WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 10:09 PM EDT

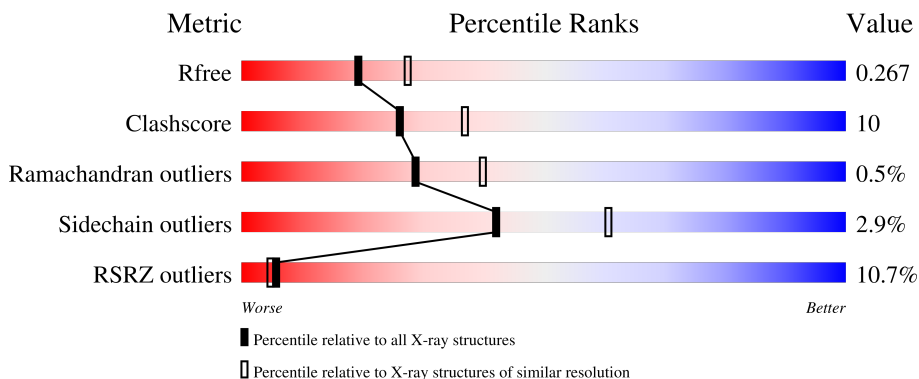|		
PDB ID	:	7K2I
Title	:	Kelch domain of human KEAP1 bound to Nrf2 cyclic peptide, c[GAPETGE]
Authors	:	Muellers, S.N.; Allen, K.N.
Deposited on	:	2020-09-08
Resolution	:	2.42 Å(reported)

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
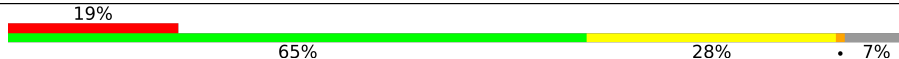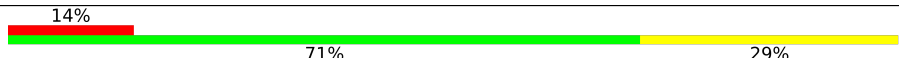*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.42 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	Percentile Ranks	Value
Rfree		0.267
Clashscore		10
Ramachandran outliers		0.5%
Sidechain outliers		2.9%
RSRZ outliers		10.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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 <=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	% 77% 17% • 5%
1	B	301	19% 65% 28% • 7%
2	P	7	14% 71% 29%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4579 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	285	Total 2260	C 1416	N 406	O 419	S 19	0	17	0
1	B	280	Total 2196	C 1374	N 393	O 410	S 19	0	16	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	613	SER	CYS	conflict	UNP Q14145
A	622	SER	CYS	conflict	UNP Q14145
A	624	SER	-	expression tag	UNP Q14145
B	613	SER	CYS	conflict	UNP Q14145
B	622	SER	CYS	conflict	UNP Q14145
B	624	SER	-	expression tag	UNP Q14145

- Molecule 2 is a protein called Nrf2 cyclic peptide,c[GAPETGE].

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	7	Total 45	C 26	N 7	O 12	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	67	Total 67	O 67	0	0
3	B	11	Total 11	O 11	0	0

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
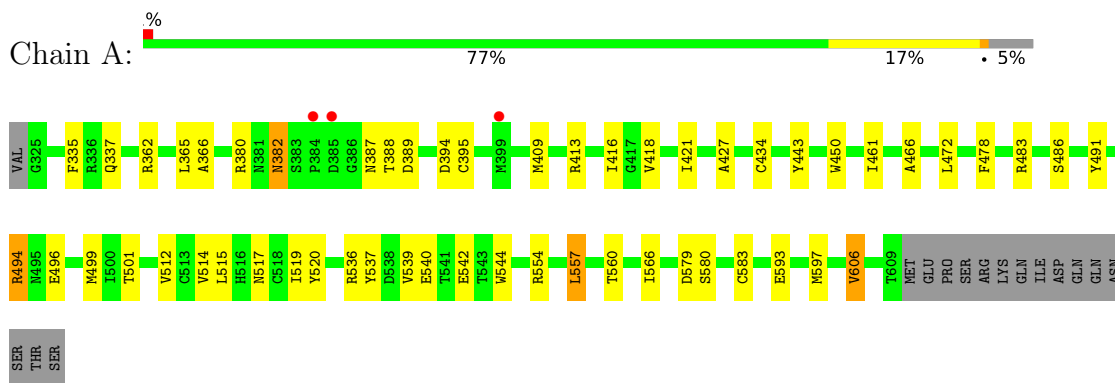
• Molecule 1: Kelch-like ECH-associated protein 1
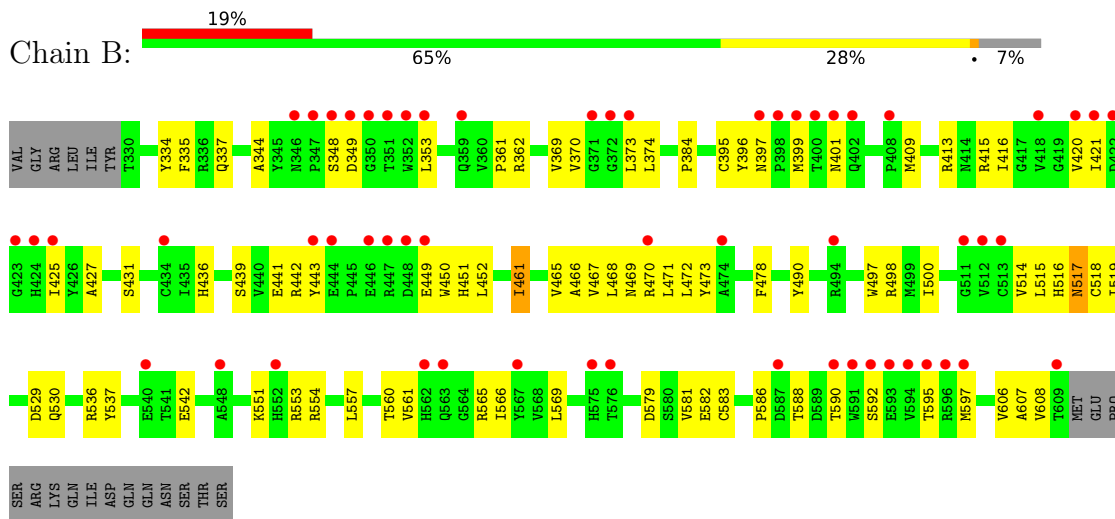
• Molecule 2: Nrf2 cyclic peptide,c[GAPETGE]

4   Data and refinement statistics   ⓘ

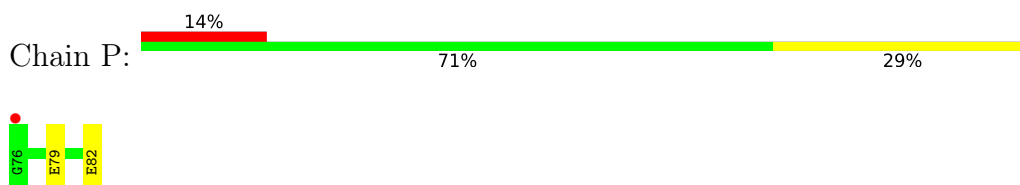| Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	77.18Å 68.62Å 143.53Å 90.00° 90.88° 90.00°	Depositor
Resolution (Å)	34.20 – 2.42 34.20 – 2.42	Depositor EDS
% Data completeness (in resolution range)	98.8 (34.20-2.42) 98.8 (34.20-2.42)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.216 , 0.267 0.217 , 0.267	Depositor DCC
R_{free} test set	1461 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å^2)	42.3	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.0	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.004 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4579	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.46	1/2361 (0.0%)	0.62	0/3215
1	B	0.39	0/2295	0.61	0/3127
2	P	0.99	0/45	0.87	0/60
All	All	0.44	1/4701 (0.0%)	0.62	0/6402

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	395	CYS	CB-SG	-6.47	1.71	1.82

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2260	0	2196	34	0
1	B	2196	0	2126	62	0
2	P	45	0	36	3	0
3	A	67	0	0	1	0
3	B	11	0	0	0	0
All	All	4579	0	4358	92	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 (92) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:561:VAL:HG22	1:B:566:ILE:HG12	1.63	0.80
1:B:466:ALA:HB1	1:B:514[B]:VAL:HG23	1.65	0.76
1:B:425:ILE:HB	1:B:443:TYR:HB3	1.67	0.75
1:B:515:LEU:HB2	1:B:566:ILE:HD11	1.70	0.74
1:A:491:TYR:HB3	1:B:516:HIS:HE1	1.52	0.73
1:B:415:ARG:NH2	2:P:79:GLU:OE2	2.22	0.71
1:A:466:ALA:HB1	1:A:514[B]:VAL:HG23	1.71	0.70
1:B:441:GLU:HB3	1:B:452:LEU:HD23	1.76	0.67
1:A:491:TYR:HB3	1:B:516:HIS:CE1	2.31	0.66
1:B:415:ARG:HH22	2:P:79:GLU:CD	2.00	0.65
1:B:472:LEU:HB3	1:B:490:TYR:HB3	1.77	0.65
1:B:369:VAL:HG21	1:B:608:VAL:O	1.98	0.64
1:B:468:LEU:HD12	1:B:469:ASN:H	1.64	0.62
1:B:436:HIS:CD2	1:B:461[B]:ILE:HD12	2.35	0.61
1:A:380:ARG:HD3	1:A:387:ASN:OD1	2.01	0.61
1:B:413:ARG:HH22	1:B:439:SER:HB2	1.66	0.61
1:A:421:ILE:HD11	1:A:472:LEU:HB2	1.84	0.59
1:B:516:HIS:O	1:B:517:ASN:HB2	2.03	0.59
1:A:515:LEU:HD22	1:A:566:ILE:HG13	1.84	0.58
1:A:554:ARG:HH22	1:A:580[B]:SER:HG	1.52	0.58
1:A:434[A]:CYS:SG	3:A:718:HOH:O	2.58	0.55
1:A:409:MET:SD	1:A:413:ARG:HD2	2.48	0.54
1:B:530:GLN:O	1:B:553[B]:ARG:HD3	2.08	0.53
1:B:579:ASP:O	1:B:597[A]:MET:HG3	2.08	0.53
1:B:468:LEU:HD12	1:B:469:ASN:N	2.23	0.53
1:A:365:LEU:HD23	1:A:365:LEU:H	1.75	0.52
1:A:416:ILE:HD11	1:A:427:ALA:HB1	1.92	0.52
1:B:436:HIS:HD2	1:B:461[B]:ILE:HD12	1.75	0.52
1:A:557:LEU:HD23	1:A:557:LEU:H	1.76	0.51
1:B:490:TYR:HB2	1:B:497:TRP:CH2	2.47	0.50
1:A:362:ARG:NH1	1:A:394:ASP:OD2	2.44	0.50
1:B:369:VAL:HG23	1:B:607:ALA:HB1	1.93	0.50
1:B:442:ARG:HH21	1:B:451:HIS:HB2	1.78	0.49
1:A:560:THR:HB	1:A:606[A]:VAL:HG23	1.94	0.49
1:B:443:TYR:HA	1:B:449:GLU:O	2.12	0.49
1:B:530:GLN:O	1:B:553[B]:ARG:NH1	2.40	0.49
1:B:581:VAL:HB	1:B:595:THR:OG1	2.12	0.49
1:A:335:PHE:C	1:A:337:GLN:H	2.17	0.48
1:B:344:ALA:HB3	1:B:353:LEU:HD21	1.95	0.48
1:B:551:LYS:N	1:B:582:GLU:OE2	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:ASP:O	1:A:597[A]:MET:HG3	2.14	0.47
1:A:512:VAL:HA	1:A:520:TYR:O	2.14	0.47
1:B:361:PRO:O	1:B:362:ARG:HG3	2.15	0.47
1:A:388:THR:HG22	1:A:389:ASP:O	2.14	0.47
1:A:443:TYR:HB2	1:A:450:TRP:CE2	2.50	0.46
1:B:349:ASP:N	1:B:349:ASP:OD1	2.48	0.46
1:A:380:ARG:HD2	1:A:382:ASN:HB2	1.98	0.46
1:B:443:TYR:HB2	1:B:450:TRP:CE2	2.51	0.46
1:B:416:ILE:HD11	1:B:427:ALA:HB1	1.98	0.46
1:B:560:THR:HB	1:B:606[B]:VAL:HG22	1.97	0.46
1:B:396:TYR:CE1	1:B:401:ASN:HA	2.51	0.45
1:A:466:ALA:HB2	1:A:512:VAL:HG12	1.98	0.45
1:A:494:ARG:HA	1:A:494:ARG:HD3	1.83	0.45
1:B:431:SER:HB3	1:B:461[B]:ILE:HG21	1.99	0.45
1:B:461[B]:ILE:HD13	1:B:478:PHE:HB3	1.99	0.45
1:B:582:GLU:HA	1:B:592:SER:O	2.17	0.45
1:B:443:TYR:HB2	1:B:450:TRP:CD2	2.52	0.44
1:B:583:CYS:N	1:B:592:SER:O	2.46	0.44
1:B:409:MET:HE1	1:B:413:ARG:HD2	1.98	0.44
1:A:519:ILE:O	1:A:536:ARG:HA	2.18	0.44
1:B:518:CYS:SG	1:B:536:ARG:HD2	2.58	0.44
1:B:519:ILE:O	1:B:536:ARG:HA	2.18	0.44
1:A:560:THR:HB	1:A:606[B]:VAL:HG22	1.99	0.43
1:B:588:THR:OG1	1:B:590:THR:OG1	2.26	0.43
1:B:554:ARG:NH2	1:B:582:GLU:OE1	2.52	0.42
1:A:537:TYR:HB2	1:A:544:TRP:CE3	2.54	0.42
1:A:501:THR:OG1	1:A:542:GLU:HG2	2.19	0.42
1:A:566:ILE:O	1:A:583:CYS:HA	2.20	0.42
1:B:370:VAL:HG22	1:B:420:VAL:HG21	2.01	0.42
1:A:478:PHE:CD1	1:A:483:ARG:HG3	2.54	0.42
1:B:334:TYR:CG	2:P:82:GLU:HG2	2.54	0.42
1:A:540:GLU:HB2	1:B:471:LEU:HD11	2.01	0.42
1:B:498:ARG:HD3	1:B:498:ARG:HA	1.86	0.42
1:A:366:ALA:HB1	1:A:418:VAL:HG22	2.02	0.41
1:B:421:ILE:HG12	1:B:467:VAL:HG11	2.02	0.41
1:B:515:LEU:HD21	1:B:586:PRO:HB3	2.02	0.41
1:B:397:ASN:OD1	1:B:399:MET:HB2	2.19	0.41
1:B:465:VAL:HA	1:B:473:TYR:O	2.20	0.41
1:A:580[A]:SER:OG	1:A:593:GLU:OE2	2.25	0.41
1:B:472:LEU:HD12	1:B:473:TYR:H	1.86	0.41
1:B:374:LEU:O	1:B:395:CYS:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:SER:HB3	1:B:461[A]:ILE:HG21	2.03	0.41
1:B:373:LEU:HD23	1:B:373:LEU:HA	1.98	0.41
1:B:409:MET:HE2	1:B:409:MET:HB2	1.81	0.41
1:B:537:TYR:OH	1:B:542:GLU:HG3	2.21	0.41
1:B:335:PHE:C	1:B:337:GLN:H	2.24	0.41
1:B:490:TYR:HB2	1:B:497:TRP:CZ3	2.56	0.40
1:B:515:LEU:CB	1:B:566:ILE:HD11	2.46	0.40
1:B:465:VAL:HG13	1:B:472:LEU:HD11	2.03	0.40
1:A:517:ASN:CB	1:B:470[B]:ARG:HD3	2.52	0.40
1:A:443:TYR:HB2	1:A:450:TRP:CZ2	2.55	0.40
1:A:486:SER:HB2	1:A:499[B]:MET:HE1	2.02	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	300/301 (100%)	291 (97%)	9 (3%)	0	100	100
1	B	294/301 (98%)	279 (95%)	11 (4%)	4 (1%)	11	14
2	P	5/7 (71%)	5 (100%)	0	0	100	100
All	All	599/609 (98%)	575 (96%)	20 (3%)	4 (1%)	29	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	517	ASN
1	B	348[A]	SER
1	B	348[B]	SER
1	B	500	ILE

5.3.2 Protein sidechains ⓘ

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	243/247 (98%)	233 (96%)	10 (4%)	30	47
1	B	236/247 (96%)	228 (97%)	8 (3%)	37	54
2	P	4/4 (100%)	4 (100%)	0	100	100
All	All	483/498 (97%)	465 (96%)	18 (4%)	42	51

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	382	ASN
1	A	461[A]	ILE
1	A	461[B]	ILE
1	A	494	ARG
1	A	496	GLU
1	A	539[A]	VAL
1	A	539[B]	VAL
1	A	557	LEU
1	A	606[A]	VAL
1	A	606[B]	VAL
1	B	384	PRO
1	B	461[A]	ILE
1	B	461[B]	ILE
1	B	529[A]	ASP
1	B	529[B]	ASP
1	B	557	LEU
1	B	565	ARG
1	B	569	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	436	HIS
1	A	469	ASN
1	B	402	GLN

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 monosaccharides 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, 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	285/301 (94%)	-0.11	3 (1%)	80	78	22, 36, 59, 107	0
1	B	280/301 (93%)	0.92	57 (20%)	1	0	30, 71, 116, 129	0
2	P	7/7 (100%)	1.32	1 (14%)	2	2	77, 90, 94, 121	0
All	All	572/609 (93%)	0.41	61 (10%)	6	5	22, 46, 110, 129	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	371	GLY	9.7
1	B	351	THR	7.9
1	B	346	ASN	6.8
1	A	385	ASP	5.8
1	B	446	GLU	5.5
1	B	399	MET	5.5
1	B	353	LEU	5.1
1	B	595	THR	4.7
1	B	423	GLY	4.5
1	A	399	MET	4.5
1	B	575	HIS	4.4
1	A	384	PRO	4.3
1	B	350	GLY	4.2
1	B	402	GLN	4.0
1	B	421	ILE	4.0
1	B	352	TRP	3.9
1	B	422	ASP	3.6
1	B	349	ASP	3.5
1	B	609	THR	3.5
1	B	408	PRO	3.5
1	B	576	THR	3.4
1	B	448	ASP	3.3
1	B	470[A]	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	443	TYR	3.1
1	B	444	GLU	3.1
1	B	424	HIS	3.1
1	B	513	CYS	3.0
2	P	76	GLY	2.9
1	B	597[A]	MET	2.9
1	B	401	ASN	2.9
1	B	425	ILE	2.7
1	B	434[A]	CYS	2.7
1	B	552	HIS	2.7
1	B	397	ASN	2.6
1	B	447	ARG	2.6
1	B	594	VAL	2.5
1	B	400	THR	2.4
1	B	449	GLU	2.4
1	B	590	THR	2.3
1	B	420	VAL	2.3
1	B	596	ARG	2.3
1	B	494	ARG	2.3
1	B	567	TYR	2.3
1	B	348[A]	SER	2.3
1	B	562	HIS	2.3
1	B	347	PRO	2.2
1	B	512	VAL	2.2
1	B	592	SER	2.2
1	B	372	GLY	2.2
1	B	591	TRP	2.2
1	B	563[A]	GLN	2.2
1	B	359	GLN	2.2
1	B	373	LEU	2.2
1	B	511	GLY	2.1
1	B	587	ASP	2.1
1	B	540	GLU	2.1
1	B	548	ALA	2.1
1	B	398	PRO	2.1
1	B	418	VAL	2.1
1	B	593	GLU	2.1
1	B	474	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 monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.