



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2021 – 12:07 PM EDT

PDB ID : 7K2H
Title : Kelch domain of human KEAP1 bound to Nrf2 cyclic peptide, c[GDPETGE]
Authors : Muellers, S.N.; Allen, K.N.
Deposited on : 2020-09-08
Resolution : 2.09 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.18
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

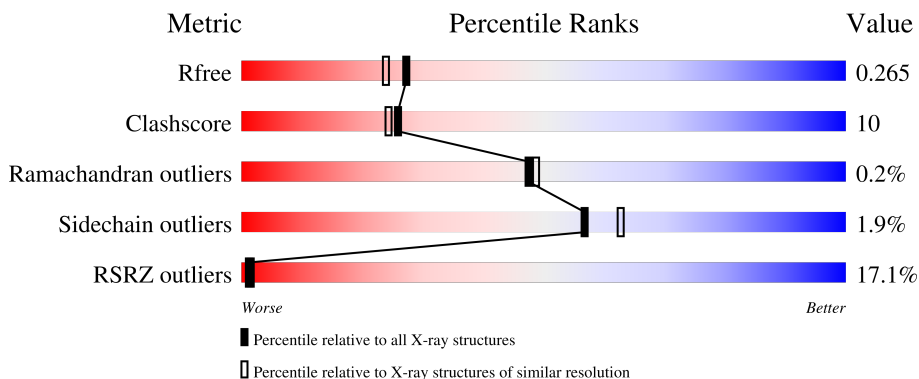
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	301	<div> <div>4%</div> <div>83%</div> <div>12%</div> <div>••</div> </div>
1	B	301	<div> <div>29%</div> <div>68%</div> <div>26%</div> <div>6%</div> </div>
2	P	7	<div> <div>86%</div> <div>14%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4652 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 Kelch-like ECH-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2211	1375	400	420	16			
1	B	283	Total	C	N	O	S	0	0	0
			2158	1343	392	408	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	613	SER	CYS	conflict	UNP Q14145
B	613	SER	CYS	conflict	UNP Q14145

- Molecule 2 is a protein called GLY-ASP-PRO-GLU-THR-GLY-GLU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	7	Total	C	N	O	0	0	0
			48	27	7	14			

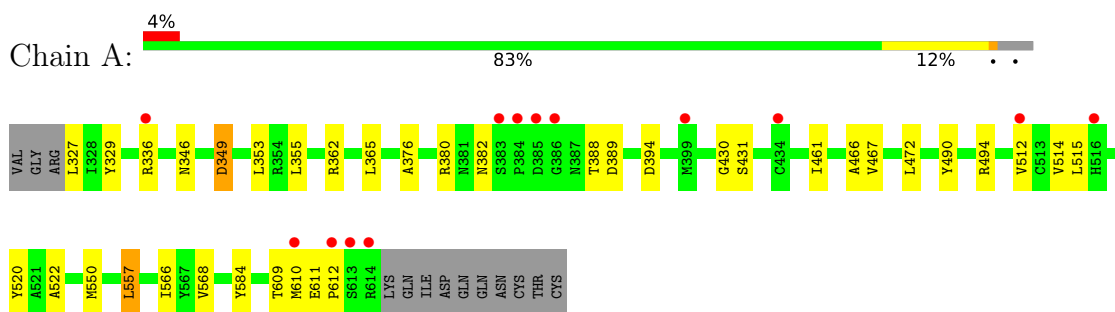
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	168	Total	O	0	0
			168	168		
3	B	64	Total	O	0	0
			64	64		
3	P	3	Total	O	0	0
			3	3		

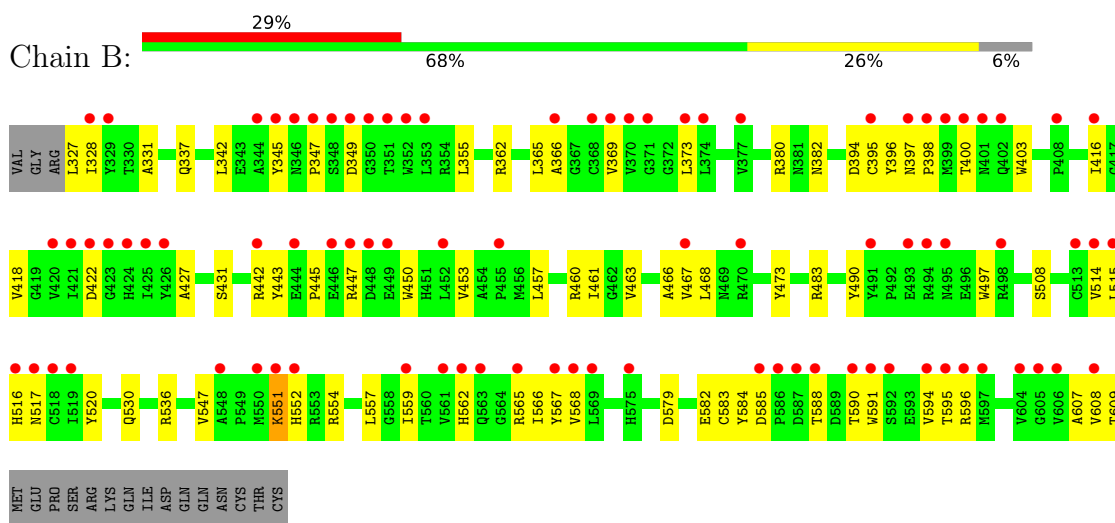
3 Residue-property plots

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.

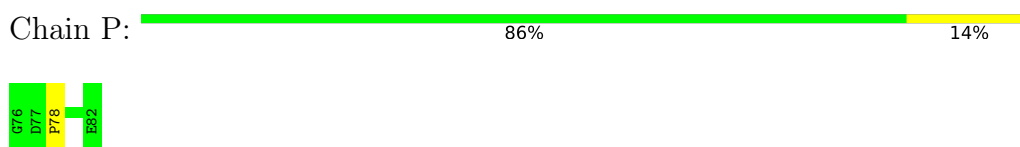
• Molecule 1: Kelch-like ECH-associated protein 1



• Molecule 1: Kelch-like ECH-associated protein 1



• Molecule 2: GLY-ASP-PRO-GLU-THR-GLY-GLU



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.24Å 68.60Å 77.27Å 90.00° 117.74° 90.00°	Depositor
Resolution (Å)	27.67 – 2.09 27.67 – 2.09	Depositor EDS
% Data completeness (in resolution range)	97.8 (27.67-2.09) 97.8 (27.67-2.09)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.225 , 0.265 0.225 , 0.265	Depositor DCC
R_{free} test set	1992 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4652	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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	0.44	0/2265	0.62	0/3085
1	B	0.41	0/2210	0.62	1/3012 (0.0%)
2	P	0.40	0/48	0.55	0/64
All	All	0.43	0/4523	0.62	1/6161 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	447	ARG	NE-CZ-NH2	-6.38	117.11	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	551	LYS	Peptide

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	2211	0	2100	32	0
1	B	2158	0	2046	58	0
2	P	48	0	35	1	0
3	A	168	0	0	0	0
3	B	64	0	0	0	0
3	P	3	0	0	0	0
All	All	4652	0	4181	90	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 10.

All (90) 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:327:LEU:HD11	1:A:611:GLU:HG3	1.44	0.97
1:B:328:ILE:HG12	1:B:608:VAL:HG12	1.60	0.82
1:B:466:ALA:HB1	1:B:514:VAL:HG23	1.61	0.81
1:B:515:LEU:HD22	1:B:566:ILE:HG13	1.63	0.80
1:A:327:LEU:CD1	1:A:611:GLU:HG3	2.15	0.76
1:A:550:MET:HE2	1:A:568:VAL:HG11	1.70	0.74
1:A:329:TYR:CE1	1:A:609:THR:HG22	2.24	0.71
1:A:466:ALA:HB1	1:A:514:VAL:HG23	1.72	0.71
1:A:550:MET:CE	1:A:568:VAL:HG11	2.23	0.68
1:A:353:LEU:HD22	1:A:355:LEU:HD21	1.75	0.67
1:B:466:ALA:HB1	1:B:514:VAL:CG2	2.26	0.66
1:B:559:ILE:HD12	1:B:568:VAL:HG12	1.78	0.64
1:A:557:LEU:HD23	1:A:557:LEU:H	1.64	0.62
1:A:329:TYR:CE1	1:A:609:THR:CG2	2.82	0.62
1:B:483:ARG:HG2	1:B:508:SER:HB2	1.82	0.62
1:B:468:LEU:HB3	1:B:473:TYR:HE1	1.65	0.61
1:A:329:TYR:OH	1:A:612:PRO:HD3	2.00	0.61
1:B:551:LYS:HB2	1:B:582:GLU:OE1	2.02	0.60
1:B:457:LEU:HD22	1:B:497:TRP:HB3	1.83	0.59
1:A:522:ALA:HB1	1:A:550:MET:HE3	1.84	0.59
1:B:369:VAL:HG21	1:B:608:VAL:O	2.04	0.56
1:B:565:ARG:HG2	1:B:584:TYR:O	2.06	0.55
1:A:515:LEU:HD22	1:A:566:ILE:HG13	1.89	0.55
1:A:329:TYR:CD1	1:A:609:THR:HG22	2.42	0.54
1:A:522:ALA:HB1	1:A:550:MET:CE	2.37	0.54
1:B:467:VAL:O	1:B:514:VAL:HG21	2.08	0.54
1:A:388:THR:HG22	1:A:389:ASP:O	2.08	0.53
1:A:430:GLY:O	1:A:461:ILE:HG22	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:LEU:HD23	1:B:396:TYR:OH	2.08	0.53
1:B:365:LEU:H	1:B:365:LEU:HD23	1.74	0.53
1:A:353:LEU:HD22	1:A:355:LEU:CD2	2.38	0.52
1:A:611:GLU:CG	1:A:612:PRO:HD2	2.38	0.52
1:B:416:ILE:HD11	1:B:427:ALA:HB1	1.91	0.52
1:B:562:HIS:HB3	1:B:567:TYR:CE2	2.45	0.52
1:B:362:ARG:NH1	1:B:394:ASP:OD2	2.43	0.52
1:B:562:HIS:HB3	1:B:567:TYR:HE2	1.74	0.52
1:B:584:TYR:HB2	1:B:591:TRP:CE2	2.46	0.51
1:B:584:TYR:HB2	1:B:591:TRP:CZ2	2.46	0.51
1:B:396:TYR:CE2	1:B:398:PRO:HA	2.46	0.50
1:A:346:ASN:CG	1:A:349:ASP:HB2	2.32	0.50
1:B:369:VAL:HG23	1:B:607:ALA:HB1	1.92	0.50
1:B:457:LEU:CD2	1:B:497:TRP:HB3	2.41	0.49
1:A:430:GLY:C	1:A:461:ILE:HG22	2.32	0.49
1:B:551:LYS:HB2	1:B:582:GLU:CD	2.32	0.49
1:B:397:ASN:HB2	1:B:400:THR:OG1	2.13	0.49
1:B:552:HIS:HB2	1:B:554:ARG:HH21	1.78	0.49
1:B:585:ASP:HB3	1:B:590:THR:OG1	2.13	0.48
1:B:442:ARG:HH11	1:B:453:VAL:HG12	1.79	0.48
1:B:443:TYR:HB2	1:B:450:TRP:CE2	2.49	0.48
1:B:551:LYS:HB3	1:B:552:HIS:CD2	2.49	0.48
1:B:516:HIS:CE1	1:B:520:TYR:CE1	3.02	0.47
1:A:353:LEU:CD2	1:A:355:LEU:HD21	2.41	0.47
1:B:460:ARG:HB3	1:B:463:VAL:HB	1.97	0.47
1:B:520:TYR:OH	1:B:536:ARG:NH1	2.45	0.47
1:B:342:LEU:HG	1:B:403:TRP:HZ2	1.80	0.47
1:A:611:GLU:HG2	1:A:612:PRO:HD2	1.97	0.46
1:A:467:VAL:O	1:A:514:VAL:HG21	2.15	0.46
1:B:331:ALA:HB2	1:B:342:LEU:HD23	1.98	0.46
1:B:516:HIS:CE1	1:B:520:TYR:HE1	2.34	0.46
1:B:366:ALA:HB1	1:B:418:VAL:HG22	1.96	0.46
1:A:362:ARG:NH1	1:A:394:ASP:OD1	2.48	0.46
1:B:551:LYS:HB3	1:B:552:HIS:CG	2.51	0.46
1:B:345:TYR:CE2	1:B:595:THR:HG21	2.50	0.45
1:A:512:VAL:HA	1:A:520:TYR:O	2.17	0.45
1:A:566:ILE:HB	1:A:584:TYR:HB3	1.98	0.45
1:B:327:LEU:N	1:B:609:THR:O	2.50	0.45
1:B:530:GLN:NE2	2:P:78:PRO:O	2.49	0.45
1:B:443:TYR:HB2	1:B:450:TRP:CD2	2.52	0.45
1:B:579:ASP:OD2	1:B:596:ARG:HB3	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:LEU:CD2	1:A:355:LEU:CD2	2.96	0.44
1:A:365:LEU:HD12	1:A:376:ALA:HB1	1.99	0.44
1:B:396:TYR:HB2	1:B:403:TRP:CE3	2.52	0.44
1:B:584:TYR:HA	1:B:590:THR:O	2.18	0.44
1:A:472:LEU:HB3	1:A:490:TYR:HB3	1.99	0.43
1:B:373:LEU:HB3	1:B:395:CYS:SG	2.58	0.43
1:B:516:HIS:HB2	1:B:517:ASN:H	1.54	0.43
1:A:431:SER:HB3	1:A:461:ILE:HG21	2.00	0.43
1:B:347:PRO:HG2	1:B:562:HIS:CE1	2.54	0.43
1:B:443:TYR:CE2	1:B:445:PRO:HA	2.55	0.42
1:B:337:GLN:HA	1:B:382:ASN:O	2.20	0.41
1:B:516:HIS:HE1	1:B:520:TYR:CE1	2.38	0.41
1:B:468:LEU:HD21	1:B:517:ASN:O	2.20	0.41
1:B:585:ASP:HB3	1:B:588:THR:OG1	2.21	0.41
1:A:550:MET:HE2	1:A:568:VAL:HG21	2.03	0.40
1:B:457:LEU:HD22	1:B:497:TRP:CB	2.50	0.40
1:B:431:SER:HB3	1:B:461:ILE:HG21	2.03	0.40
1:B:490:TYR:HB2	1:B:497:TRP:CZ2	2.56	0.40
1:B:583:CYS:HB3	1:B:594:VAL:HG21	2.03	0.40
1:B:328:ILE:HD11	1:B:562:HIS:HB2	2.04	0.40
1:A:380:ARG:HD3	1:A:382:ASN:OD1	2.21	0.40

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	286/301 (95%)	277 (97%)	9 (3%)	0	100	100
1	B	281/301 (93%)	266 (95%)	14 (5%)	1 (0%)	34	32
2	P	5/7 (71%)	5 (100%)	0	0	100	100
All	All	572/609 (94%)	548 (96%)	23 (4%)	1 (0%)	47	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	547	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	233/247 (94%)	228 (98%)	5 (2%)	53	59
1	B	225/247 (91%)	221 (98%)	4 (2%)	59	65
2	P	5/5 (100%)	5 (100%)	0	100	100
All	All	463/499 (93%)	454 (98%)	9 (2%)	57	63

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	336	ARG
1	A	349	ASP
1	A	494	ARG
1	A	557	LEU
1	A	610	MET
1	B	349	ASP
1	B	380	ARG
1	B	422	ASP
1	B	557	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	387	ASN
1	B	516	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	288/301 (95%)	0.14	13 (4%) 33 38	15, 24, 48, 101	0
1	B	283/301 (94%)	1.48	86 (30%) 0 0	18, 51, 85, 104	0
2	P	7/7 (100%)	-0.23	0 100 100	24, 33, 36, 38	0
All	All	578/609 (94%)	0.79	99 (17%) 1 1	15, 32, 79, 104	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	351	THR	7.1
1	B	592	SER	6.8
1	B	518	CYS	6.6
1	B	353	LEU	6.4
1	A	610	MET	6.4
1	B	399	MET	6.4
1	B	421	ILE	6.3
1	B	595	THR	6.0
1	A	613	SER	5.7
1	B	491	TYR	5.6
1	B	591	TRP	5.5
1	B	516	HIS	5.3
1	B	515	LEU	5.2
1	B	370	VAL	5.1
1	B	594	VAL	5.0
1	B	371	GLY	5.0
1	B	346	ASN	5.0
1	B	352	TRP	4.9
1	B	606	VAL	4.8
1	B	552	HIS	4.8
1	A	614	ARG	4.7
1	B	402	GLN	4.7
1	B	447	ARG	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	373	LEU	4.6
1	B	452	LEU	4.6
1	B	422	ASP	4.5
1	B	347	PRO	4.4
1	B	348	SER	4.3
1	B	575	HIS	4.2
1	B	397	ASN	4.2
1	A	336	ARG	4.2
1	B	400	THR	4.1
1	B	349	ASP	4.0
1	B	493	GLU	3.9
1	B	586	PRO	3.8
1	B	328	ILE	3.7
1	A	386	GLY	3.7
1	B	550	MET	3.6
1	B	350	GLY	3.6
1	A	385	ASP	3.5
1	A	384	PRO	3.5
1	B	567	TYR	3.5
1	B	494	ARG	3.4
1	B	395	CYS	3.4
1	B	548	ALA	3.3
1	B	517	ASN	3.3
1	B	608	VAL	3.3
1	B	398	PRO	3.3
1	B	561	VAL	3.3
1	B	596	ARG	3.2
1	B	568	VAL	3.2
1	B	562	HIS	3.1
1	B	444	GLU	3.1
1	B	565	ARG	3.1
1	B	426	TYR	3.1
1	B	514	VAL	3.1
1	B	590	THR	3.0
1	B	597	MET	3.0
1	B	424	HIS	3.0
1	B	408	PRO	2.9
1	A	399	MET	2.9
1	B	604	VAL	2.9
1	B	585	ASP	2.8
1	B	442	ARG	2.8
1	B	446	GLU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	345	TYR	2.8
1	B	455	PRO	2.8
1	B	368	CYS	2.8
1	B	425	ILE	2.7
1	B	563	GLN	2.7
1	B	448	ASP	2.6
1	B	449	GLU	2.6
1	B	401	ASN	2.6
1	B	377	VAL	2.5
1	B	374	LEU	2.5
1	B	569	LEU	2.5
1	B	495	ASN	2.5
1	B	467	VAL	2.5
1	A	383	SER	2.4
1	B	588	THR	2.4
1	B	416	ILE	2.4
1	B	513	CYS	2.4
1	B	420	VAL	2.4
1	B	366	ALA	2.3
1	A	434	CYS	2.3
1	B	551	LYS	2.2
1	A	516	HIS	2.2
1	B	587	ASP	2.2
1	B	559	ILE	2.1
1	B	329	TYR	2.1
1	B	423	GLY	2.1
1	B	470	ARG	2.1
1	B	519	ILE	2.1
1	A	512	VAL	2.1
1	B	369	VAL	2.1
1	B	605	GLY	2.1
1	A	612	PRO	2.0
1	B	498	ARG	2.0
1	B	344	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 [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.