Full wwPDB X-ray Structure Validation Report (i)

Oct 8, 2023 – 11:32 PM EDT

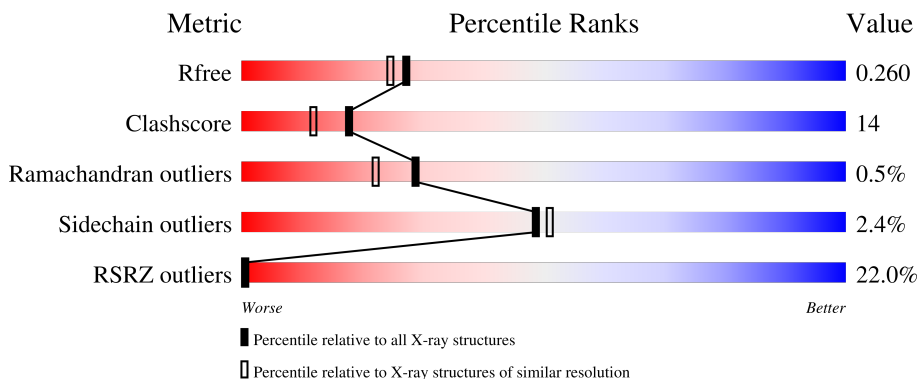|		
PDB ID	:	7K2G
Title	:	Kelch domain of human KEAP1 bound to Nrf2 cyclic peptide, c[GDEEAGE]
Authors	:	Muellers, S.N.; Allen, K.N.
Deposited on	:	2020-09-08
Resolution	:	2.15 Å(reported)

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 2.15 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		0.260
Clashscore		14
Ramachandran outliers		0.5%
Sidechain outliers		2.4%
RSRZ outliers		22.0%

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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	7% / 81% 14% · ·
1	B	301	34% / 72% 21% · 6%
2	P	7	43% / 71% 29%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4570 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
			2140	1333	387	406	14			

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 GLY-ASP-GLU-GLU-ALA-GLY-GLU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	7	Total	C	N	O	0	0	0
			48	26	7	15			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	133	Total	O	0	0
			133	133		
3	B	36	Total	O	0	0
			36	36		
3	P	2	Total	O	0	0
			2	2		

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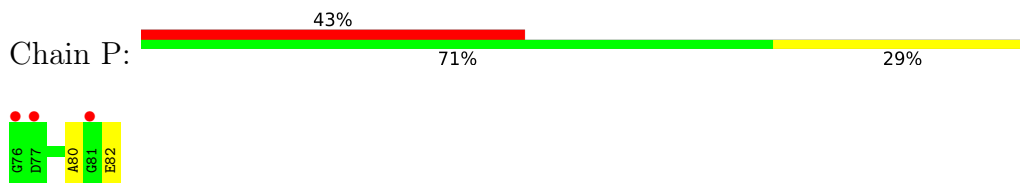
- Molecule 1: Kelch-like ECH-associated protein 1

Chain A:

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

Chain B:
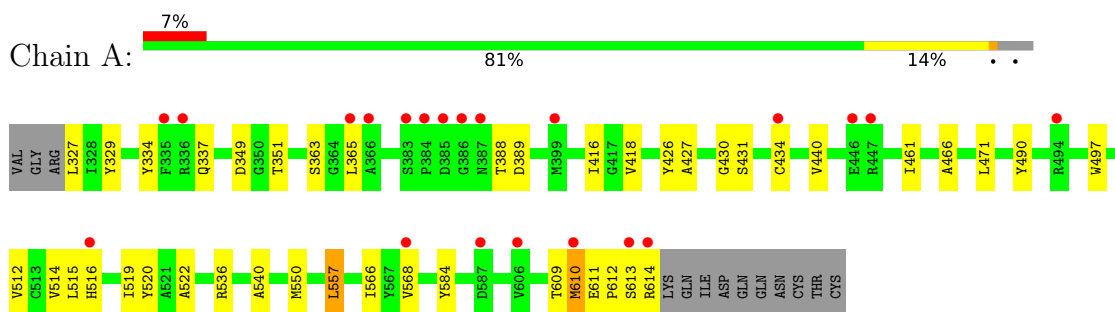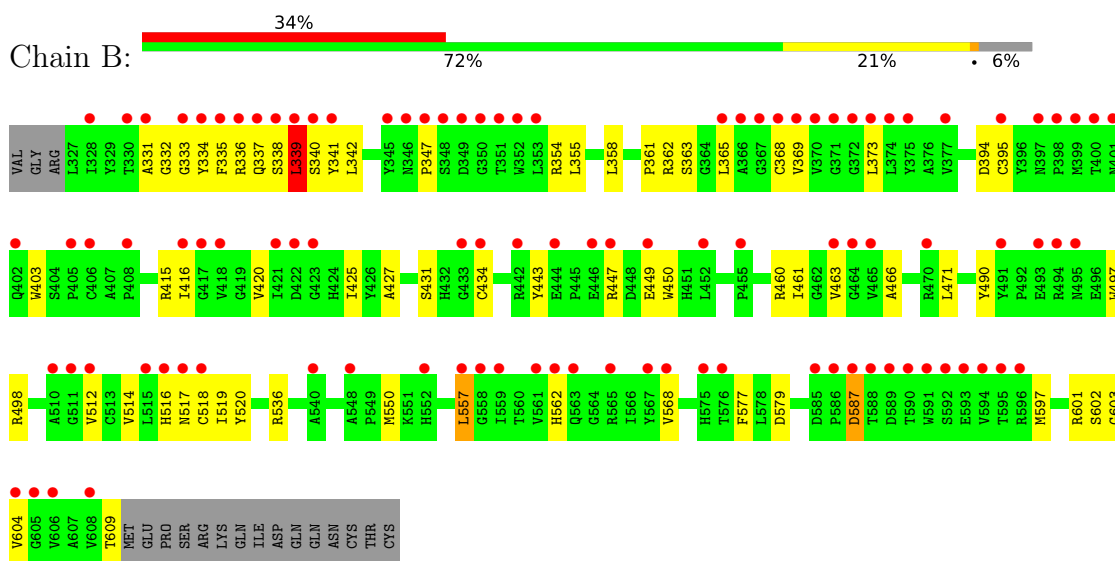
- Molecule 2: GLY-ASP-GLU-GLU-ALA-GLY-GLU

Chain P:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	161.58Å 68.67Å 77.18Å 90.00° 117.50° 90.00°	Depositor
Resolution (Å)	27.03 – 2.15 27.03 – 2.15	Depositor EDS
% Data completeness (in resolution range)	91.8 (27.03-2.15) 91.9 (27.03-2.15)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 2.15Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.230 , 0.260 0.230 , 0.260	Depositor DCC
R_{free} test set	2014 reflections (5.37%)	wwPDB-VP
Wilson B-factor (Å^2)	28.1	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 50.3	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.021 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4570	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 5.16% 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	0.31	1/2265 (0.0%)	0.53	0/3085
1	B	0.27	0/2191	0.50	0/2989
2	P	0.25	0/47	0.48	0/61
All	All	0.29	1/4503 (0.0%)	0.52	0/6135

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	610	MET	C-N	-5.69	1.21	1.34

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	2211	0	2105	38	0
1	B	2140	0	2021	80	0
2	P	48	0	32	3	0
3	A	133	0	0	1	0
3	B	36	0	0	2	0
3	P	2	0	0	0	0
All	All	4570	0	4158	116	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 14.

All (116) 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:334:TYR:O	1:B:601:ARG:HA	1.49	1.10
1:B:334:TYR:CE1	1:B:577:PHE:CZ	2.40	1.09
1:B:340:SER:CB	1:B:361:PRO:HA	1.83	1.08
1:B:334:TYR:CE1	1:B:577:PHE:CE1	2.44	1.05
1:B:340:SER:HB3	1:B:361:PRO:HA	1.13	1.04
1:B:334:TYR:N	1:B:602:SER:O	1.91	1.04
1:B:334:TYR:CD1	1:B:577:PHE:CE1	2.45	1.03
1:B:341:TYR:CE1	1:B:354:ARG:NH2	2.27	1.03
1:B:466:ALA:HB1	1:B:514:VAL:HG23	1.41	1.02
1:B:333:GLY:O	1:B:363:SER:HB3	1.60	1.00
1:A:466:ALA:HB1	1:A:514:VAL:HG23	1.41	0.99
1:B:340:SER:HB2	1:B:358:LEU:CD1	1.92	0.99
1:B:334:TYR:CD1	1:B:577:PHE:HE1	1.86	0.90
1:B:340:SER:HB2	1:B:358:LEU:HD12	1.53	0.89
1:B:334:TYR:O	1:B:601:ARG:CA	2.21	0.89
1:B:334:TYR:HE1	1:B:577:PHE:CZ	1.96	0.83
1:B:340:SER:HB3	1:B:361:PRO:CA	2.05	0.81
1:A:550:MET:SD	3:A:775:HOH:O	2.38	0.80
1:B:342:LEU:HD22	1:B:403:TRP:CZ2	2.16	0.79
1:B:331:ALA:HA	1:B:341:TYR:O	1.84	0.78
1:A:471:LEU:HD11	1:B:517:ASN:CB	2.16	0.76
1:B:334:TYR:CE1	1:B:577:PHE:HZ	2.02	0.76
1:B:341:TYR:HE1	1:B:354:ARG:NH2	1.84	0.74
1:B:334:TYR:HB3	1:B:602:SER:OG	1.88	0.73
1:B:340:SER:CB	1:B:358:LEU:HD12	2.20	0.70
1:A:416:ILE:HD11	1:A:427:ALA:HB1	1.73	0.70
1:B:362:ARG:NH2	1:B:394:ASP:OD2	2.23	0.70
1:A:550:MET:HE2	1:A:568:VAL:HG21	1.73	0.69
1:B:340:SER:HB2	1:B:358:LEU:HD13	1.74	0.69
1:B:341:TYR:CD1	1:B:354:ARG:NH2	2.61	0.68
1:B:332:GLY:HA2	1:B:340:SER:HA	1.76	0.68
1:B:333:GLY:O	1:B:363:SER:CB	2.41	0.68
1:B:333:GLY:HA3	1:B:604:VAL:HG12	1.78	0.66
1:B:334:TYR:O	1:B:602:SER:N	2.27	0.66
1:B:425:ILE:HB	1:B:443:TYR:HB3	1.79	0.64
1:A:329:TYR:OH	1:A:612:PRO:HD3	1.98	0.64
1:B:340:SER:HB2	1:B:358:LEU:HB2	1.80	0.63
1:B:362:ARG:HD2	1:B:365:LEU:HD13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:CYS:SG	1:B:425:ILE:CD1	2.87	0.62
1:B:334:TYR:HD1	1:B:577:PHE:HE1	1.42	0.62
1:B:333:GLY:C	1:B:602:SER:O	2.38	0.62
1:B:334:TYR:HD1	1:B:602:SER:OG	1.83	0.61
1:B:340:SER:CA	1:B:358:LEU:HD12	2.30	0.61
1:B:518:CYS:SG	1:B:536:ARG:HD3	2.41	0.60
1:A:466:ALA:HB1	1:A:514:VAL:CG2	2.24	0.60
1:B:335:PHE:HB3	1:B:339:LEU:HD11	1.83	0.59
1:B:416:ILE:HD11	1:B:427:ALA:HB1	1.85	0.59
1:B:334:TYR:HD1	1:B:602:SER:HG	1.49	0.57
1:A:550:MET:HE2	1:A:568:VAL:HG11	1.86	0.56
1:A:334:TYR:HB2	1:A:363:SER:HB3	1.87	0.56
1:B:340:SER:CB	1:B:358:LEU:HB2	2.35	0.56
1:B:373:LEU:HD13	1:B:395:CYS:SG	2.46	0.56
1:A:329:TYR:CE1	1:A:609:THR:HG22	2.41	0.56
1:A:515:LEU:HD22	1:A:566:ILE:HG13	1.87	0.55
1:B:334:TYR:HE1	1:B:577:PHE:HZ	1.42	0.55
1:A:430:GLY:O	1:A:461:ILE:HG22	2.08	0.53
1:A:431:SER:HB3	1:A:461:ILE:HG21	1.90	0.53
1:A:557:LEU:HD23	1:A:557:LEU:H	1.73	0.53
1:A:349:ASP:HB3	1:A:351:THR:HG23	1.91	0.52
1:A:522:ALA:HB1	1:A:550:MET:HE3	1.91	0.52
1:B:334:TYR:CE2	2:P:82:GLU:HG2	2.45	0.52
1:B:347:PRO:HG2	1:B:562:HIS:ND1	2.25	0.52
1:B:340:SER:OG	1:B:361:PRO:HA	2.07	0.51
1:A:550:MET:CE	1:A:568:VAL:HG11	2.41	0.50
1:A:430:GLY:C	1:A:461:ILE:HG22	2.31	0.50
1:A:334:TYR:HB2	1:A:363:SER:CB	2.42	0.50
1:B:334:TYR:CD1	1:B:602:SER:OG	2.64	0.50
1:B:514:VAL:HG22	1:B:519:ILE:HG12	1.95	0.49
1:B:579:ASP:HA	1:B:597:MET:HE2	1.94	0.49
1:B:342:LEU:O	1:B:355:LEU:HB2	2.13	0.49
1:B:333:GLY:CA	1:B:604:VAL:HG12	2.40	0.49
1:B:550:MET:HE2	1:B:568:VAL:HG21	1.93	0.48
1:B:342:LEU:HD22	1:B:403:TRP:HZ2	1.72	0.48
1:A:514:VAL:HG12	1:A:514:VAL:O	2.13	0.48
1:B:334:TYR:CZ	2:P:82:GLU:HG2	2.49	0.48
1:B:466:ALA:HB1	1:B:514:VAL:CG2	2.30	0.48
1:B:365:LEU:H	1:B:365:LEU:HD23	1.80	0.47
1:A:329:TYR:CE1	1:A:609:THR:CG2	2.99	0.46
1:B:340:SER:HB2	1:B:358:LEU:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:SER:O	1:A:614:ARG:HG2	2.15	0.46
1:B:431:SER:HB3	1:B:461:ILE:HG21	1.96	0.46
1:A:519:ILE:O	1:A:536:ARG:HA	2.17	0.45
1:A:329:TYR:CD1	1:A:609:THR:HG22	2.52	0.45
1:A:327:LEU:HD12	1:A:612:PRO:HD2	1.99	0.45
1:B:460:ARG:HB3	1:B:463:VAL:HB	1.99	0.45
1:A:327:LEU:HG	1:A:611:GLU:HB3	1.99	0.44
1:A:515:LEU:HB3	1:A:520:TYR:CE1	2.51	0.44
1:A:540:ALA:HB1	1:B:471:LEU:HD11	1.99	0.44
1:B:340:SER:C	1:B:358:LEU:HD12	2.37	0.44
1:A:512:VAL:HA	1:A:520:TYR:O	2.17	0.44
1:B:420:VAL:N	3:B:703:HOH:O	2.50	0.44
1:B:334:TYR:HB3	1:B:602:SER:HG	1.80	0.44
1:B:490:TYR:HB2	1:B:497:TRP:CE2	2.53	0.43
1:B:557:LEU:H	1:B:557:LEU:HD23	1.83	0.43
1:B:334:TYR:CE1	1:B:577:PHE:HE1	2.08	0.43
1:B:587:ASP:OD2	1:B:587:ASP:N	2.52	0.43
1:A:514:VAL:HG22	1:A:519:ILE:HG12	2.00	0.43
1:B:369:VAL:HG21	1:B:609:THR:HB	2.00	0.43
1:A:522:ALA:HB1	1:A:550:MET:CE	2.50	0.42
1:A:566:ILE:HB	1:A:584:TYR:HB3	2.01	0.42
1:B:512:VAL:HA	1:B:520:TYR:O	2.20	0.42
1:A:440:VAL:HG21	1:A:497:TRP:CZ2	2.55	0.42
1:B:443:TYR:HB2	1:B:450:TRP:CE2	2.54	0.42
1:A:334:TYR:CD1	1:A:334:TYR:C	2.93	0.42
1:A:388:THR:HG22	1:A:389:ASP:O	2.20	0.42
1:B:415:ARG:HH21	2:P:80:ALA:HB3	1.84	0.41
1:A:490:TYR:HB2	1:A:497:TRP:CE2	2.55	0.41
1:B:368:CYS:SG	1:B:425:ILE:HD12	2.60	0.41
1:B:338:SER:HB2	3:B:721:HOH:O	2.19	0.41
1:A:365:LEU:HD23	1:A:365:LEU:H	1.85	0.41
1:B:333:GLY:HA3	1:B:604:VAL:CG1	2.49	0.41
1:B:341:TYR:HE1	1:B:354:ARG:HH22	1.63	0.41
1:A:418:VAL:HA	1:A:426:TYR:O	2.21	0.41
1:B:340:SER:OG	1:B:358:LEU:HB2	2.20	0.40
1:B:333:GLY:HA2	1:B:603:GLY:C	2.41	0.40
1:B:447:ARG:NH1	1:B:449:GLU:OE2	2.54	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%)	273 (96%)	12 (4%)	1 (0%)	41	37
1	B	281/301 (93%)	265 (94%)	14 (5%)	2 (1%)	22	15
2	P	5/7 (71%)	5 (100%)	0	0	100	100
All	All	572/609 (94%)	543 (95%)	26 (4%)	3 (0%)	29	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	516	HIS
1	B	339	LEU
1	B	516	HIS

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	233/245 (95%)	229 (98%)	4 (2%)	60	65
1	B	220/245 (90%)	213 (97%)	7 (3%)	39	38
2	P	4/4 (100%)	4 (100%)	0	100	100
All	All	457/494 (92%)	446 (98%)	11 (2%)	49	51

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	337	GLN
1	A	434	CYS
1	A	557	LEU
1	A	610	MET
1	B	336	ARG
1	B	337	GLN
1	B	339	LEU
1	B	434	CYS
1	B	498	ARG
1	B	557	LEU
1	B	587	ASP

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	563	GLN
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 (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(Å²)	Q<0.9
1	A	288/301 (95%)	0.39	21 (7%)	15	21	15, 26, 48, 77	0
1	B	283/301 (94%)	1.73	103 (36%)	0	0	24, 60, 107, 126	0
2	P	7/7 (100%)	1.63	3 (42%)	0	0	61, 62, 72, 75	0
All	All	578/609 (94%)	1.06	127 (21%)	0	0	15, 38, 99, 126	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	334	TYR	10.7
1	B	341	TYR	9.4
1	B	335	PHE	8.3
1	B	337	GLN	7.0
1	B	399	MET	7.0
1	B	333	GLY	6.4
1	B	518	CYS	6.4
1	A	386	GLY	6.3
1	B	516	HIS	6.1
1	B	348	SER	6.0
1	A	385	ASP	6.0
1	B	351	THR	5.7
1	A	384	PRO	5.6
1	B	353	LEU	5.5
1	A	610	MET	5.4
1	B	575	HIS	5.1
1	B	422	ASP	5.0
1	B	336	ARG	5.0
1	A	336	ARG	5.0
1	B	346	ASN	4.9
1	B	402	GLN	4.9
1	B	562	HIS	4.7
1	B	339	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	491	TYR	4.6
1	B	372	GLY	4.5
1	B	340	SER	4.5
1	B	352	TRP	4.4
1	B	587	ASP	4.3
1	B	591	TRP	4.3
1	B	604	VAL	4.3
1	B	397	ASN	4.3
2	P	76	GLY	4.0
1	B	494	ARG	3.9
1	B	370	VAL	3.9
1	B	470	ARG	3.9
1	B	416	ILE	3.9
1	A	614	ARG	3.9
1	B	328	ILE	3.9
1	B	338	SER	3.8
1	B	421	ILE	3.8
1	B	452	LEU	3.8
1	B	418	VAL	3.8
1	B	447	ARG	3.7
1	A	613	SER	3.7
1	B	517	ASN	3.7
1	B	347	PRO	3.7
1	B	590	THR	3.6
1	B	557	LEU	3.6
1	B	434	CYS	3.6
1	A	399	MET	3.5
1	B	369	VAL	3.5
1	B	493	GLU	3.5
1	B	548	ALA	3.5
1	B	565	ARG	3.4
1	B	349	ASP	3.4
1	B	366	ALA	3.3
1	B	373	LEU	3.3
1	B	377	VAL	3.2
1	B	408	PRO	3.2
1	B	400	THR	3.2
1	B	567	TYR	3.1
1	B	374	LEU	3.1
1	A	335	PHE	3.1
1	A	383	SER	3.1
1	B	592	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	365	LEU	3.0
1	B	568	VAL	3.0
1	B	588	THR	3.0
1	A	587	ASP	3.0
1	B	442	ARG	2.9
1	B	395	CYS	2.9
1	B	594	VAL	2.9
1	B	371	GLY	2.8
1	B	596	ARG	2.8
1	B	446	GLU	2.8
1	A	434	CYS	2.8
1	B	463	VAL	2.8
1	B	552	HIS	2.8
1	B	405	PRO	2.7
1	B	444	GLU	2.7
1	B	449	GLU	2.7
1	B	368	CYS	2.7
1	A	387	ASN	2.7
1	B	515	LEU	2.7
1	B	563	GLN	2.6
1	B	595	THR	2.6
1	B	350	GLY	2.6
1	B	605	GLY	2.6
1	B	593	GLU	2.5
1	B	558	GLY	2.5
1	B	511	GLY	2.5
1	B	540	ALA	2.4
1	B	465	VAL	2.3
1	A	366	ALA	2.3
1	B	331	ALA	2.3
2	P	81	GLY	2.3
1	B	559	ILE	2.3
1	B	345	TYR	2.3
1	B	608	VAL	2.3
1	B	495	ASN	2.3
1	B	589	ASP	2.3
1	B	576	THR	2.2
1	B	401	ASN	2.2
1	B	330	THR	2.2
1	B	455	PRO	2.2
2	P	77	ASP	2.2
1	A	516	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	417	GLY	2.2
1	A	365	LEU	2.1
1	A	606	VAL	2.1
1	B	367	GLY	2.1
1	B	375	TYR	2.1
1	B	464	GLY	2.1
1	B	586	PRO	2.1
1	A	446	GLU	2.1
1	B	423	GLY	2.1
1	A	447	ARG	2.1
1	B	406	CYS	2.1
1	B	512	VAL	2.0
1	B	606	VAL	2.0
1	B	398	PRO	2.0
1	B	510	ALA	2.0
1	A	568	VAL	2.0
1	B	561	VAL	2.0
1	A	494	ARG	2.0
1	B	433	GLY	2.0
1	B	585	ASP	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.