



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:11 AM UTC

PDB ID : 2QZV / pdb_00002qzv
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

<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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

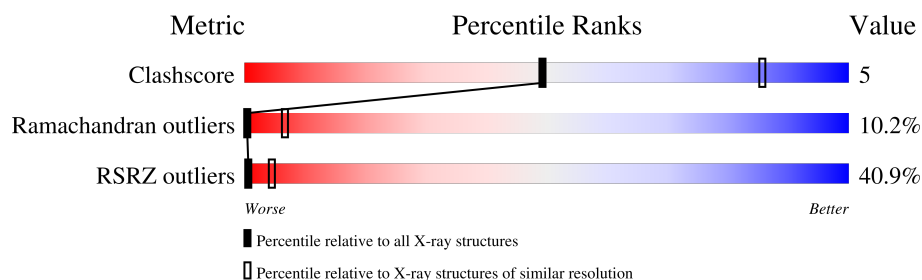
1 Overall quality at a glance

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	190562	1001 (11.50-4.06)
Ramachandran outliers	187476	1055 (11.50-4.00)
RSRZ outliers	180081	1162 (11.50-4.00)

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 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	873	34% 69% 14% 14%
1	B	873	36% 70% 14% 14%

2 Entry composition [i](#)

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			

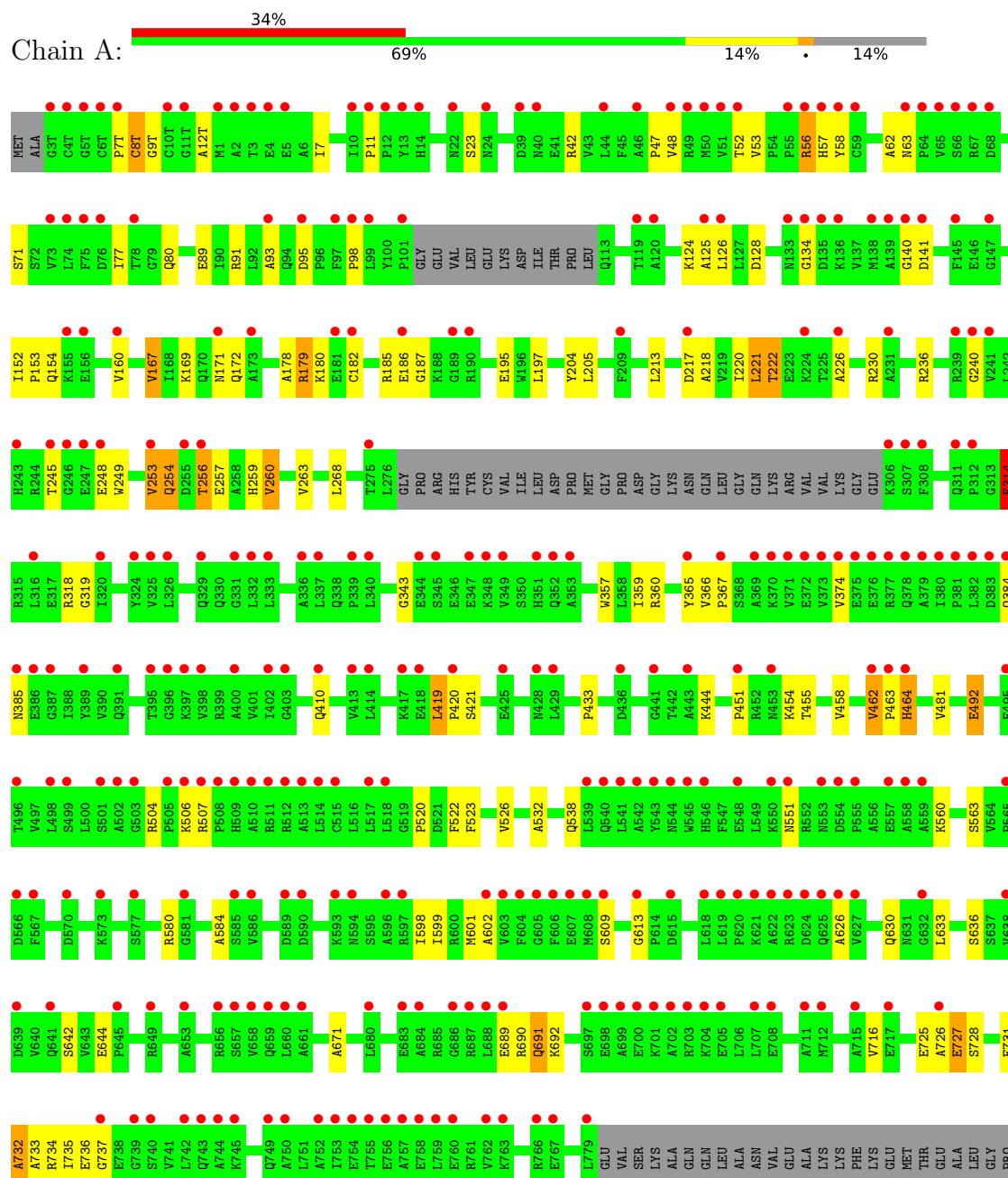
There are 24 discrepancies between the modelled and reference sequences:

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, 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: 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 – 9.00 200.00 – 9.00	Depositor EDS
% Data completeness (in resolution range)	98.0 (200.00-9.00) 91.2 (200.00-9.00)	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) 0.545 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	-1.2	Xtriage
Anisotropy	4.910	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 0.0	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	0.38	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

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	0.53	0/3699	1.18	30/5148 (0.6%)
1	B	0.52	0/3699	1.18	29/5148 (0.6%)
All	All	0.53	0/7398	1.18	59/10296 (0.6%)

There are no bond length outliers.

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	THR	N-CA-C	10.63	125.87	108.96
1	B	222	THR	N-CA-C	10.63	125.86	108.96
1	B	366	VAL	N-CA-C	9.29	116.74	107.55
1	A	366	VAL	N-CA-C	9.28	116.74	107.55
1	A	259	HIS	N-CA-C	7.62	119.59	111.28
1	A	197	LEU	N-CA-C	7.60	121.79	109.40
1	B	197	LEU	N-CA-C	7.59	121.77	109.40
1	B	259	HIS	N-CA-C	7.59	119.55	111.28
1	A	419	LEU	N-CA-C	7.13	123.41	113.57
1	B	419	LEU	N-CA-C	7.13	123.41	113.57
1	A	601	MET	N-CA-C	7.03	119.15	107.20
1	B	601	MET	N-CA-C	7.01	119.12	107.20
1	A	220	ILE	CA-C-N	6.89	134.71	121.54
1	A	220	ILE	C-N-CA	6.89	134.71	121.54
1	B	220	ILE	CA-C-N	6.88	134.68	121.54
1	B	220	ILE	C-N-CA	6.88	134.68	121.54
1	A	410	GLN	N-CA-C	-6.80	103.80	111.14
1	B	410	GLN	N-CA-C	-6.80	103.80	111.14
1	B	8(T)	CYS	N-CA-C	6.79	125.27	110.80
1	A	8(T)	CYS	N-CA-C	6.79	125.25	110.80
1	A	602	ALA	N-CA-C	-6.69	105.68	114.31
1	B	602	ALA	N-CA-C	-6.69	105.68	114.31
1	B	221	LEU	N-CA-C	5.96	123.49	110.80
1	A	221	LEU	N-CA-C	5.95	123.48	110.80
1	B	506	LYS	N-CA-C	5.93	118.05	108.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	506	LYS	N-CA-C	5.93	118.04	108.32
1	A	727	GLU	N-CA-C	5.86	123.28	110.80
1	A	451	PRO	N-CA-C	-5.80	105.83	113.65
1	B	451	PRO	N-CA-C	-5.79	105.83	113.65
1	B	195	GLU	N-CA-C	5.75	116.67	108.74
1	A	195	GLU	N-CA-C	5.74	116.66	108.74
1	B	385	ASN	N-CA-C	-5.61	99.16	108.75
1	A	385	ASN	N-CA-C	-5.59	99.18	108.75
1	B	613	GLY	CA-C-N	5.56	125.53	120.03
1	B	613	GLY	C-N-CA	5.56	125.53	120.03
1	A	613	GLY	CA-C-N	5.52	125.50	120.03
1	A	613	GLY	C-N-CA	5.52	125.50	120.03
1	A	728	SER	N-CA-C	5.50	118.95	110.42
1	A	726	ALA	N-CA-C	5.50	122.51	110.80
1	A	9(T)	GLY	N-CA-C	-5.49	100.17	113.18
1	B	9(T)	GLY	N-CA-C	-5.49	100.18	113.18
1	A	314	GLU	N-CA-C	5.46	122.42	110.80
1	B	314	GLU	N-CA-C	5.45	122.41	110.80
1	B	733	ALA	N-CA-C	5.42	116.91	110.19
1	B	245	THR	N-CA-C	5.41	117.03	107.61
1	A	245	THR	N-CA-C	5.41	117.02	107.61
1	A	167	VAL	N-CA-C	5.38	120.54	109.34
1	B	167	VAL	N-CA-C	5.38	120.52	109.34
1	B	492	GLU	N-CA-C	5.36	122.21	110.80
1	A	492	GLU	N-CA-C	5.35	122.20	110.80
1	B	260	VAL	N-CA-C	5.21	120.13	108.88
1	A	260	VAL	N-CA-C	5.19	120.09	108.88
1	B	56	ARG	N-CA-C	5.18	117.67	109.96
1	A	56	ARG	N-CA-C	5.16	117.64	109.96
1	B	256	THR	N-CA-C	-5.07	100.20	108.76
1	B	726	ALA	N-CA-C	5.06	116.41	107.61
1	A	256	THR	N-CA-C	-5.05	100.23	108.76
1	A	140	GLY	N-CA-C	5.04	121.65	110.66
1	B	140	GLY	N-CA-C	5.04	121.64	110.66

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
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:B:690:ARG:O	1:B:691:GLN:C	2.55	0.50
1:A:462:VAL:O	1:A:464:HIS:N	2.45	0.49
1:A:690:ARG:O	1:A:691:GLN:C	2.55	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:A:256:THR:O	1:A:257:GLU:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:256:THR:O	1:B:257:GLU:C	2.57	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
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: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: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: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%)	0	6
1	B	743/873 (85%)	528 (71%)	142 (19%)	73 (10%)	0	7
All	All	1486/1746 (85%)	1052 (71%)	283 (19%)	151 (10%)	0	7

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

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Mol	Chain	Res	Type
1	B	360	ARG
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

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Mol	Chain	Res	Type
1	A	523	PHE
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

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Mol	Chain	Res	Type
1	A	736	GLU
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 oligosaccharides 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%)	1.98	295 (39%) 1 5	50, 50, 50, 50	0
1	B	749/873 (85%)	2.18	317 (42%) 0 4	50, 50, 50, 50	0
All	All	1498/1746 (85%)	2.08	612 (40%) 0 4	50, 50, 50, 50	0

All (612) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	713	SER	15.8
1	A	756	GLU	14.7
1	B	351	HIS	14.6
1	B	416	GLU	14.0
1	A	544	ASN	13.4
1	A	353	ALA	12.6
1	B	596	ALA	12.2
1	B	415	TRP	11.7
1	B	98	PRO	11.3
1	A	463	PRO	11.2
1	A	380	ILE	11.2
1	B	375	GLU	10.2
1	A	336	ALA	10.0
1	A	743	GLN	10.0
1	B	464	HIS	10.0
1	B	192	THR	9.8
1	B	245	THR	9.7
1	A	391	GLN	9.6
1	A	593	LYS	9.6
1	B	638	VAL	9.4
1	B	595	SER	9.4
1	A	558	ALA	9.3
1	A	708	GLU	9.3
1	B	597	ARG	9.2

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Mol	Chain	Res	Type	RSRZ
1	B	669	GLN	8.9
1	B	247	GLU	8.9
1	A	375	GLU	8.9
1	A	760	GLU	8.9
1	A	543	TYR	8.8
1	B	343	GLY	8.8
1	A	542	ALA	8.7
1	B	397	LYS	8.7
1	A	508	PRO	8.7
1	A	155	LYS	8.7
1	B	589	ASP	8.6
1	A	511	ARG	8.5
1	B	87	ASP	8.3
1	B	91	ARG	8.3
1	A	554	ASP	8.3
1	A	239	ARG	8.3
1	B	593	LYS	8.2
1	B	171	ASN	8.1
1	A	605	GLY	8.0
1	B	3(T)	GLY	8.0
1	B	325	VAL	7.9
1	B	326	LEU	7.8
1	A	506	LYS	7.8
1	B	89	GLU	7.8
1	B	178	ALA	7.7
1	B	592	HIS	7.7
1	A	417	LYS	7.7
1	A	753	ILE	7.7
1	A	607	GLU	7.7
1	B	93	ALA	7.6
1	B	70	GLN	7.6
1	A	429	LEU	7.5
1	A	507	ARG	7.4
1	A	705	GLU	7.4
1	A	502	ALA	7.4
1	A	332	LEU	7.3
1	B	463	PRO	7.3
1	A	134	GLY	7.3
1	A	396	GLY	7.3
1	B	428	ASN	7.3
1	B	374	VAL	7.2
1	A	711	ALA	7.2

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Mol	Chain	Res	Type	RSRZ
1	B	4(T)	CYS	7.2
1	A	597	ARG	7.2
1	A	369	ALA	7.2
1	B	696	GLN	7.2
1	B	558	ALA	7.1
1	B	391	GLN	7.1
1	B	652	ASP	7.1
1	B	100	TYR	7.0
1	B	389	TYR	7.0
1	B	5(T)	GLY	6.9
1	A	349	VAL	6.9
1	A	596	ALA	6.8
1	A	246	GLY	6.8
1	A	606	PHE	6.7
1	A	464	HIS	6.7
1	B	46	ALA	6.7
1	A	701	LYS	6.7
1	B	700	GLU	6.7
1	B	71	SER	6.6
1	A	546	HIS	6.6
1	A	370	LYS	6.6
1	B	398	VAL	6.6
1	A	3	THR	6.6
1	A	590	ASP	6.6
1	A	245	THR	6.6
1	A	704	LYS	6.5
1	A	389	TYR	6.5
1	B	754	GLU	6.5
1	A	3(T)	GLY	6.5
1	B	412	GLU	6.5
1	B	678	GLN	6.4
1	A	382	LEU	6.4
1	A	247	GLU	6.4
1	B	68	ASP	6.4
1	B	655	GLN	6.4
1	A	13	TYR	6.4
1	A	602	ALA	6.4
1	B	695	ASP	6.4
1	A	119	THR	6.4
1	A	57	HIS	6.3
1	A	58	TYR	6.3
1	A	514	LEU	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	509	HIS	6.3
1	B	639	ASP	6.3
1	A	755	THR	6.3
1	A	4(T)	CYS	6.3
1	A	499	SER	6.2
1	B	425	GLU	6.2
1	B	682	GLN	6.2
1	A	66	SER	6.1
1	B	239	ARG	6.1
1	A	762	VAL	6.1
1	B	47	PRO	6.1
1	A	372	GLU	6.1
1	B	569	GLY	6.1
1	A	657	SER	6.0
1	A	510	ALA	6.0
1	A	615	ASP	6.0
1	B	324	TYR	6.0
1	B	72	SER	6.0
1	B	485	GLU	6.0
1	B	750	ALA	6.0
1	A	387	GLY	5.8
1	B	508	PRO	5.8
1	B	173	ALA	5.8
1	A	621	LYS	5.7
1	B	502	ALA	5.7
1	A	428	ASN	5.7
1	A	12	PRO	5.6
1	A	402	ILE	5.6
1	A	550	LYS	5.6
1	B	114	VAL	5.6
1	A	624	ASP	5.6
1	B	13	TYR	5.6
1	A	548	GLU	5.6
1	B	190	ARG	5.6
1	B	327	SER	5.5
1	B	347	GLU	5.5
1	A	515	CYS	5.5
1	A	698	GLU	5.5
1	A	381	PRO	5.5
1	A	425	GLU	5.5
1	B	99	LEU	5.5
1	A	739	GLY	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	194	GLU	5.5
1	B	566	ASP	5.4
1	A	49	ARG	5.3
1	A	5(T)	GLY	5.3
1	B	636	SER	5.3
1	B	598	ILE	5.3
1	B	157	VAL	5.2
1	B	496	THR	5.2
1	A	759	LEU	5.2
1	B	246	GLY	5.2
1	A	618	LEU	5.2
1	A	397	LYS	5.1
1	A	512	ARG	5.1
1	A	462	VAL	5.1
1	B	499	SER	5.1
1	A	540	GLN	5.1
1	B	380	ILE	5.1
1	B	216	VAL	5.1
1	B	58	TYR	5.1
1	B	692	LYS	5.1
1	B	429	LEU	5.1
1	B	392	ASP	5.1
1	B	354	GLY	5.0
1	B	707	LEU	5.0
1	B	382	LEU	5.0
1	B	675	HIS	4.9
1	B	748	ALA	4.9
1	B	411	ASP	4.9
1	B	624	ASP	4.9
1	A	702	ALA	4.9
1	B	134	GLY	4.9
1	A	505	PRO	4.9
1	B	217	ASP	4.9
1	A	67	ARG	4.9
1	A	384	GLN	4.8
1	A	737	GLY	4.8
1	A	4	GLU	4.8
1	B	671	ALA	4.8
1	B	738	GLU	4.7
1	A	97	PHE	4.7
1	B	703	ARG	4.7
1	A	740	SER	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	76	ASP	4.7
1	B	6(T)	CYS	4.7
1	A	545	TRP	4.7
1	B	506	LYS	4.6
1	B	576	ALA	4.6
1	A	156	GLU	4.6
1	A	240	GLY	4.6
1	B	686	GLY	4.6
1	B	12	PRO	4.6
1	B	627	VAL	4.6
1	B	640	VAL	4.6
1	B	648	GLN	4.6
1	B	465	ASN	4.6
1	A	707	LEU	4.6
1	A	403	GLY	4.6
1	B	376	GLU	4.6
1	B	507	ARG	4.5
1	B	755	THR	4.5
1	B	97	PHE	4.5
1	B	580	ARG	4.5
1	B	350	SER	4.5
1	B	119	THR	4.5
1	A	603	VAL	4.5
1	A	557	GLU	4.5
1	B	120	ALA	4.5
1	A	39	ASP	4.5
1	B	562	PHE	4.5
1	A	125	ALA	4.5
1	B	581	GLY	4.5
1	B	726	ALA	4.4
1	A	65	VAL	4.4
1	B	336	ALA	4.4
1	B	57	HIS	4.4
1	A	98	PRO	4.4
1	A	256	THR	4.4
1	A	383	ASP	4.4
1	B	373	VAL	4.4
1	A	577	SER	4.4
1	B	683	GLU	4.4
1	A	74	LEU	4.4
1	B	393	VAL	4.3
1	A	59	CYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	395	THR	4.3
1	A	517	LEU	4.3
1	A	6(T)	CYS	4.3
1	A	639	ASP	4.3
1	B	381	PRO	4.3
1	B	631	ASN	4.3
1	B	658	VAL	4.3
1	B	509	HIS	4.3
1	B	372	GLU	4.3
1	B	417	LYS	4.3
1	A	386	GLU	4.2
1	B	462	VAL	4.2
1	B	409	THR	4.2
1	A	687	ARG	4.2
1	B	122	HIS	4.2
1	A	567	PHE	4.2
1	A	641	GLN	4.1
1	B	431	HIS	4.1
1	A	374	VAL	4.1
1	B	1	MET	4.1
1	B	33	LYS	4.1
1	B	583	VAL	4.1
1	A	570	ASP	4.0
1	A	173	ALA	4.0
1	B	612	THR	4.0
1	B	243	HIS	4.0
1	B	408	LEU	4.0
1	A	660	LEU	4.0
1	A	326	LEU	4.0
1	B	742	LEU	4.0
1	B	20	ASP	4.0
1	A	55	PRO	4.0
1	B	656	ARG	4.0
1	A	589	ASP	4.0
1	B	113	GLN	4.0
1	B	151	TYR	4.0
1	B	442	THR	4.0
1	A	700	GLU	3.9
1	B	557	GLU	3.9
1	A	414	LEU	3.9
1	A	441	GLY	3.9
1	B	88	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	691	GLN	3.9
1	B	379	ALA	3.9
1	A	625	GLN	3.9
1	B	588	PHE	3.9
1	B	651	ARG	3.9
1	A	64	PRO	3.9
1	B	323	VAL	3.9
1	A	312	PRO	3.9
1	A	619	LEU	3.8
1	A	209	PHE	3.8
1	B	400	ALA	3.8
1	A	413	VAL	3.8
1	B	699	ALA	3.8
1	B	494	GLN	3.8
1	B	659	GLN	3.8
1	B	565	PRO	3.8
1	A	656	ARG	3.8
1	B	200	SER	3.8
1	A	241	VAL	3.8
1	A	551	ASN	3.7
1	B	11(T)	GLY	3.7
1	B	378	GLN	3.7
1	A	243	HIS	3.7
1	A	626	ALA	3.7
1	B	716	VAL	3.7
1	B	226	ALA	3.7
1	A	73	VAL	3.7
1	A	50	MET	3.7
1	B	413	VAL	3.6
1	B	69	THR	3.6
1	B	80	GLN	3.6
1	B	330	GLN	3.6
1	B	395	THR	3.6
1	A	348	LYS	3.6
1	A	325	VAL	3.6
1	B	201	VAL	3.6
1	B	693	ILE	3.6
1	B	224	LYS	3.6
1	B	585	SER	3.6
1	A	2	ALA	3.6
1	B	150	THR	3.6
1	B	579	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	637	SER	3.6
1	A	340	LEU	3.5
1	A	586	VAL	3.5
1	A	745	LYS	3.5
1	A	758	GLU	3.5
1	B	396	GLY	3.5
1	A	253	VAL	3.5
1	B	594	ASN	3.5
1	A	5	GLU	3.5
1	A	101	PRO	3.5
1	B	149	GLY	3.5
1	B	138	MET	3.5
1	A	518	LEU	3.5
1	A	140	GLY	3.4
1	B	704	LYS	3.4
1	A	63	ASN	3.4
1	B	133	ASN	3.4
1	A	138	MET	3.4
1	B	49	ARG	3.4
1	A	712	MET	3.4
1	B	584	ALA	3.4
1	B	159	VAL	3.4
1	A	311	GLN	3.4
1	A	352	GLN	3.4
1	B	587	THR	3.4
1	A	1	MET	3.4
1	B	690	ARG	3.4
1	A	553	ASN	3.4
1	B	779	LEU	3.4
1	B	626	ALA	3.3
1	A	373	VAL	3.3
1	B	230	ARG	3.3
1	A	541	LEU	3.3
1	A	555	PRO	3.3
1	B	233	GLN	3.3
1	A	182	CYS	3.3
1	B	621	LYS	3.3
1	B	202	GLY	3.3
1	B	361	GLY	3.3
1	A	141	ASP	3.3
1	B	394	LYS	3.3
1	B	573	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	590	ASP	3.3
1	A	120	ALA	3.3
1	A	661	ALA	3.3
1	A	699	ALA	3.3
1	B	670	GLU	3.3
1	A	410	GLN	3.3
1	A	565	PRO	3.3
1	B	10	ILE	3.3
1	B	387	GLY	3.3
1	B	720	GLY	3.3
1	B	369	ALA	3.3
1	B	577	SER	3.3
1	B	778	GLU	3.2
1	B	8	ILE	3.2
1	A	331	GLY	3.2
1	A	24	ASN	3.2
1	B	641	GLN	3.2
1	B	319	GLY	3.2
1	A	594	ASN	3.2
1	A	513	ALA	3.2
1	B	66	SER	3.2
1	B	757	ALA	3.2
1	B	269	GLY	3.2
1	B	568	VAL	3.2
1	A	52	THR	3.1
1	A	496	THR	3.1
1	B	763	LYS	3.1
1	A	189	GLY	3.1
1	B	248	GLU	3.1
1	B	241	VAL	3.1
1	B	86	ALA	3.1
1	A	255	ASP	3.1
1	A	653	ALA	3.1
1	A	135	ASP	3.1
1	B	10(T)	CYS	3.1
1	A	345	SER	3.1
1	A	139	ALA	3.1
1	B	346	GLU	3.1
1	A	171	ASN	3.1
1	A	750	ALA	3.1
1	B	92	LEU	3.1
1	B	18	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	275	THR	3.0
1	B	501	SER	3.0
1	A	226	ALA	3.0
1	B	495	PHE	3.0
1	B	189	GLY	3.0
1	A	585	SER	3.0
1	A	306	LYS	3.0
1	A	99	LEU	3.0
1	A	697	SER	3.0
1	B	115	VAL	3.0
1	B	486	LEU	3.0
1	A	686	GLY	3.0
1	B	711	ALA	3.0
1	A	609	SER	3.0
1	A	333	LEU	3.0
1	B	35	TYR	3.0
1	B	512	ARG	3.0
1	A	744	ALA	3.0
1	B	479	ARG	3.0
1	B	679	ARG	3.0
1	B	344	GLU	3.0
1	B	725	GLU	3.0
1	B	154	GLN	3.0
1	B	383	ASP	2.9
1	B	390	VAL	2.9
1	B	421	SER	2.9
1	A	51	VAL	2.9
1	A	93	ALA	2.9
1	B	737	GLY	2.9
1	A	501	SER	2.9
1	B	16	ILE	2.9
1	B	24	ASN	2.9
1	A	11	PRO	2.9
1	A	766	ARG	2.9
1	B	542	ALA	2.9
1	B	161	GLU	2.9
1	A	385	ASN	2.9
1	A	231	ALA	2.9
1	A	715	ALA	2.9
1	B	30	VAL	2.8
1	B	634	VAL	2.8
1	A	573	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	376	GLU	2.8
1	A	498	LEU	2.8
1	A	703	ARG	2.8
1	A	379	ALA	2.8
1	B	353	ALA	2.8
1	A	95	ASP	2.8
1	A	566	ASP	2.8
1	B	717	GLU	2.8
1	A	377	ARG	2.8
1	B	662	ILE	2.8
1	B	685	ARG	2.8
1	A	224	LYS	2.8
1	A	742	LEU	2.8
1	B	228	HIS	2.8
1	A	136	LYS	2.8
1	A	398	VAL	2.8
1	B	160	VAL	2.8
1	B	710	GLU	2.8
1	B	649	ARG	2.8
1	B	3	THR	2.8
1	B	196	TRP	2.8
1	B	225	THR	2.8
1	B	625	GLN	2.8
1	A	400	ALA	2.8
1	A	316	LEU	2.8
1	A	22	ASN	2.7
1	A	48	VAL	2.7
1	A	659	GLN	2.7
1	A	689	GLU	2.7
1	A	11(T)	GLY	2.7
1	A	351	HIS	2.7
1	B	19	LEU	2.7
1	B	26	SER	2.7
1	B	152	ILE	2.7
1	B	262	ASP	2.7
1	B	15	TYR	2.7
1	A	688	LEU	2.7
1	B	709	LEU	2.7
1	A	40	ASN	2.7
1	B	264	TYR	2.7
1	A	371	VAL	2.7
1	B	746	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	406	TYR	2.7
1	B	728	SER	2.7
1	B	586	VAL	2.6
1	B	697	SER	2.6
1	B	271	VAL	2.6
1	B	7(T)	PRO	2.6
1	B	272	PRO	2.6
1	A	726	ALA	2.6
1	B	719	THR	2.6
1	B	267	VAL	2.6
1	B	619	LEU	2.6
1	A	181	GLU	2.6
1	B	156	GLU	2.6
1	B	11	PRO	2.6
1	B	129	PHE	2.6
1	B	739	GLY	2.6
1	A	539	LEU	2.6
1	B	95	ASP	2.6
1	B	570	ASP	2.6
1	A	75	PHE	2.6
1	A	190	ARG	2.6
1	B	340	LEU	2.6
1	A	10	ILE	2.6
1	A	186	GLU	2.6
1	A	453	ASN	2.6
1	A	757	ALA	2.6
1	B	766	ARG	2.5
1	A	337	LEU	2.5
1	A	779	LEU	2.5
1	B	17	HIS	2.5
1	A	559	ALA	2.5
1	B	455	THR	2.5
1	A	307	SER	2.5
1	A	683	GLU	2.5
1	B	29	GLU	2.5
1	A	503	GLY	2.5
1	B	515	CYS	2.5
1	A	44	LEU	2.5
1	A	324	TYR	2.5
1	B	511	ARG	2.5
1	B	630	GLN	2.4
1	A	649	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	9	ARG	2.4
1	B	355	ASP	2.4
1	B	121	LEU	2.4
1	A	767	GLU	2.4
1	A	68	ASP	2.4
1	A	147	GLY	2.4
1	B	193	GLY	2.4
1	A	632	GLY	2.4
1	B	124	LYS	2.4
1	A	752	ALA	2.4
1	B	268	LEU	2.4
1	A	56	ARG	2.4
1	A	14	HIS	2.4
1	A	418	GLU	2.4
1	B	439	GLN	2.4
1	A	749	GLN	2.4
1	B	261	PRO	2.4
1	A	717	GLU	2.3
1	B	348	LYS	2.3
1	A	623	ARG	2.3
1	B	741	VAL	2.3
1	A	347	GLU	2.3
1	B	317	GLU	2.3
1	B	22	ASN	2.3
1	B	143	TRP	2.3
1	A	495	PHE	2.3
1	A	638	VAL	2.3
1	B	727	GLU	2.3
1	B	90	ILE	2.3
1	B	605	GLY	2.3
1	A	367	PRO	2.3
1	B	14	HIS	2.3
1	B	198	VAL	2.3
1	B	532	ALA	2.3
1	B	384	GLN	2.3
1	A	10(T)	CYS	2.2
1	A	320	ILE	2.2
1	A	620	PRO	2.2
1	A	443	ALA	2.2
1	A	604	PHE	2.2
1	B	613	GLY	2.2
1	B	712	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	339	PRO	2.2
1	A	451	PRO	2.2
1	A	684	ALA	2.2
1	A	344	GLU	2.2
1	B	36	ILE	2.2
1	A	627	VAL	2.2
1	A	645	PRO	2.2
1	A	329	GLN	2.2
1	B	322	ASP	2.2
1	A	378	GLN	2.2
1	A	248	GLU	2.2
1	A	7(T)	PRO	2.2
1	A	78	THR	2.2
1	A	308	PHE	2.2
1	B	567	PHE	2.2
1	B	653	ALA	2.1
1	A	145	PHE	2.1
1	B	31	GLY	2.1
1	A	763	LYS	2.1
1	B	244	ARG	2.1
1	A	622	ALA	2.1
1	B	128	ASP	2.1
1	A	658	VAL	2.1
1	B	457	VAL	2.1
1	A	613	GLY	2.1
1	A	754	GLU	2.1
1	A	160	VAL	2.1
1	A	420	PRO	2.1
1	A	46	ALA	2.0
1	A	133	ASN	2.0
1	B	191	VAL	2.0
1	A	581	GLY	2.0
1	B	63	ASN	2.0
1	B	629	PRO	2.0
1	A	608	MET	2.0
1	B	561	LEU	2.0
1	A	365	TYR	2.0
1	A	217	ASP	2.0
1	A	436	ASP	2.0
1	B	603	VAL	2.0
1	A	126	LEU	2.0
1	A	680	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 oligosaccharides 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.