



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2021 – 12:01 PM EDT

PDB ID : 7K2J
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 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

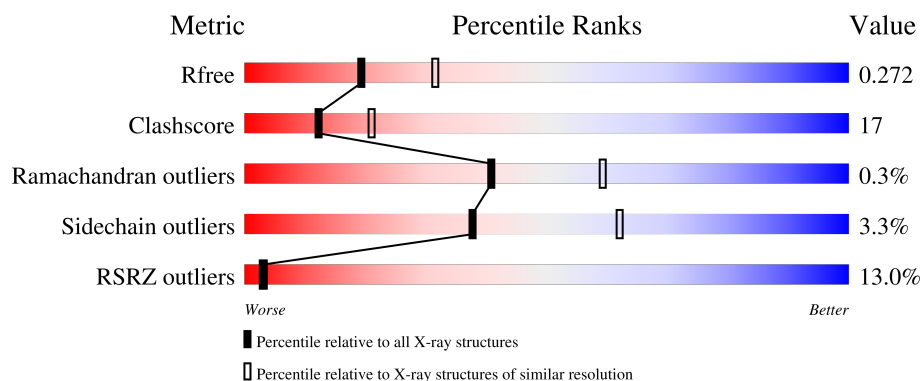
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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}	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (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	<div> <div>3%</div> <div>78%</div> <div>20%</div> <div>..</div> </div>
1	B	290	<div> <div>22%</div> <div>61%</div> <div>32%</div> <div>..</div> </div>
2	P	7	<div> <div>86%</div> <div>14%</div> </div>

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			

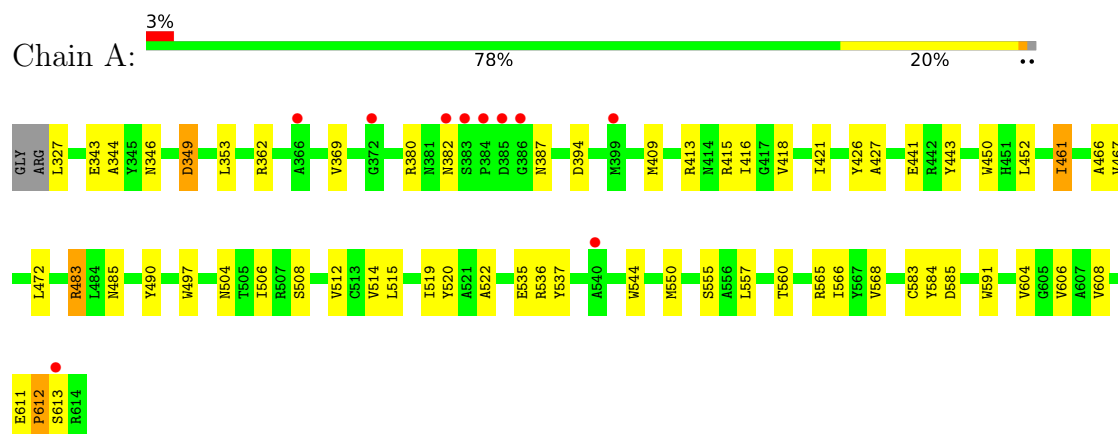
- Molecule 3 is water.

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

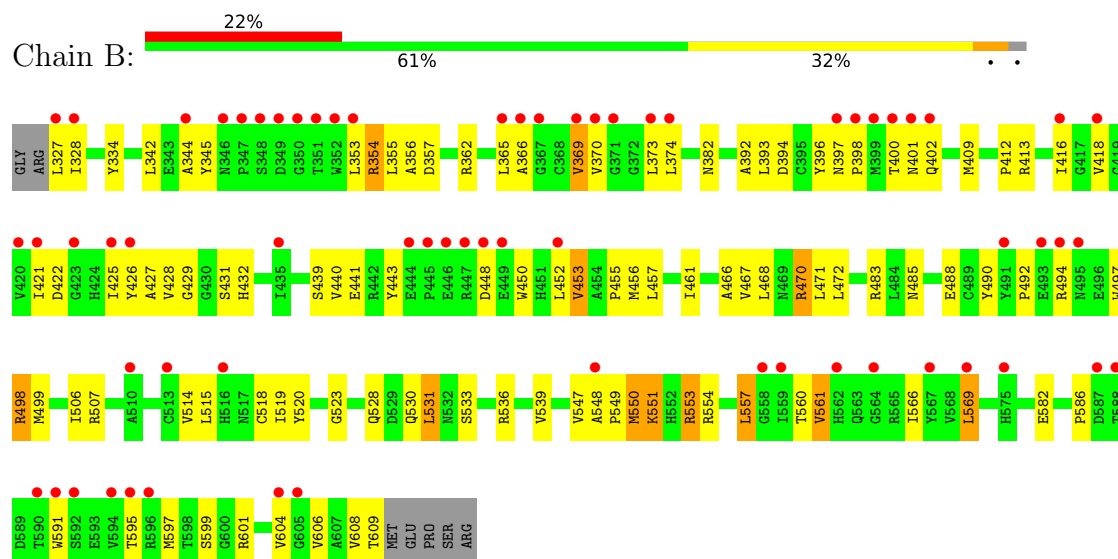
3 Residue-property plots

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.

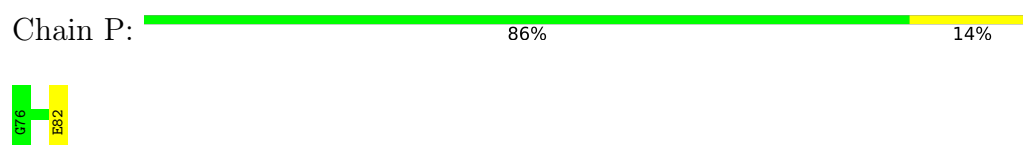
- Molecule 1: Kelch-like ECH-associated protein 1



- 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) 97.9 (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 0.225 , 0.272	Depositor DCC
R_{free} test set	1999 reflections (7.93%)	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)	0.37 , 51.5	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

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	0.69	0/2259	0.71	0/3078
1	B	0.60	2/2173 (0.1%)	0.94	13/2961 (0.4%)
2	P	0.44	0/46	0.56	0/61
All	All	0.64	2/4478 (0.0%)	0.83	13/6100 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	453	VAL	CB-CG2	-9.04	1.33	1.52
1	B	498	ARG	CG-CD	-5.45	1.38	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	354	ARG	NE-CZ-NH2	-17.29	111.66	120.30
1	B	354	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	B	498	ARG	CB-CG-CD	-8.52	89.45	111.60
1	B	354	ARG	CD-NE-CZ	8.05	134.87	123.60
1	B	354	ARG	CG-CD-NE	6.80	126.08	111.80
1	B	369	VAL	CG1-CB-CG2	-6.72	100.15	110.90
1	B	382	ASN	C-N-CA	5.86	136.34	121.70
1	B	498	ARG	CD-NE-CZ	-5.71	115.60	123.60
1	B	561	VAL	CG1-CB-CG2	5.58	119.83	110.90
1	B	453	VAL	CA-CB-CG2	-5.42	102.76	110.90
1	B	498	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	B	327	LEU	CA-CB-CG	5.04	126.89	115.30
1	B	551	LYS	CD-CE-NZ	5.02	123.24	111.70

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	41	0
1	B	2124	0	2007	104	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	145	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 17.

All (145) 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:B:569:LEU:HD12	1:B:597:MET:HE1	1.62	0.82
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:409:MET:HB3	1:B:441:GLU:CD	2.21	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: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:362:ARG:HH21	1:B:392:ALA:CB	2.07	0.56
1:A:550:MET:HE1	1:A:568:VAL:HG21	1.88	0.55
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
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:515:LEU:HD22	1:B:566:ILE:CD1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:370:VAL:HG21	1:B:425:ILE:CD1	2.42	0.50
1:A:522:ALA:HB1	1:A:550:MET:HE3	1.92	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:HD13	1:B:499:MET:HE2	1.93	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:461:ILE:O	1:A:461:ILE:HG13	2.14	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:MET:HG2	1:B:450:TRP:CE2	2.52	0.45
1:B:550:MET:HE2	1:B:554:ARG:HD2	1.99	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: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:A:550:MET:HE1	1:A:568:VAL:HG11	2.00	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:346:ASN:CG	1:A:349:ASP:HB2	2.38	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: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: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
1:A:565:ARG:HG2	1:A:585:ASP:HA	2.02	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: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 [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%)	274 (96%)	11 (4%)	1 (0%)	41	59
1	B	281/290 (97%)	265 (94%)	15 (5%)	1 (0%)	34	53
2	P	5/7 (71%)	4 (80%)	1 (20%)	0	100	100
All	All	572/587 (97%)	543 (95%)	27 (5%)	2 (0%)	41	59

All (2) Ramachandran outliers are listed below:

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

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	232/234 (99%)	225 (97%)	7 (3%)	41	66
1	B	218/234 (93%)	210 (96%)	8 (4%)	34	57
2	P	4/4 (100%)	4 (100%)	0	100	100
All	All	454/472 (96%)	439 (97%)	15 (3%)	38	62

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	349	ASP
1	A	415	ARG
1	A	461	ILE
1	A	483	ARG
1	A	555	SER
1	A	557	LEU
1	A	613	SER
1	B	448	ASP
1	B	470	ARG
1	B	528	GLN
1	B	531	LEU
1	B	550	MET
1	B	553	ARG
1	B	557	LEU
1	B	569	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

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%)	0.13	10 (3%)	44 48	25, 41, 66, 140	0
1	B	283/290 (97%)	1.16	65 (22%)	0 0	36, 73, 123, 154	0
2	P	7/7 (100%)	0.39	0	100 100	59, 60, 73, 80	0
All	All	578/587 (98%)	0.64	75 (12%)	3 3	25, 53, 112, 154	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	351	THR	9.9
1	B	347	PRO	6.0
1	B	588	THR	5.1
1	B	421	ILE	4.8
1	B	494	ARG	4.7
1	B	348	SER	4.4
1	A	386	GLY	4.2
1	B	416	ILE	4.1
1	B	591	TRP	4.1
1	B	399	MET	4.0
1	A	385	ASP	4.0
1	B	371	GLY	4.0
1	B	353	LEU	4.0
1	B	366	ALA	3.9
1	B	491	TYR	3.9
1	B	402	GLN	3.9
1	B	590	THR	3.8
1	B	373	LEU	3.7
1	B	575	HIS	3.7
1	B	587	ASP	3.7
1	B	444	GLU	3.6
1	B	397	ASN	3.6
1	B	495	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	604	VAL	3.4
1	B	446	GLU	3.4
1	B	493	GLU	3.3
1	B	452	LEU	3.3
1	B	558	GLY	3.2
1	B	423	GLY	3.2
1	B	449	GLU	3.2
1	B	400	THR	3.1
1	A	383	SER	3.1
1	B	559	ILE	3.1
1	A	384	PRO	3.0
1	B	516	HIS	3.0
1	B	447	ARG	3.0
1	B	569	LEU	2.9
1	B	352	TRP	2.9
1	B	567	TYR	2.9
1	B	435	ILE	2.8
1	B	365	LEU	2.8
1	B	328	ILE	2.8
1	B	605	GLY	2.8
1	A	613	SER	2.7
1	B	592	SER	2.7
1	B	426	TYR	2.7
1	B	344	ALA	2.6
1	B	398	PRO	2.6
1	B	595	THR	2.6
1	B	350	GLY	2.6
1	B	596	ARG	2.5
1	B	349	ASP	2.5
1	B	418	VAL	2.5
1	A	366	ALA	2.5
1	A	382	ASN	2.4
1	B	374	LEU	2.4
1	B	369	VAL	2.4
1	B	562	HIS	2.3
1	A	399	MET	2.3
1	B	548	ALA	2.3
1	A	372	GLY	2.3
1	B	327	LEU	2.3
1	B	510	ALA	2.3
1	A	540	ALA	2.2
1	B	445	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	448	ASP	2.2
1	B	594	VAL	2.2
1	B	346	ASN	2.1
1	B	367	GLY	2.1
1	B	420	VAL	2.1
1	B	370	VAL	2.1
1	B	513	CYS	2.1
1	B	401	ASN	2.1
1	B	425	ILE	2.0
1	B	564	GLY	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 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.