



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:57 PM UTC

PDB ID : 7K2J / pdb_00007k2j
Title : Kelch domain of human KEAP1 bound to Nrf2 cyclic peptide, c[GDPEAGE]
Authors : Muellers, S.N.; Allen, K.N.
Deposited on : 2020-09-08
Resolution : 2.52 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

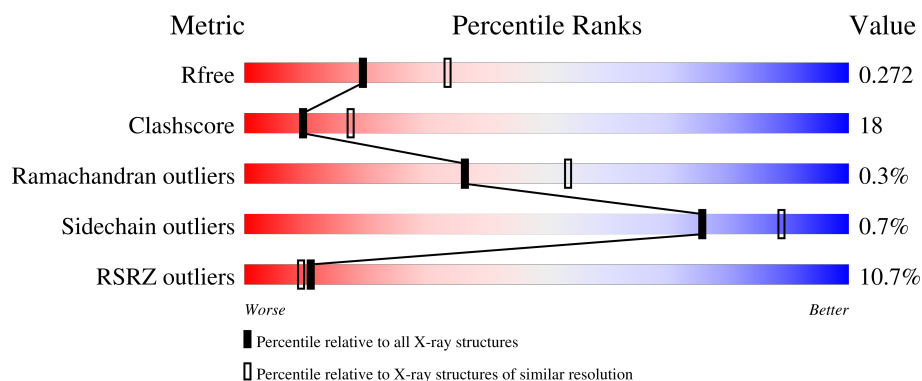
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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}	180053	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	2% 76% 22% ..
1	B	290	20% 61% 35% ..
2	P	7	71% 29%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4422 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
			2205	1372	397	420	16			
1	B	283	Total	C	N	O	S	0	0	0
			2124	1322	384	403	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 Nrf2 cyclic peptide,c[GDPEAGE].

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	7	Total	C	N	O	0	0	0
			46	26	7	13			

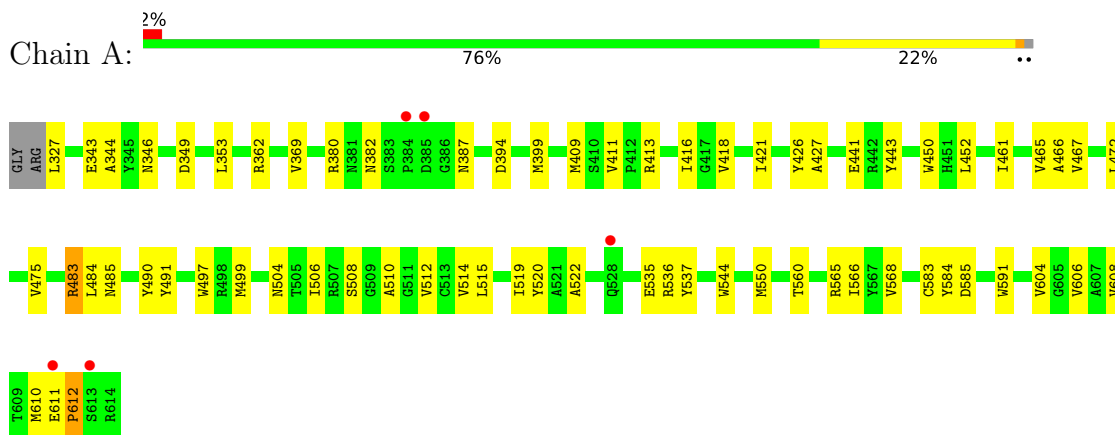
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	40	Total	O	0	0
			40	40		
3	B	7	Total	O	0	0
			7	7		

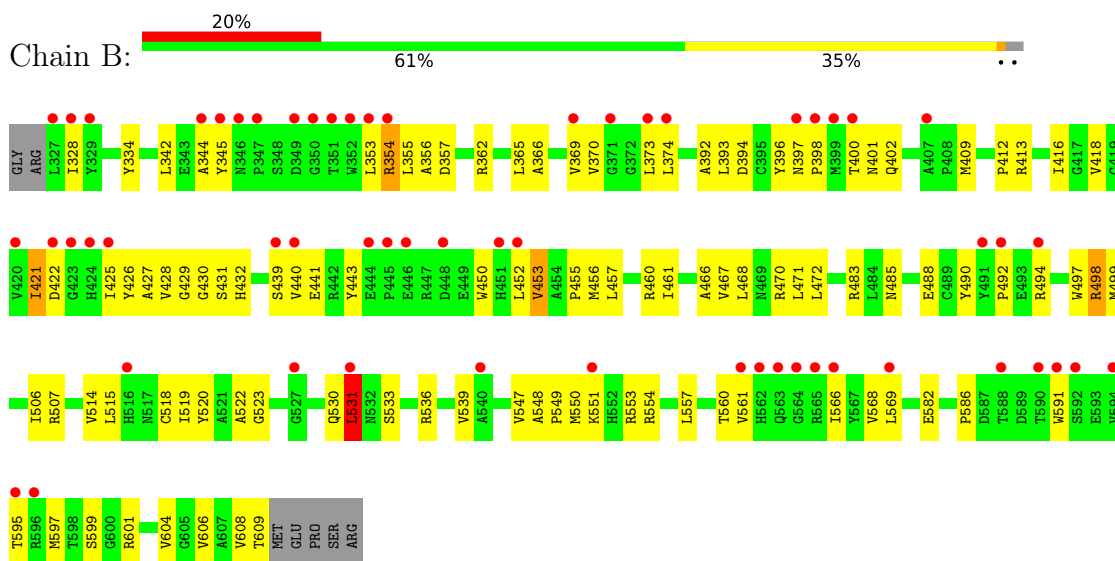
3 Residue-property plots

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.

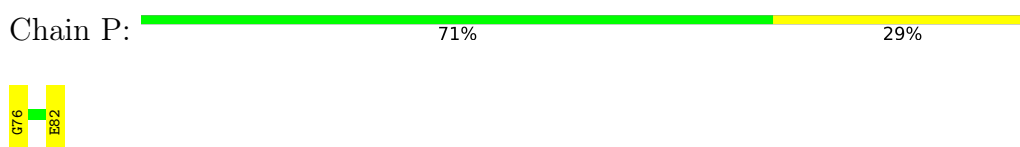
- Molecule 1: Kelch-like ECH-associated protein 1



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



- Molecule 2: Nrf2 cyclic peptide,c[GDPEAGE]



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.18Å 68.87Å 77.40Å 90.00° 117.54° 90.00°	Depositor
Resolution (Å)	27.78 – 2.52 27.78 – 2.52	Depositor EDS
% Data completeness (in resolution range)	97.9 (27.78-2.52) 97.8 (27.78-2.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.224 , 0.274 0.226 , 0.272	Depositor DCC
R_{free} test set	2003 reflections (7.78%)	wwPDB-VP
Wilson B-factor (Å ²)	43.2	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 61.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4422	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% 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](#)

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	0.83	5/2259 (0.2%)	0.82	5/3078 (0.2%)
1	B	0.55	1/2173 (0.0%)	0.94	8/2961 (0.3%)
2	P	0.31	0/46	4.78	1/61 (1.6%)
All	All	0.70	6/4478 (0.1%)	1.00	14/6100 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	411	VAL	C-O	-8.38	1.17	1.24
1	A	510	ALA	C-N	-5.97	1.30	1.33
1	A	465	VAL	C-O	-5.85	1.18	1.24
1	B	453	VAL	CB-CG2	-5.66	1.33	1.52
1	A	475	VAL	C-O	-5.50	1.18	1.24
1	A	411	VAL	CA-C	5.11	1.57	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	76	GLY	O-C-N	-36.90	63.96	123.00
1	B	498	ARG	CB-CG-CD	-9.50	89.45	111.30
1	B	354	ARG	NE-CZ-NH2	-8.38	111.66	119.20
1	B	354	ARG	CD-NE-CZ	7.47	134.87	124.40
1	A	475	VAL	N-CA-C	7.01	117.93	108.11
1	A	484	LEU	N-CA-C	6.83	120.82	109.95
1	A	411	VAL	O-C-N	6.83	126.50	121.72
1	B	354	ARG	CG-CD-NE	6.40	126.08	112.00
1	B	498	ARG	CD-NE-CZ	-6.29	115.60	124.40
1	B	531	LEU	N-CA-C	6.12	119.45	109.24
1	B	421	ILE	CA-C-N	5.89	132.79	121.54
1	B	421	ILE	C-N-CA	5.89	132.79	121.54
1	A	491	TYR	CA-C-N	5.78	125.46	119.05
1	A	491	TYR	C-N-CA	5.78	125.46	119.05

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	2205	0	2095	43	0
1	B	2124	0	2007	108	0
2	P	46	0	33	2	0
3	A	40	0	0	0	0
3	B	7	0	0	0	0
All	All	4422	0	4135	151	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 18.

All (151) 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:515:LEU:HB2	1:B:566:ILE:HD11	1.27	1.09
1:B:362:ARG:HH21	1:B:392:ALA:HB3	1.20	1.03
1:B:354:ARG:NH2	1:B:357:ASP:OD1	1.91	1.02
1:B:400:THR:HG22	1:B:402:GLN:HB2	1.48	0.93
1:B:515:LEU:CB	1:B:566:ILE:HD11	2.01	0.90
1:B:425:ILE:HG13	1:B:443:TYR:HD2	1.37	0.90
1:B:428:VAL:HA	1:B:440:VAL:HG23	1.52	0.88
1:B:397:ASN:HB3	1:B:400:THR:HB	1.60	0.84
1:A:550:MET:HE2	1:A:568:VAL:HG21	1.64	0.79
1:B:362:ARG:NH2	1:B:392:ALA:HB3	1.97	0.79
1:B:328:ILE:HG21	1:B:560:THR:HG21	1.67	0.76
1:B:369:VAL:HG11	1:B:609:THR:HB	1.70	0.74
1:B:518:CYS:HB3	1:B:536:ARG:HB2	1.70	0.74
1:B:441:GLU:HB3	1:B:452:LEU:HD23	1.71	0.72
1:B:569:LEU:HD12	1:B:597:MET:HE1	1.70	0.72
1:B:561:VAL:HG22	1:B:566:ILE:HG12	1.72	0.71
1:B:441:GLU:HG3	1:B:450:TRP:CZ3	2.25	0.71
1:B:393:LEU:HD22	1:B:450:TRP:HE1	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:ILE:HB	1:B:443:TYR:HB3	1.74	0.70
1:B:441:GLU:HG3	1:B:450:TRP:CE3	2.27	0.68
1:B:441:GLU:HB3	1:B:452:LEU:CD2	2.23	0.68
1:B:569:LEU:HD12	1:B:597:MET:CE	2.23	0.68
1:B:561:VAL:HG22	1:B:566:ILE:CG1	2.26	0.66
1:B:409:MET:HB3	1:B:441:GLU:CD	2.21	0.66
1:B:523:GLY:HA2	1:B:531:LEU:O	1.94	0.66
1:B:328:ILE:HG12	1:B:608:VAL:HG22	1.78	0.65
1:B:466:ALA:HB1	1:B:514:VAL:HG23	1.78	0.64
1:A:467:VAL:HG22	1:A:472:LEU:HD12	1.80	0.64
1:A:327:LEU:HD13	1:A:611:GLU:HB3	1.80	0.64
1:B:425:ILE:HG13	1:B:443:TYR:CD2	2.27	0.63
1:B:515:LEU:HD22	1:B:566:ILE:HD12	1.81	0.63
1:B:472:LEU:HB3	1:B:490:TYR:HB3	1.81	0.63
1:A:380:ARG:HD3	1:A:382:ASN:OD1	1.99	0.63
1:A:515:LEU:HD22	1:A:566:ILE:HG13	1.82	0.62
1:A:550:MET:CE	1:A:568:VAL:HG11	2.30	0.61
1:B:421:ILE:HB	1:B:426:TYR:HE2	1.65	0.61
1:B:440:VAL:HG13	1:B:453:VAL:HG21	1.82	0.61
1:B:416:ILE:HD11	1:B:427:ALA:HB1	1.82	0.60
1:A:522:ALA:HB1	1:A:550:MET:HE3	1.85	0.59
1:B:345:TYR:OH	1:B:595:THR:OG1	2.03	0.58
1:B:497:TRP:O	1:B:498:ARG:HG3	2.03	0.58
1:B:431:SER:HB3	1:B:461:ILE:HG21	1.84	0.57
1:B:515:LEU:HD23	1:B:520:TYR:CZ	2.39	0.57
1:B:470:ARG:N	1:B:470:ARG:HE	2.03	0.56
1:B:440:VAL:HG13	1:B:453:VAL:CG2	2.36	0.56
1:B:522:ALA:HB1	1:B:550:MET:HE3	1.88	0.56
1:B:362:ARG:HH21	1:B:392:ALA:CB	2.07	0.56
1:B:356:ALA:HB2	1:B:401:ASN:OD1	2.06	0.55
1:B:530:GLN:O	1:B:553:ARG:HD2	2.06	0.55
1:B:554:ARG:HG3	1:B:557:LEU:HD22	1.88	0.55
1:B:514:VAL:O	1:B:561:VAL:HG21	2.07	0.55
1:A:560:THR:HB	1:A:606:VAL:HG12	1.88	0.54
1:B:507:ARG:HH22	1:B:533:SER:HB2	1.72	0.54
1:B:397:ASN:CB	1:B:400:THR:HB	2.33	0.54
1:A:490:TYR:HB2	1:A:497:TRP:CE2	2.43	0.53
1:B:393:LEU:HD22	1:B:450:TRP:NE1	2.23	0.53
1:B:428:VAL:CA	1:B:440:VAL:HG23	2.33	0.53
1:A:485:ASN:HB3	1:A:506:ILE:CG1	2.38	0.53
1:B:362:ARG:NH2	1:B:394:ASP:OD1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:548:ALA:O	1:B:591:TRP:NE1	2.41	0.52
1:A:416:ILE:HD11	1:A:427:ALA:HB1	1.91	0.52
1:B:342:LEU:HD12	1:B:355:LEU:HB2	1.92	0.52
1:A:485:ASN:HB3	1:A:506:ILE:HA	1.91	0.52
1:B:443:TYR:HB2	1:B:450:TRP:CE2	2.45	0.52
1:B:456:MET:HE1	1:B:460:ARG:HB2	1.92	0.51
1:A:399:MET:SD	1:A:610:MET:HE1	2.50	0.51
1:B:515:LEU:HD22	1:B:566:ILE:CD1	2.40	0.51
1:B:355:LEU:HD22	1:B:396:TYR:OH	2.11	0.51
1:B:470:ARG:N	1:B:470:ARG:NE	2.59	0.51
1:B:370:VAL:HG21	1:B:425:ILE:HD11	1.93	0.51
1:A:519:ILE:O	1:A:536:ARG:HA	2.11	0.51
1:B:550:MET:HE2	1:B:568:VAL:HG21	1.94	0.50
1:B:370:VAL:HG21	1:B:425:ILE:CD1	2.42	0.50
1:B:373:LEU:CD1	1:B:397:ASN:HA	2.42	0.50
1:B:373:LEU:HD13	1:B:398:PRO:HD3	1.93	0.50
1:A:566:ILE:O	1:A:583:CYS:HA	2.12	0.49
1:A:380:ARG:NH2	1:A:387:ASN:HB3	2.27	0.49
1:B:536:ARG:HE	1:B:547:VAL:HG11	1.78	0.49
1:B:457:LEU:HD11	1:B:498:ARG:HA	1.95	0.49
1:B:520:TYR:CZ	1:B:536:ARG:HD3	2.48	0.48
1:A:512:VAL:HA	1:A:520:TYR:O	2.12	0.48
1:B:365:LEU:H	1:B:365:LEU:HD23	1.78	0.48
1:B:328:ILE:CG2	1:B:560:THR:HG21	2.40	0.48
1:B:560:THR:HB	1:B:606:VAL:HG12	1.95	0.48
1:B:421:ILE:HB	1:B:426:TYR:CE2	2.46	0.48
1:B:485:ASN:HB3	1:B:506:ILE:HA	1.96	0.48
1:B:494:ARG:O	1:B:494:ARG:HG2	2.14	0.47
1:A:346:ASN:CG	1:A:349:ASP:HB2	2.38	0.47
1:A:550:MET:HE2	1:A:568:VAL:HG11	1.96	0.47
1:A:409:MET:SD	1:A:413:ARG:HD2	2.55	0.46
1:B:440:VAL:CG1	1:B:453:VAL:HG21	2.44	0.46
1:B:366:ALA:HB1	1:B:418:VAL:HG22	1.96	0.46
1:B:412:PRO:HG2	1:B:432:HIS:CE1	2.50	0.46
1:A:441:GLU:HB3	1:A:452:LEU:HD23	1.97	0.46
1:B:599:SER:O	1:B:601:ARG:HG2	2.15	0.46
1:B:362:ARG:NH2	1:B:392:ALA:CB	2.73	0.45
1:B:418:VAL:HA	1:B:426:TYR:O	2.16	0.45
1:A:421:ILE:HD11	1:A:472:LEU:HB2	1.97	0.45
1:A:346:ASN:HB3	1:A:349:ASP:HB2	1.98	0.45
1:A:490:TYR:HB2	1:A:497:TRP:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:TYR:CZ	1:B:595:THR:OG1	2.67	0.45
1:B:498:ARG:HH11	1:B:498:ARG:HD3	1.53	0.45
1:B:440:VAL:CG1	1:B:453:VAL:CG2	2.94	0.45
1:B:470:ARG:NE	1:B:470:ARG:H	2.15	0.45
1:A:327:LEU:HD22	1:A:612:PRO:HD3	1.98	0.45
1:B:344:ALA:HB3	1:B:353:LEU:HB3	1.99	0.45
1:B:374:LEU:HB3	1:B:396:TYR:HB3	1.99	0.45
1:B:490:TYR:HB2	1:B:497:TRP:CH2	2.52	0.45
1:B:409:MET:HG2	1:B:450:TRP:CE2	2.52	0.45
1:B:515:LEU:HB3	1:B:520:TYR:CE1	2.52	0.44
1:A:418:VAL:HA	1:A:426:TYR:O	2.18	0.44
1:A:362:ARG:NH1	1:A:394:ASP:OD2	2.51	0.44
1:B:468:LEU:CD2	1:B:539:VAL:HG21	2.48	0.44
1:B:604:VAL:HG23	1:B:606:VAL:HG23	1.99	0.44
1:A:327:LEU:HD23	1:A:344:ALA:HB1	1.99	0.44
1:A:515:LEU:HB3	1:A:520:TYR:CE1	2.53	0.44
1:B:519:ILE:O	1:B:536:ARG:HA	2.17	0.43
1:A:604:VAL:HG23	1:A:606:VAL:HG23	2.00	0.43
1:B:413:ARG:NH1	1:B:429:GLY:O	2.47	0.43
1:B:430:GLY:C	1:B:461:ILE:HG22	2.43	0.43
1:B:549:PRO:O	1:B:591:TRP:CD1	2.71	0.43
1:B:409:MET:HB3	1:B:441:GLU:OE2	2.18	0.43
1:B:467:VAL:HA	1:B:471:LEU:O	2.19	0.43
1:B:490:TYR:CE2	1:B:492:PRO:HA	2.54	0.43
1:A:504:ASN:ND2	1:A:535:GLU:OE1	2.41	0.43
1:B:425:ILE:CG1	1:B:443:TYR:HD2	2.20	0.43
1:A:343:GLU:HA	1:A:353:LEU:O	2.19	0.43
1:B:456:MET:HB3	1:B:488:GLU:OE2	2.19	0.43
1:B:551:LYS:N	1:B:582:GLU:OE2	2.51	0.42
1:A:537:TYR:HB2	1:A:544:TRP:CE2	2.54	0.42
1:B:334:TYR:CG	2:P:82:GLU:HG2	2.55	0.42
1:B:439:SER:HA	1:B:455:PRO:HA	2.00	0.42
1:A:499:MET:HE2	1:A:499:MET:HB2	1.87	0.42
1:B:483:ARG:HB3	1:B:506:ILE:CG2	2.50	0.42
1:A:466:ALA:HB1	1:A:514:VAL:HG23	2.01	0.41
1:B:499:MET:HB2	1:B:499:MET:HE2	1.83	0.41
1:B:428:VAL:HG22	1:B:440:VAL:CG2	2.49	0.41
1:A:483:ARG:HG2	1:A:508:SER:HB3	2.01	0.41
1:B:515:LEU:HD21	1:B:586:PRO:HB3	2.03	0.41
1:B:334:TYR:CD1	2:P:82:GLU:HG2	2.56	0.41
1:A:485:ASN:HB3	1:A:506:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:ARG:HG2	1:A:585:ASP:HA	2.02	0.41
1:B:569:LEU:HB2	1:B:597:MET:HE3	2.03	0.41
1:A:369:VAL:HG21	1:A:608:VAL:O	2.21	0.41
1:A:416:ILE:HD13	1:A:416:ILE:HG21	1.89	0.41
1:A:443:TYR:HB2	1:A:450:TRP:CD2	2.56	0.41
1:A:584:TYR:HB2	1:A:591:TRP:CZ3	2.55	0.41
1:A:399:MET:HE2	1:A:399:MET:HB2	1.82	0.40
1:B:400:THR:CG2	1:B:402:GLN:HB2	2.33	0.40
1:B:397:ASN:HA	1:B:398:PRO:HD3	1.95	0.40
1:B:490:TYR:HB2	1:B:497:TRP:CZ3	2.57	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	286/290 (99%)	274 (96%)	11 (4%)	1 (0%)	36	53
1	B	281/290 (97%)	265 (94%)	15 (5%)	1 (0%)	30	47
2	P	5/7 (71%)	4 (80%)	1 (20%)	0	100	100
All	All	572/587 (97%)	543 (95%)	27 (5%)	2 (0%)	36	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	422	ASP
1	A	612	PRO

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	232/234 (99%)	230 (99%)	2 (1%)	70	86
1	B	218/234 (93%)	217 (100%)	1 (0%)	81	91
2	P	4/4 (100%)	4 (100%)	0	100	100
All	All	454/472 (96%)	451 (99%)	3 (1%)	76	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	461	ILE
1	A	483	ARG
1	B	531	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	402	GLN
1	A	432	HIS
1	A	437	HIS
1	A	485	ASN
1	A	552	HIS
1	B	397	ASN
1	B	414	ASN
1	B	451	HIS
1	B	504	ASN
1	B	575	HIS

5.3.3 RNA ⓘ

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	288/290 (99%)	-0.02	5 (1%) 69 66	25, 41, 66, 140	0
1	B	283/290 (97%)	1.14	57 (20%) 3 2	36, 73, 123, 154	0
2	P	7/7 (100%)	0.74	0 100 100	59, 60, 73, 80	0
All	All	578/587 (98%)	0.56	62 (10%) 11 9	25, 53, 112, 154	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	564	GLY	5.3
1	B	329	TYR	5.2
1	B	351	THR	5.1
1	B	347	PRO	4.6
1	B	346	ASN	4.5
1	B	399	MET	4.5
1	B	327	LEU	4.3
1	B	563	GLN	4.3
1	B	373	LEU	4.2
1	B	344	ALA	3.9
1	B	591	TRP	3.9
1	B	588	THR	3.6
1	B	420	VAL	3.5
1	B	516	HIS	3.4
1	B	400	THR	3.4
1	B	444	GLU	3.4
1	B	491	TYR	3.3
1	B	371	GLY	3.2
1	B	439	SER	3.1
1	B	350	GLY	3.1
1	B	445	PRO	3.0
1	B	424	HIS	3.0
1	A	385	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	566	ILE	2.8
1	A	384	PRO	2.8
1	B	349	ASP	2.8
1	B	565	ARG	2.7
1	B	425	ILE	2.7
1	B	590	THR	2.6
1	B	446	GLU	2.6
1	B	423	GLY	2.5
1	B	448	ASP	2.5
1	B	374	LEU	2.5
1	B	369	VAL	2.5
1	B	596	ARG	2.5
1	B	531	LEU	2.5
1	B	595	THR	2.4
1	B	551	LYS	2.4
1	B	451	HIS	2.4
1	B	594	VAL	2.4
1	B	562	HIS	2.4
1	B	397	ASN	2.4
1	B	353	LEU	2.4
1	A	528	GLN	2.3
1	B	540	ALA	2.3
1	A	613	SER	2.3
1	B	592	SER	2.3
1	B	345	TYR	2.3
1	A	611	GLU	2.2
1	B	440	VAL	2.2
1	B	354	ARG	2.2
1	B	407	ALA	2.2
1	B	422	ASP	2.2
1	B	561	VAL	2.2
1	B	398	PRO	2.1
1	B	527	GLY	2.1
1	B	492	PRO	2.1
1	B	569	LEU	2.1
1	B	352	TRP	2.1
1	B	452	LEU	2.1
1	B	494	ARG	2.1
1	B	328	ILE	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.