



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2021 – 12:01 PM EDT

PDB ID : 7K2Q
Title : Kelch domain of human KEAP1 bound to Nrf2 cyclic peptide, c[Ahx-DPETGE]
Authors : Muellers, S.N.; Allen, K.N.
Deposited on : 2020-09-08
Resolution : 2.37 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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
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

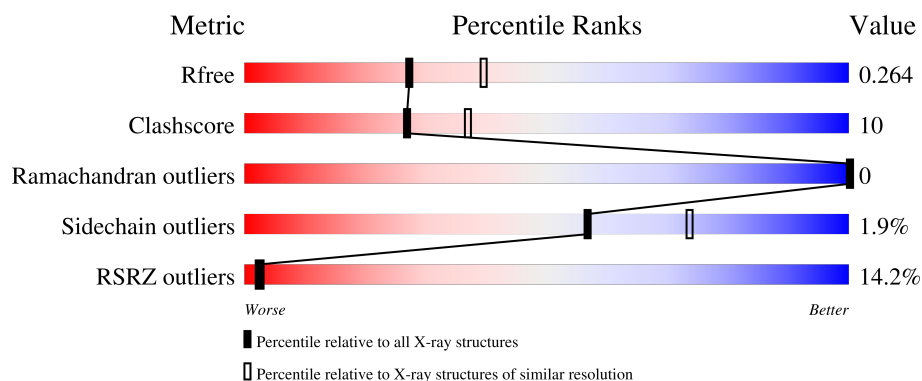
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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	290	<div> <div>2%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
1	B	290	<div> <div>27%</div> <div>70%</div> <div>28%</div> <div>.</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 4558 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
			2154	1342	388	409	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	540	ALA	GLU	conflict	UNP Q14145
A	542	ALA	GLU	conflict	UNP Q14145
A	613	SER	CYS	conflict	UNP Q14145
B	540	ALA	GLU	conflict	UNP Q14145
B	542	ALA	GLU	conflict	UNP Q14145
B	613	SER	CYS	conflict	UNP Q14145

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	7	Total	C	N	O	0	0	0
			52	31	7	14			

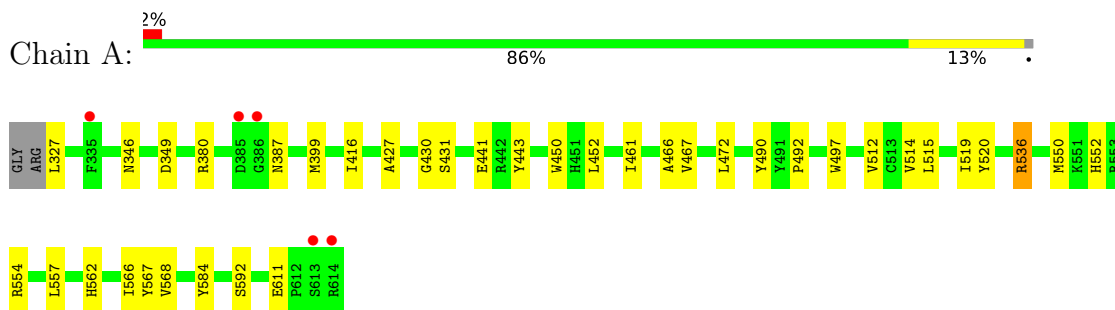
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	95	Total	O	0	0
			95	95		
3	B	42	Total	O	0	0
			42	42		
3	P	4	Total	O	0	0
			4	4		

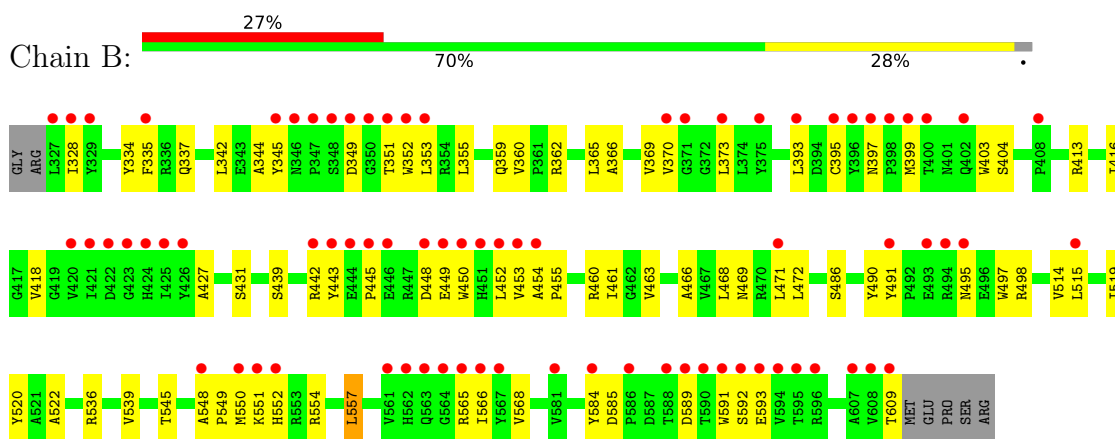
3 Residue-property plots [i](#)

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.

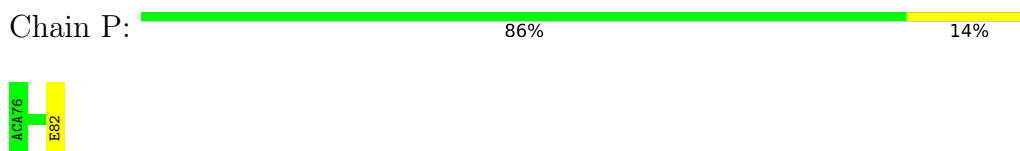
• Molecule 1: Kelch-like ECH-associated protein 1



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



• Molecule 2: ACA-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	162.15Å 68.75Å 77.59Å 90.00° 117.43° 90.00°	Depositor
Resolution (Å)	42.12 – 2.37 42.12 – 2.37	Depositor EDS
% Data completeness (in resolution range)	96.6 (42.12-2.37) 96.6 (42.12-2.37)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.218 , 0.264 0.218 , 0.264	Depositor DCC
R_{free} test set	1990 reflections (6.63%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4558	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACA

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	0.30	0/2265	0.55	0/3085
1	B	0.28	0/2207	0.55	0/3009
2	P	0.28	0/44	0.49	0/59
All	All	0.29	0/4516	0.55	0/6153

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2211	0	2106	28	0
1	B	2154	0	2038	60	0
2	P	52	0	42	1	0
3	A	95	0	0	1	0
3	B	42	0	0	1	0
3	P	4	0	0	0	0
All	All	4558	0	4186	88	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 (88) 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:342:LEU:HD12	1:B:403:TRP:CZ2	2.11	0.86
1:B:342:LEU:HD12	1:B:403:TRP:HZ2	1.45	0.80
1:B:548:ALA:O	1:B:591:TRP:NE1	2.15	0.79
1:A:550:MET:HE1	1:A:568:VAL:HG21	1.73	0.69
1:B:549:PRO:O	1:B:591:TRP:CD1	2.46	0.69
1:B:359:GLN:HE21	1:B:360:VAL:HG23	1.60	0.66
1:B:472:LEU:HB3	1:B:490:TYR:HB3	1.78	0.65
1:A:515:LEU:HD22	1:A:566:ILE:HG13	1.81	0.62
1:A:466:ALA:HB1	1:A:514:VAL:HG23	1.81	0.62
1:B:469:ASN:O	1:B:471:LEU:HD12	2.01	0.61
1:B:442:ARG:HE	1:B:453:VAL:CG1	2.12	0.61
1:A:416:ILE:HD11	1:A:427:ALA:HB1	1.82	0.61
1:A:552:HIS:HB2	1:A:554:ARG:HH21	1.67	0.59
1:B:554:ARG:HG3	1:B:557:LEU:HD22	1.84	0.59
1:A:327:LEU:HD11	1:A:611:GLU:HG2	1.82	0.59
1:B:416:ILE:HD11	1:B:427:ALA:HB1	1.85	0.59
1:B:552:HIS:HB2	1:B:554:ARG:HH21	1.68	0.59
1:B:454:ALA:HB3	1:B:490:TYR:HE1	1.67	0.58
1:B:442:ARG:HE	1:B:453:VAL:HG12	1.68	0.58
1:B:565:ARG:NH1	1:B:585:ASP:OD2	2.36	0.58
1:B:468:LEU:HD21	1:B:539:VAL:HG21	1.86	0.57
1:A:399:MET:HE2	3:A:717:HOH:O	2.03	0.57
1:B:397:ASN:OD1	1:B:399:MET:HG2	2.05	0.57
1:B:362:ARG:HG3	1:B:365:LEU:HD13	1.85	0.57
1:B:551:LYS:HZ2	1:B:593:GLU:H	1.52	0.56
1:B:442:ARG:NE	1:B:453:VAL:CG1	2.71	0.54
1:B:455:PRO:O	1:B:497:TRP:CD1	2.60	0.54
1:A:431:SER:HB3	1:A:461:ILE:HG21	1.88	0.54
1:B:373:LEU:HD12	1:B:397:ASN:HA	1.88	0.54
1:B:466:ALA:HB1	1:B:514:VAL:HG23	1.90	0.53
1:B:369:VAL:HG11	1:B:609:THR:HB	1.90	0.53
1:B:335:PHE:C	1:B:337:GLN:H	2.12	0.53
1:B:550:MET:HE1	1:B:568:VAL:HG21	1.91	0.53
1:B:515:LEU:HB3	1:B:520:TYR:CE1	2.44	0.53
1:A:512:VAL:HA	1:A:520:TYR:O	2.09	0.52
1:B:551:LYS:HZ1	1:B:592:SER:HA	1.74	0.52
1:A:550:MET:HE1	1:A:568:VAL:HG11	1.92	0.52
1:B:490:TYR:OH	1:B:495:ASN:OD1	2.26	0.51
1:A:472:LEU:HB3	1:A:490:TYR:HB3	1.93	0.51
1:B:370:VAL:HG11	1:B:445:PRO:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:MET:CE	1:A:568:VAL:HG11	2.40	0.51
1:B:413:ARG:NH2	1:B:439:SER:OG	2.42	0.51
1:A:566:ILE:HB	1:A:584:TYR:HB3	1.94	0.50
1:B:443:TYR:HB2	1:B:450:TRP:CE2	2.47	0.50
1:B:460:ARG:HB3	1:B:463:VAL:HB	1.94	0.50
1:B:519:ILE:O	1:B:536:ARG:HA	2.12	0.49
1:B:365:LEU:H	1:B:365:LEU:HD23	1.78	0.48
1:B:431:SER:HB3	1:B:461:ILE:HG21	1.95	0.48
1:A:490:TYR:HB2	1:A:497:TRP:CE2	2.50	0.47
1:B:442:ARG:NE	1:B:453:VAL:HG12	2.30	0.47
1:B:548:ALA:HB3	1:B:584:TYR:HE1	1.80	0.47
1:A:430:GLY:C	1:A:461:ILE:HG22	2.34	0.47
1:B:443:TYR:HA	1:B:449:GLU:O	2.15	0.47
1:B:548:ALA:HB2	1:B:589:ASP:CG	2.35	0.46
1:B:393:LEU:HD22	1:B:450:TRP:HZ2	1.80	0.46
1:B:393:LEU:HD22	1:B:450:TRP:CZ2	2.50	0.46
1:B:373:LEU:CD1	1:B:397:ASN:HA	2.46	0.45
1:B:471:LEU:CD2	1:B:491:TYR:CD2	3.00	0.45
1:B:515:LEU:HD22	1:B:566:ILE:HG13	1.97	0.45
1:B:395:CYS:O	1:B:403:TRP:HA	2.17	0.45
1:A:515:LEU:HB3	1:A:520:TYR:CE1	2.52	0.45
1:A:467:VAL:O	1:A:514:VAL:HG21	2.17	0.45
1:B:442:ARG:O	1:B:450:TRP:HA	2.16	0.45
1:B:353:LEU:HD23	1:B:355:LEU:HD11	1.98	0.45
1:A:441:GLU:HB3	1:A:452:LEU:HD23	1.99	0.44
1:B:551:LYS:NZ	1:B:593:GLU:H	2.15	0.44
1:A:519:ILE:O	1:A:536:ARG:HA	2.17	0.44
1:A:562:HIS:HB3	1:A:567:TYR:CE2	2.53	0.43
1:B:468:LEU:CD2	1:B:539:VAL:HG21	2.48	0.43
1:A:443:TYR:HB2	1:A:450:TRP:CD2	2.54	0.43
1:A:443:TYR:HB2	1:A:450:TRP:CE2	2.53	0.42
1:B:345:TYR:HB2	1:B:352:TRP:CH2	2.54	0.42
1:A:430:GLY:O	1:A:461:ILE:HG22	2.20	0.42
1:A:552:HIS:HB2	1:A:554:ARG:NH2	2.34	0.42
1:B:454:ALA:HB3	1:B:490:TYR:CE1	2.51	0.42
1:B:349:ASP:HB3	1:B:351:THR:HG22	2.00	0.42
1:B:522:ALA:HB1	1:B:550:MET:HE3	2.02	0.42
1:B:328:ILE:O	1:B:344:ALA:HA	2.19	0.42
1:B:471:LEU:CD2	1:B:491:TYR:CE2	3.02	0.42
1:A:346:ASN:CG	1:A:349:ASP:HB2	2.40	0.41
1:B:466:ALA:HB1	1:B:514:VAL:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:TYR:CE2	1:A:492:PRO:HA	2.55	0.41
1:B:366:ALA:HB1	1:B:418:VAL:HG22	2.03	0.41
1:B:443:TYR:HB2	1:B:450:TRP:CD2	2.56	0.41
1:B:486:SER:HA	3:B:707:HOH:O	2.21	0.40
1:A:380:ARG:NH2	1:A:387:ASN:HB3	2.36	0.40
1:B:334:TYR:CG	2:P:82:GLU:HG2	2.57	0.40
1:A:346:ASN:HB3	1:A:349:ASP:HB2	2.03	0.40

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	286/290 (99%)	273 (96%)	13 (4%)	0	100	100
1	B	281/290 (97%)	268 (95%)	13 (5%)	0	100	100
2	P	4/7 (57%)	4 (100%)	0	0	100	100
All	All	571/587 (97%)	545 (95%)	26 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	233/234 (100%)	230 (99%)	3 (1%)	69	82
1	B	224/234 (96%)	218 (97%)	6 (3%)	44	62
2	P	5/5 (100%)	5 (100%)	0	100	100
All	All	462/473 (98%)	453 (98%)	9 (2%)	57	73

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

Mol	Chain	Res	Type
1	A	536	ARG
1	A	557	LEU
1	A	592	SER
1	B	404	SER
1	B	448	ASP
1	B	452	LEU
1	B	498	ARG
1	B	545	THR
1	B	557	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	451	HIS
1	A	563	GLN
1	B	359	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACA	P	76	2	7,7,8	0.57	0	6,6,8	0.84	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACA	P	76	2	-	4/4/5/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	76	ACA	C3-C4-C5-C6
2	P	76	ACA	C4-C5-C6-N6
2	P	76	ACA	C1-C2-C3-C4
2	P	76	ACA	C2-C3-C4-C5

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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	288/290 (99%)	0.12	5 (1%) 70 71	22, 32, 52, 88	0
1	B	283/290 (97%)	1.36	77 (27%) 0 0	27, 55, 93, 117	0
2	P	6/7 (85%)	-0.03	0 100 100	36, 38, 38, 41	0
All	All	577/587 (98%)	0.72	82 (14%) 2 3	22, 39, 88, 117	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	329	TYR	9.2
1	B	562	HIS	7.4
1	B	351	THR	7.0
1	B	423	GLY	6.5
1	B	595	THR	6.1
1	B	347	PRO	6.1
1	B	567	TYR	6.1
1	B	592	SER	5.9
1	B	452	LEU	5.4
1	B	446	GLU	5.2
1	B	373	LEU	5.2
1	B	590	THR	5.1
1	B	422	ASP	5.1
1	B	591	TRP	4.9
1	B	421	ILE	4.8
1	B	443	TYR	4.8
1	B	424	HIS	4.7
1	B	402	GLN	4.6
1	B	398	PRO	4.5
1	B	395	CYS	4.5
1	B	594	VAL	4.5
1	B	494	ARG	4.5
1	B	399	MET	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	371	GLY	4.4
1	B	370	VAL	4.1
1	B	353	LEU	4.1
1	B	397	ASN	4.1
1	B	350	GLY	4.1
1	B	328	ILE	4.1
1	B	449	GLU	4.0
1	B	495	ASN	4.0
1	B	445	PRO	3.9
1	B	442	ARG	3.9
1	B	352	TRP	3.9
1	B	346	ASN	3.9
1	B	607	ALA	3.8
1	B	588	THR	3.6
1	B	444	GLU	3.6
1	B	425	ILE	3.5
1	B	581	VAL	3.5
1	A	335	PHE	3.5
1	B	375	TYR	3.5
1	B	349	ASP	3.4
1	B	345	TYR	3.4
1	B	491	TYR	3.4
1	B	454	ALA	3.4
1	B	608	VAL	3.4
1	B	451	HIS	3.3
1	B	593	GLU	3.3
1	B	426	TYR	3.3
1	B	565	ARG	3.3
1	B	408	PRO	3.2
1	B	348	SER	3.1
1	B	596	ARG	2.9
1	B	561	VAL	2.9
1	A	614	ARG	2.8
1	B	551	LYS	2.8
1	B	566	ILE	2.7
1	B	515	LEU	2.7
1	B	552	HIS	2.7
1	A	385	ASP	2.6
1	B	563	GLN	2.6
1	B	493	GLU	2.6
1	B	420	VAL	2.6
1	B	335	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	386	GLY	2.6
1	A	613	SER	2.5
1	B	586	PRO	2.5
1	B	448	ASP	2.4
1	B	584	TYR	2.3
1	B	400	THR	2.3
1	B	471	LEU	2.3
1	B	450	TRP	2.2
1	B	393	LEU	2.2
1	B	548	ALA	2.2
1	B	589	ASP	2.2
1	B	453	VAL	2.1
1	B	550	MET	2.1
1	B	396	TYR	2.1
1	B	327	LEU	2.1
1	B	609	THR	2.1
1	B	564	GLY	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ACA	P	76	8/9	0.91	0.20	34,43,46,53	0

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.