LYS	12.0
1	A	536	ARG	11.9
1	B	518	LEU	11.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	564	VAL	11.9
1	B	472	ASP	11.9
1	A	537	LEU	11.9
1	A	206	PRO	11.9
1	B	471	TYR	11.9
1	B	468	VAL	11.8
1	B	431	HIS	11.8
1	B	79	GLY	11.8
1	B	636	SER	11.8
1	A	352	GLN	11.8
1	B	460	TYR	11.8
1	A	351	HIS	11.7
1	A	625	GLN	11.7
1	A	629	PRO	11.7
1	A	571	ALA	11.7
1	A	718	SER	11.7
1	A	607	GLU	11.6
1	B	710	GLU	11.6
1	A	87	ASP	11.6
1	A	424	GLU	11.5
1	B	529	ILE	11.5
1	B	475	ALA	11.5
1	A	427	LEU	11.5
1	B	733	ALA	11.5
1	B	64	PRO	11.5
1	A	518	LEU	11.4
1	A	43	VAL	11.4
1	A	708	GLU	11.4
1	A	73	VAL	11.4
1	A	529	ILE	11.4
1	A	637	SER	11.4
1	A	46	ALA	11.4
1	B	556	ALA	11.4
1	A	445	PRO	11.4
1	B	535	ALA	11.4
1	B	481	VAL	11.4
1	A	714	MET	11.4
1	B	469	GLN	11.4
1	A	69	THR	11.4
1	A	711	ALA	11.3
1	A	528	THR	11.3
1	A	436	ASP	11.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	467	ALA	11.2
1	A	29	GLU	11.2
1	A	83	LEU	11.2
1	A	422	GLY	11.2
1	A	141	ASP	11.2
1	A	608	MET	11.2
1	A	619	LEU	11.2
1	A	159	VAL	11.1
1	B	499	SER	11.1
1	A	740	SER	11.1
1	A	124	LYS	11.1
1	A	460	TYR	11.1
1	B	561	LEU	11.1
1	A	522	PHE	11.1
1	B	753	ILE	11.1
1	A	514	LEU	11.1
1	A	354	GLY	11.1
1	A	501	SER	11.1
1	B	755	THR	11.1
1	A	423	VAL	11.1
1	B	624	ASP	11.0
1	B	513	ALA	11.0
1	A	75	PHE	11.0
1	A	562	PHE	11.0
1	A	246	GLY	11.0
1	B	743	GLN	11.0
1	B	711	ALA	11.0
1	A	636	SER	11.0
1	A	506	LYS	11.0
1	A	125	ALA	10.9
1	B	515	CYS	10.9
1	A	716	VAL	10.9
1	B	750	ALA	10.9
1	B	554	ASP	10.9
1	A	332	LEU	10.9
1	B	754	GLU	10.9
1	B	491	PRO	10.9
1	A	451	PRO	10.8
1	B	514	LEU	10.8
1	B	621	LYS	10.8
1	A	74	LEU	10.8
1	A	614	PRO	10.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	72	SER	10.8
1	A	490	ASP	10.8
1	A	37	ARG	10.8
1	B	580	ARG	10.8
1	A	523	PHE	10.8
1	B	48	VAL	10.8
1	A	729	ARG	10.7
1	B	563	SER	10.7
1	A	505	PRO	10.7
1	A	717	GLU	10.7
1	A	345	SER	10.7
1	B	50	MET	10.7
1	A	453	ASN	10.6
1	B	553	ASN	10.6
1	B	483	GLY	10.6
1	B	574	ALA	10.6
1	B	479	ARG	10.6
1	A	551	ASN	10.6
1	A	81	VAL	10.6
1	B	517	LEU	10.6
1	B	488	THR	10.6
1	A	512	ARG	10.5
1	A	552	ARG	10.5
1	A	564	VAL	10.5
1	B	570	ASP	10.5
1	A	705	GLU	10.5
1	A	84	ARG	10.5
1	A	158	GLU	10.5
1	A	349	VAL	10.4
1	B	728	SER	10.4
1	B	579	VAL	10.4
1	B	44	LEU	10.4
1	B	462	VAL	10.4
1	A	725	GLU	10.4
1	B	712	MET	10.4
1	B	572	CYS	10.4
1	B	11(T)	GLY	10.4
1	B	581	GLY	10.4
1	A	534	HIS	10.4
1	B	474	ARG	10.3
1	A	335	LYS	10.3
1	B	433	PRO	10.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	447	GLN	10.3
1	B	47	PRO	10.3
1	B	610	GLU	10.3
1	A	504	ARG	10.2
1	B	453	ASN	10.2
1	A	350	SER	10.2
1	B	534	HIS	10.2
1	B	81	VAL	10.2
1	A	88	GLN	10.2
1	B	716	VAL	10.1
1	A	207	ALA	10.1
1	A	733	ALA	10.1
1	A	491	PRO	10.1
1	A	570	ASP	10.1
1	A	338	GLN	10.1
1	A	584	ALA	10.1
1	A	743	GLN	10.1
1	B	80	GLN	10.1
1	B	490	ASP	10.1
1	A	430	GLY	10.1
1	B	708	GLU	10.1
1	A	356	CYS	10.0
1	A	80	GLN	10.0
1	B	71	SER	10.0
1	B	42	ARG	10.0
1	A	713	SER	10.0
1	A	140	GLY	10.0
1	A	34	THR	10.0
1	A	630	GLN	10.0
1	A	477	ARG	9.9
1	B	473	TYR	9.9
1	A	30	VAL	9.9
1	A	613	GLY	9.8
1	A	44	LEU	9.8
1	B	457	VAL	9.8
1	B	744	ALA	9.8
1	A	156	GLU	9.8
1	B	67	ARG	9.8
1	B	495	PHE	9.8
1	A	618	LEU	9.8
1	B	528	THR	9.7
1	A	210	GLU	9.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	331	GLY	9.7
1	A	511	ARG	9.7
1	A	609	SER	9.7
1	A	470	VAL	9.7
1	B	562	PHE	9.7
1	A	736	GLU	9.7
1	A	560	LYS	9.7
1	A	86	ALA	9.6
1	B	703	ARG	9.6
1	A	624	ASP	9.6
1	A	247	GLU	9.6
1	B	705	GLU	9.6
1	B	530	GLU	9.6
1	B	713	SER	9.6
1	B	43	VAL	9.6
1	B	551	ASN	9.6
1	A	45	PHE	9.6
1	B	536	ARG	9.6
1	B	430	GLY	9.6
1	A	31	GLY	9.5
1	B	701	LYS	9.5
1	B	626	ALA	9.5
1	B	734	ARG	9.5
1	B	555	PRO	9.5
1	B	737	GLY	9.5
1	A	154	GLN	9.5
1	A	703	ARG	9.5
1	B	10(T)	CYS	9.5
1	B	532	ALA	9.5
1	A	517	LEU	9.5
1	B	77	ILE	9.5
1	A	631	ASN	9.5
1	A	38	GLN	9.4
1	A	706	LEU	9.4
1	B	560	LYS	9.4
1	B	531	THR	9.4
1	B	552	ARG	9.4
1	B	78	THR	9.4
1	A	85	HIS	9.4
1	A	462	VAL	9.4
1	B	748	ALA	9.3
1	A	42	ARG	9.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	123	LEU	9.3
1	B	638	VAL	9.3
1	A	244	ARG	9.3
1	B	583	VAL	9.3
1	B	749	GLN	9.3
1	A	483	GLY	9.3
1	B	492	GLU	9.3
1	B	584	ALA	9.2
1	A	433	PRO	9.2
1	A	41	GLU	9.2
1	A	448	PRO	9.2
1	A	458	VAL	9.2
1	A	531	THR	9.2
1	A	432	ASP	9.2
1	A	232	LEU	9.2
1	A	245	THR	9.2
1	B	395	THR	9.2
1	B	585	SER	9.2
1	B	448	PRO	9.2
1	B	756	GLU	9.2
1	A	620	PRO	9.1
1	A	28	VAL	9.1
1	A	459	SER	9.1
1	A	488	THR	9.1
1	A	742	LEU	9.1
1	A	466	ALA	9.0
1	A	429	LEU	9.0
1	A	737	GLY	9.0
1	B	505	PRO	9.0
1	A	465	ASN	9.0
1	B	707	LEU	9.0
1	B	605	GLY	9.0
1	A	142	GLU	9.0
1	A	27	ARG	9.0
1	A	151	TYR	9.0
1	A	355	ASP	9.0
1	B	752	ALA	8.9
1	B	424	GLU	8.9
1	A	205	LEU	8.9
1	A	628	PHE	8.9
1	A	615	ASP	8.9
1	A	735	ILE	8.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	27	ARG	8.9
1	A	738	GLU	8.9
1	B	576	ALA	8.9
1	B	502	ALA	8.9
1	A	544	ASN	8.9
1	B	706	LEU	8.9
1	B	83	LEU	8.8
1	A	507	ARG	8.8
1	A	265	GLU	8.8
1	B	421	SER	8.8
1	A	495	PHE	8.8
1	A	62	ALA	8.8
1	B	493	GLU	8.8
1	A	474	ARG	8.8
1	B	82	ARG	8.8
1	A	160	VAL	8.8
1	A	344	GLU	8.8
1	B	394	LYS	8.8
1	B	420	PRO	8.7
1	A	704	LYS	8.7
1	A	745	LYS	8.7
1	B	451	PRO	8.7
1	A	468	VAL	8.7
1	A	342	GLU	8.7
1	B	550	LYS	8.7
1	A	744	ALA	8.7
1	B	435	ALA	8.7
1	B	745	LYS	8.7
1	B	480	VAL	8.7
1	A	183	PHE	8.7
1	A	707	LEU	8.7
1	A	155	LYS	8.6
1	B	445	PRO	8.6
1	B	577	SER	8.6
1	A	741	VAL	8.6
1	B	606	PHE	8.6
1	B	34	THR	8.6
1	A	503	GLY	8.6
1	A	446	LEU	8.5
1	B	523	PHE	8.5
1	B	704	LYS	8.5
1	A	348	LYS	8.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	701	LYS	8.5
1	B	573	LYS	8.5
1	A	113	GLN	8.5
1	B	497	VAL	8.5
1	A	634	VAL	8.4
1	A	143	TRP	8.4
1	A	262	ASP	8.4
1	B	69	THR	8.4
1	A	394	LYS	8.4
1	B	35	TYR	8.4
1	B	345	SER	8.4
1	A	434	LEU	8.4
1	B	699	ALA	8.4
1	B	608	MET	8.3
1	B	461	ARG	8.3
1	A	471	TYR	8.3
1	A	548	GLU	8.3
1	A	550	LYS	8.3
1	B	434	LEU	8.3
1	A	616	GLY	8.3
1	A	419	LEU	8.3
1	A	185	ARG	8.3
1	B	432	ASP	8.3
1	B	758	GLU	8.2
1	A	233	GLN	8.2
1	B	512	ARG	8.2
1	B	698	GLU	8.2
1	B	422	GLY	8.2
1	B	426	LEU	8.2
1	A	561	LEU	8.2
1	B	33	LYS	8.2
1	A	213	LEU	8.2
1	B	503	GLY	8.2
1	A	161	GLU	8.2
1	A	35	TYR	8.2
1	B	611	ASP	8.1
1	B	447	GLN	8.1
1	A	181	GLU	8.1
1	B	747	LYS	8.1
1	A	530	GLU	8.1
1	B	478	ALA	8.1
1	B	511	ARG	8.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	525	ASP	8.0
1	A	709	LEU	8.0
1	B	697	SER	8.0
1	A	343	GLY	8.0
1	B	506	LYS	8.0
1	B	459	SER	8.0
1	A	182	CYS	8.0
1	B	549	LEU	8.0
1	B	575	ILE	7.9
1	B	343	GLY	7.9
1	B	452	ARG	7.9
1	B	746	LEU	7.9
1	B	36	ILE	7.9
1	B	458	VAL	7.9
1	A	209	PHE	7.9
1	B	696	GLN	7.9
1	B	501	SER	7.9
1	A	510	ALA	7.9
1	A	475	ALA	7.9
1	B	702	ALA	7.9
1	A	585	SER	7.9
1	A	89	GLU	7.9
1	A	739	GLY	7.9
1	A	770	LEU	7.9
1	A	480	VAL	7.8
1	B	741	VAL	7.8
1	A	461	ARG	7.8
1	A	357	TRP	7.8
1	A	556	ALA	7.8
1	B	12(T)	ALA	7.8
1	B	482	PHE	7.8
1	B	396	GLY	7.8
1	B	500	LEU	7.8
1	A	243	HIS	7.8
1	B	537	LEU	7.8
1	A	473	TYR	7.7
1	A	527	ILE	7.7
1	A	547	PHE	7.7
1	A	184	ASP	7.7
1	B	73	VAL	7.7
1	A	702	ALA	7.7
1	A	396	GLY	7.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	484	PRO	7.6
1	B	700	GLU	7.6
1	A	395	THR	7.6
1	B	341	GLU	7.6
1	B	342	GLU	7.6
1	B	484	PRO	7.6
1	A	464	HIS	7.6
1	A	214	ASP	7.5
1	B	62	ALA	7.5
1	A	572	CYS	7.5
1	A	418	GLU	7.5
1	B	464	HIS	7.5
1	B	9	ARG	7.5
1	B	735	ILE	7.4
1	B	510	ALA	7.4
1	A	632	GLY	7.4
1	A	392	ASP	7.4
1	A	337	LEU	7.4
1	A	583	VAL	7.4
1	A	481	VAL	7.4
1	A	36	ILE	7.4
1	A	128	ASP	7.3
1	A	498	LEU	7.3
1	A	82	ARG	7.3
1	A	546	HIS	7.3
1	B	84	ARG	7.3
1	B	507	ARG	7.3
1	A	11(T)	GLY	7.3
1	B	627	VAL	7.3
1	A	248	GLU	7.2
1	A	493	GLU	7.2
1	A	212	VAL	7.2
1	A	263	VAL	7.2
1	B	423	VAL	7.2
1	B	740	SER	7.2
1	A	478	ALA	7.2
1	B	29	GLU	7.2
1	A	492	GLU	7.2
1	A	524	THR	7.1
1	A	549	LEU	7.1
1	A	540	GLN	7.1
1	B	31	GLY	7.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	45	PHE	7.1
1	B	489	LEU	7.1
1	A	581	GLY	7.1
1	A	482	PHE	7.1
1	A	150	THR	7.0
1	A	771	ILE	7.0
1	A	33	LYS	7.0
1	A	606	PHE	7.0
1	A	211	GLU	7.0
1	A	543	TYR	7.0
1	A	576	ALA	7.0
1	A	188	LYS	7.0
1	A	25	VAL	7.0
1	A	582	ALA	7.0
1	B	559	ALA	7.0
1	A	525	ASP	7.0
1	A	747	LYS	7.0
1	A	500	LEU	7.0
1	B	538	GLN	7.0
1	B	709	LEU	7.0
1	B	620	PRO	7.0
1	A	334	LEU	6.9
1	A	166	THR	6.9
1	A	189	GLY	6.9
1	B	26	SER	6.9
1	B	498	LEU	6.9
1	A	557	GLU	6.9
1	B	504	ARG	6.9
1	B	446	LEU	6.9
1	B	738	GLU	6.9
1	A	122	HIS	6.9
1	A	545	TRP	6.9
1	B	639	ASP	6.9
1	A	750	ALA	6.9
1	A	333	LEU	6.8
1	A	114	VAL	6.8
1	A	393	VAL	6.8
1	A	580	ARG	6.8
1	B	41	GLU	6.8
1	B	508	PRO	6.8
1	A	133	ASN	6.8
1	B	757	ALA	6.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	485	GLU	6.8
1	A	700	GLU	6.8
1	A	153	PRO	6.8
1	A	24	ASN	6.7
1	A	149	GLY	6.7
1	A	605	GLY	6.7
1	A	115	VAL	6.7
1	B	524	THR	6.7
1	B	522	PHE	6.7
1	A	186	GLU	6.6
1	A	416	GLU	6.6
1	A	91	ARG	6.6
1	B	8	ILE	6.6
1	A	54	PRO	6.6
1	A	231	ALA	6.6
1	A	486	LEU	6.6
1	A	90	ILE	6.6
1	A	261	PRO	6.6
1	A	542	ALA	6.6
1	B	739	GLY	6.5
1	A	454	LYS	6.5
1	B	428	ASN	6.5
1	B	527	ILE	6.4
1	B	736	GLU	6.4
1	A	126	LEU	6.4
1	B	486	LEU	6.4
1	B	436	ASP	6.4
1	B	542	ALA	6.4
1	A	98	PRO	6.4
1	A	208	VAL	6.4
1	A	553	ASN	6.4
1	B	586	VAL	6.4
1	A	558	ALA	6.4
1	A	746	LEU	6.4
1	A	574	ALA	6.4
1	B	587	THR	6.4
1	B	751	LEU	6.4
1	A	157	VAL	6.4
1	B	544	ASN	6.4
1	A	532	ALA	6.3
1	A	555	PRO	6.3
1	A	539	LEU	6.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	347	GLU	6.3
1	B	526	VAL	6.3
1	B	17	HIS	6.2
1	A	118	ASN	6.2
1	B	344	GLU	6.2
1	B	485	GLU	6.2
1	A	697	SER	6.2
1	A	32	PRO	6.2
1	B	742	LEU	6.2
1	A	699	ALA	6.2
1	A	10(T)	CYS	6.2
1	A	165	ALA	6.2
1	A	578	ARG	6.2
1	B	695	ASP	6.1
1	A	633	LEU	6.1
1	A	463	PRO	6.1
1	A	579	VAL	6.1
1	A	526	VAL	6.1
1	B	75	PHE	6.1
1	A	541	LEU	6.1
1	A	319	GLY	6.1
1	A	190	ARG	6.1
1	A	152	ILE	6.0
1	A	538	GLN	6.0
1	A	773	ALA	6.0
1	B	533	ASP	6.0
1	A	234	ASN	6.0
1	A	559	ALA	6.0
1	A	164	GLN	5.9
1	A	266	GLU	5.9
1	A	497	VAL	5.9
1	B	85	HIS	5.9
1	A	533	ASP	5.9
1	B	1	MET	5.9
1	A	554	ASP	5.9
1	B	346	GLU	5.8
1	B	760	GLU	5.8
1	A	264	TYR	5.8
1	B	9(T)	GLY	5.8
1	B	339	PRO	5.8
1	A	489	LEU	5.8
1	B	32	PRO	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	761	ARG	5.8
1	A	698	GLU	5.8
1	B	548	GLU	5.8
1	A	191	VAL	5.8
1	B	635	VAL	5.8
1	A	638	VAL	5.8
1	A	748	ALA	5.7
1	A	17	HIS	5.7
1	A	457	VAL	5.7
1	A	577	SER	5.7
1	A	121	LEU	5.7
1	B	30	VAL	5.7
1	A	187	GLY	5.7
1	A	452	ARG	5.7
1	B	509	HIS	5.7
1	A	249	TRP	5.7
1	A	163	ILE	5.7
1	A	193	GLY	5.7
1	A	250	LEU	5.7
1	A	120	ALA	5.6
1	A	749	GLN	5.6
1	A	194	GLU	5.6
1	B	28	VAL	5.6
1	A	162	ILE	5.6
1	B	589	ASP	5.6
1	A	415	TRP	5.6
1	B	10	ILE	5.6
1	A	444	LYS	5.6
1	A	117	PRO	5.6
1	A	53	VAL	5.5
1	A	235	PHE	5.5
1	B	18	VAL	5.5
1	A	119	THR	5.5
1	A	767	GLU	5.5
1	A	329	GLN	5.5
1	B	759	LEU	5.5
1	B	156	GLU	5.4
1	A	144	LEU	5.4
1	B	183	PHE	5.3
1	B	487	VAL	5.3
1	B	619	LEU	5.3
1	A	139	ALA	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	427	LEU	5.3
1	B	61	VAL	5.2
1	B	615	ASP	5.2
1	A	12(T)	ALA	5.2
1	A	573	LYS	5.2
1	A	437	ARG	5.2
1	A	328	GLU	5.2
1	B	763	LYS	5.2
1	A	696	GLN	5.2
1	A	318	ARG	5.2
1	A	195	GLU	5.1
1	B	37	ARG	5.1
1	A	487	VAL	5.1
1	A	134	GLY	5.1
1	A	397	LYS	5.0
1	A	752	ALA	5.0
1	A	39	ASP	5.0
1	A	180	LYS	5.0
1	A	204	TYR	5.0
1	A	101	PRO	5.0
1	A	9	ARG	4.9
1	A	330	GLN	4.9
1	A	417	LYS	4.9
1	B	614	PRO	4.9
1	A	40	ASN	4.9
1	A	509	HIS	4.9
1	A	769	GLU	4.9
1	B	184	ASP	4.9
1	B	539	LEU	4.9
1	A	95	ASP	4.8
1	A	18	VAL	4.8
1	A	131	ASP	4.8
1	A	19	LEU	4.8
1	A	175	ARG	4.8
1	B	693	ILE	4.8
1	B	541	LEU	4.8
1	B	444	LYS	4.8
1	A	92	LEU	4.7
1	A	358	LEU	4.7
1	B	602	ALA	4.7
1	B	54	PRO	4.7
1	B	546	HIS	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	612	THR	4.7
1	B	53	VAL	4.7
1	A	575	ILE	4.7
1	A	327	SER	4.7
1	B	540	GLN	4.7
1	A	192	THR	4.7
1	A	751	LEU	4.6
1	B	7	ILE	4.6
1	B	545	TRP	4.6
1	B	694	LEU	4.6
1	A	276	LEU	4.6
1	A	116	LEU	4.6
1	A	145	PHE	4.6
1	A	61	VAL	4.6
1	A	774	ARG	4.6
1	B	38	GLN	4.6
1	B	547	PHE	4.6
1	A	403	GLY	4.5
1	A	587	THR	4.5
1	A	766	ARG	4.5
1	A	398	VAL	4.5
1	A	768	MET	4.5
1	B	338	GLN	4.5
1	B	425	GLU	4.4
1	A	94	GLN	4.4
1	A	100	TYR	4.4
1	A	230	ARG	4.4
1	B	340	LEU	4.4
1	B	603	VAL	4.4
1	B	317	GLU	4.4
1	B	2	ALA	4.4
1	A	8	ILE	4.4
1	B	588	PHE	4.3
1	A	135	ASP	4.3
1	A	93	ALA	4.3
1	A	167	VAL	4.3
1	A	260	VAL	4.3
1	A	410	GLN	4.3
1	A	508	PRO	4.3
1	A	127	LEU	4.3
1	A	368	SER	4.3
1	B	543	TYR	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	19	LEU	4.2
1	A	99	LEU	4.2
1	A	242	LEU	4.2
1	B	764	LYS	4.2
1	B	689	GLU	4.2
1	A	695	ASP	4.2
1	A	251	VAL	4.2
1	A	442	THR	4.2
1	A	409	THR	4.2
1	A	443	ALA	4.1
1	A	146	GLU	4.1
1	A	10	ILE	4.1
1	A	148	PRO	4.1
1	A	772	TYR	4.1
1	A	132	LYS	4.1
1	A	97	PHE	4.1
1	B	613	GLY	4.1
1	A	179	ARG	4.0
1	B	766	ARG	4.0
1	B	604	PHE	4.0
1	A	96	PRO	4.0
1	B	429	LEU	4.0
1	B	392	ASP	4.0
1	A	23	SER	4.0
1	B	601	MET	4.0
1	A	367	PRO	4.0
1	B	86	ALA	4.0
1	A	229	LEU	4.0
1	B	393	VAL	3.9
1	A	20	ASP	3.9
1	A	228	HIS	3.9
1	A	413	VAL	3.9
1	A	400	ALA	3.9
1	B	634	VAL	3.9
1	A	147	GLY	3.8
1	A	755	THR	3.8
1	A	765	VAL	3.8
1	B	348	LYS	3.8
1	A	412	GLU	3.8
1	B	16	ILE	3.8
1	B	765	VAL	3.8
1	B	762	VAL	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	754	GLU	3.8
1	A	275	THR	3.8
1	A	404	SER	3.8
1	A	236	ARG	3.8
1	A	237	ASP	3.8
1	A	130	GLU	3.8
1	A	753	ILE	3.8
1	B	618	LEU	3.7
1	A	604	PHE	3.7
1	A	586	VAL	3.7
1	B	690	ARG	3.7
1	B	87	ASP	3.7
1	A	129	PHE	3.7
1	B	185	ARG	3.7
1	B	616	GLY	3.7
1	A	215	LEU	3.7
1	A	178	ALA	3.6
1	B	628	PHE	3.6
1	A	177	ARG	3.6
1	A	240	GLY	3.6
1	A	405	THR	3.5
1	A	414	LEU	3.5
1	A	756	GLU	3.5
1	A	138	MET	3.5
1	A	320	ILE	3.5
1	B	25	VAL	3.5
1	B	767	GLU	3.5
1	A	321	GLN	3.5
1	B	617	THR	3.5
1	A	269	GLY	3.5
1	A	359	ILE	3.5
1	A	196	TRP	3.4
1	A	218	ALA	3.4
1	A	241	VAL	3.4
1	B	419	LEU	3.4
1	A	259	HIS	3.4
1	B	113	GLN	3.4
1	A	758	GLU	3.4
1	B	629	PRO	3.4
1	A	306	LYS	3.4
1	A	391	GLN	3.4
1	A	399	ARG	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	3.4
1	A	760	GLU	3.4
1	B	590	ASP	3.3
1	A	438	GLY	3.3
1	A	402	ILE	3.3
1	A	217	ASP	3.3
1	A	759	LEU	3.3
1	A	689	GLU	3.3
1	B	210	GLU	3.3
1	A	312	PRO	3.3
1	B	155	LYS	3.2
1	B	88	GLN	3.2
1	B	691	GLN	3.2
1	B	11	PRO	3.2
1	A	757	ALA	3.2
1	B	350	SER	3.2
1	A	762	VAL	3.2
1	A	763	LYS	3.2
1	B	209	PHE	3.2
1	A	761	ARG	3.2
1	A	137	VAL	3.1
1	A	11	PRO	3.1
1	A	588	PHE	3.1
1	A	270	VAL	3.1
1	B	186	GLU	3.1
1	B	20	ASP	3.1
1	B	692	LYS	3.1
1	A	252	THR	3.1
1	A	203	ALA	3.0
1	B	349	VAL	3.0
1	A	411	ASP	3.0
1	B	89	GLU	3.0
1	B	91	ARG	3.0
1	B	40	ASN	3.0
1	A	307	SER	3.0
1	A	764	LYS	3.0
1	B	443	ALA	3.0
1	B	101	PRO	3.0
1	A	176	LEU	3.0
1	A	693	ILE	3.0
1	A	639	ASP	3.0
1	B	153	PRO	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	311	GLN	2.9
1	B	182	CYS	2.9
1	B	336	ALA	2.9
1	B	351	HIS	2.9
1	A	12	PRO	2.9
1	A	379	ALA	2.9
1	A	401	VAL	2.9
1	A	369	ALA	2.9
1	A	136	LYS	2.9
1	B	437	ARG	2.9
1	A	694	LEU	2.8
1	B	126	LEU	2.8
1	B	630	GLN	2.8
1	A	174	LEU	2.8
1	B	207	ALA	2.8
1	A	219	VAL	2.8
1	B	154	GLN	2.8
1	B	640	VAL	2.8
1	A	316	LEU	2.8
1	A	690	ARG	2.8
1	B	659	GLN	2.8
1	A	378	GLN	2.8
1	B	769	GLU	2.7
1	A	9(T)	GLY	2.7
1	B	8(T)	CYS	2.7
1	B	208	VAL	2.7
1	B	592	HIS	2.7
1	B	39	ASP	2.7
1	B	128	ASP	2.7
1	B	125	ALA	2.7
1	B	591	PHE	2.6
1	A	216	VAL	2.6
1	A	691	GLN	2.6
1	B	335	LYS	2.6
1	B	187	GLY	2.6
1	A	173	ALA	2.6
1	A	313	GLY	2.6
1	A	197	LEU	2.6
1	A	227	LEU	2.6
1	B	657	SER	2.6
1	A	325	VAL	2.6
1	B	90	ILE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	322	ASP	2.5
1	B	652	ASP	2.5
1	B	211	GLU	2.5
1	B	404	SER	2.5
1	A	590	ASP	2.5
1	A	589	ASP	2.5
1	A	310	LEU	2.5
1	B	127	LEU	2.5
1	A	274	THR	2.5
1	A	406	TYR	2.5
1	B	157	VAL	2.5
1	A	380	ILE	2.5
1	B	60	ILE	2.5
1	A	389	TYR	2.5
1	A	775	ALA	2.5
1	B	653	ALA	2.5
1	B	15	TYR	2.4
1	B	633	LEU	2.4
1	A	326	LEU	2.4
1	B	641	GLN	2.4
1	B	655	GLN	2.4
1	A	383	ASP	2.4
1	B	3	THR	2.4
1	B	688	LEU	2.4
1	B	661	ALA	2.4
1	A	314	GLU	2.4
1	A	16	ILE	2.4
1	A	365	TYR	2.4
1	B	275	THR	2.3
1	B	328	GLU	2.3
1	A	267	VAL	2.3
1	A	55	PRO	2.3
1	A	3	THR	2.3
1	A	60	ILE	2.3
1	A	198	VAL	2.3
1	A	362	PRO	2.3
1	B	12	PRO	2.3
1	A	22	ASN	2.2
1	B	150	THR	2.2
1	A	366	VAL	2.2
1	A	323	VAL	2.2
1	B	600	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	668	SER	2.2
1	B	650	THR	2.2
1	A	315	ARG	2.2
1	B	189	GLY	2.2
1	A	7	ILE	2.2
1	A	381	PRO	2.2
1	B	658	VAL	2.2
1	B	4	GLU	2.2
1	B	206	PRO	2.2
1	B	663	GLU	2.2
1	B	114	VAL	2.2
1	A	21	GLN	2.2
1	B	170	GLN	2.2
1	B	327	SER	2.2
1	A	360	ARG	2.1
1	A	671	ALA	2.1
1	B	656	ARG	2.1
1	A	692	LYS	2.1
1	B	667	ASN	2.1
1	A	388	ILE	2.1
1	A	370	LYS	2.1
1	A	670	GLU	2.1
1	B	95	ASP	2.1
1	B	642	SER	2.1
1	A	667	ASN	2.1
1	B	665	THR	2.1
1	A	226	ALA	2.1
1	B	631	ASN	2.1
1	B	632	GLY	2.1
1	A	271	VAL	2.1
1	A	171	ASN	2.0
1	B	397	LYS	2.0
1	B	151	TYR	2.0
1	A	603	VAL	2.0
1	B	768	MET	2.0
1	B	329	GLN	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 carbohydrates 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.