



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:10 PM UTC

PDB ID : 7K2R / pdb_00007k2r
Title : Kelch domain of human KEAP1 bound to Nrf2-based cyclic peptide, c[LhA-DEETGE]
Authors : Muellers, S.N.; Allen, K.N.
Deposited on : 2020-09-08
Resolution : 2.10 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

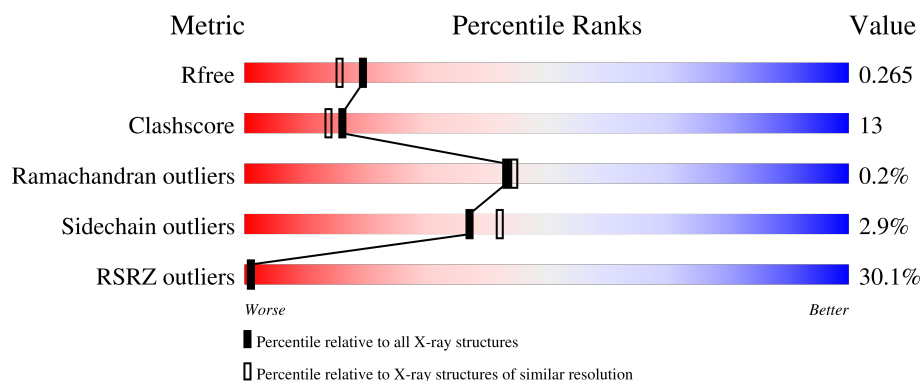
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	55% 73% 22% ..
1	B	290	5% 85% 14% .
2	P	7	71% 29%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4496 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	B	289	Total	C	N	O	S	0	1	0
			2225	1383	404	421	17			
1	A	284	Total	C	N	O	S	0	1	0
			2101	1306	378	402	15			

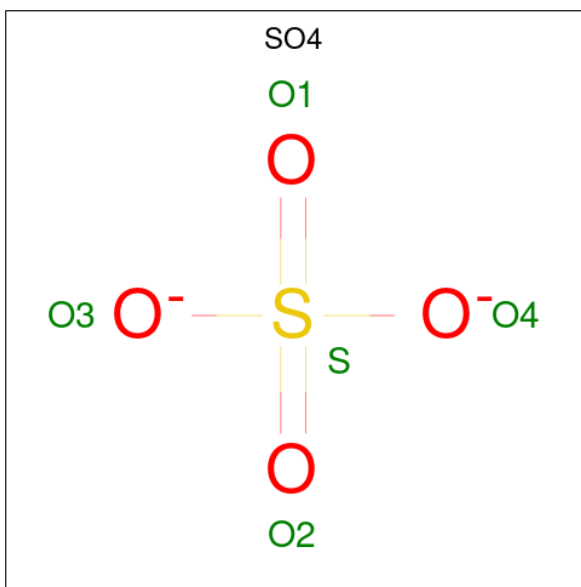
There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called B3A-ASP-PRO-GLU-THR-GLY-GLU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	7	Total	C	N	O	0	0	0
			50	29	7	14			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

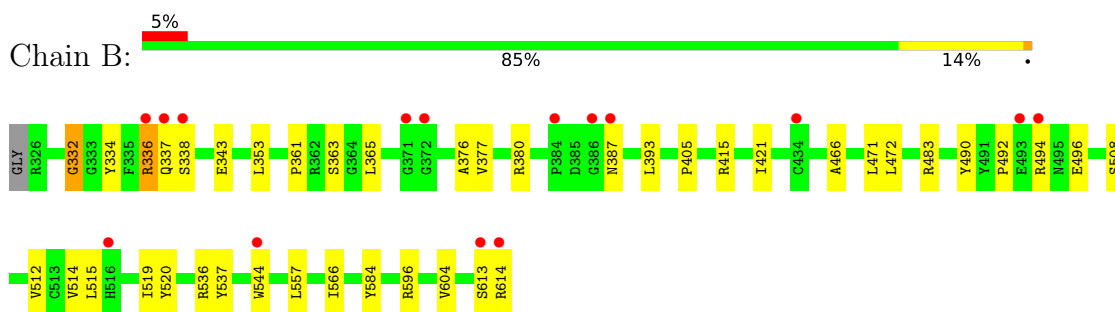
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	91	Total	O	0	0
			91	91		
4	A	18	Total	O	0	0
			18	18		
4	P	6	Total	O	0	0
			6	6		

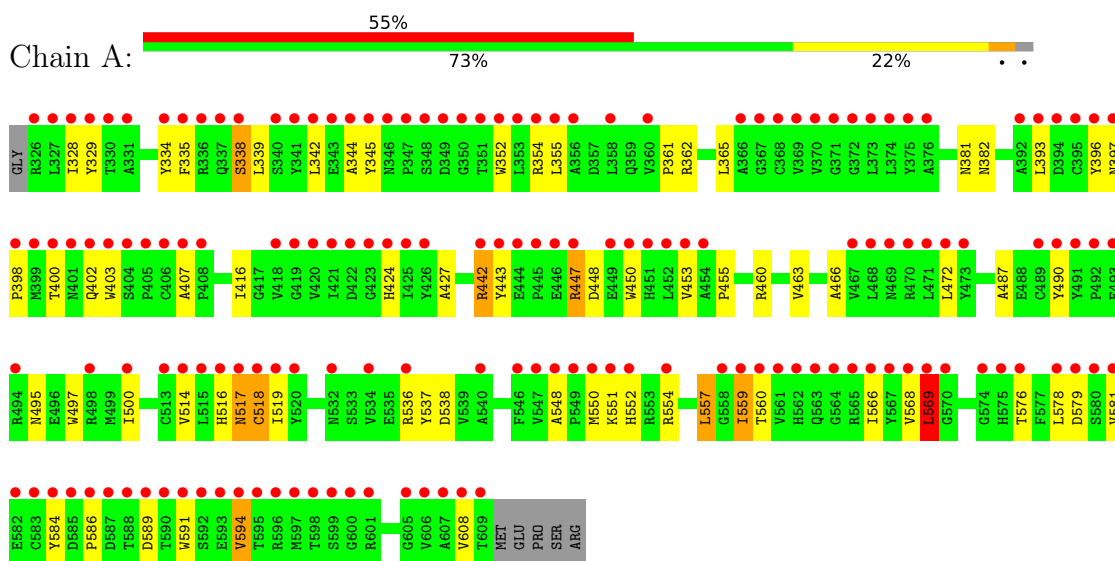
3 Residue-property plots [i](#)

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.

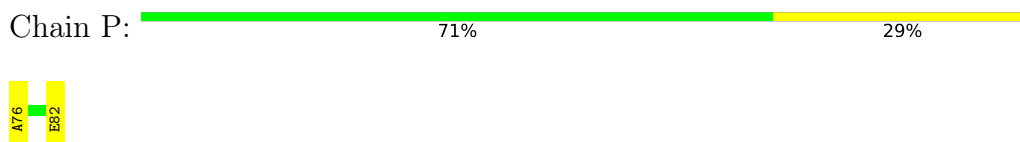
- Molecule 1: Kelch-like ECH-associated protein 1



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



- Molecule 2: B3A-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	162.75Å 68.76Å 77.13Å 90.00° 117.89° 90.00°	Depositor
Resolution (Å)	29.52 – 2.10 29.52 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.52-2.10) 99.5 (29.52-2.10)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.240 , 0.262 0.241 , 0.265	Depositor DCC
R_{free} test set	2001 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.010 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4496	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% 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

Bond lengths and bond angles in the following residue types are not validated in this section: B3A, SO4

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	0.52	0/2152	0.75	4/2938 (0.1%)
1	B	0.49	0/2282	0.63	1/3107 (0.0%)
2	P	0.31	0/44	0.40	0/59
All	All	0.50	0/4478	0.69	5/6104 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	332	GLY	O-C-N	6.67	130.01	122.67
1	A	579	ASP	N-CA-C	-5.99	106.10	113.41
1	A	578	LEU	N-CA-C	5.62	119.07	110.20
1	A	569	LEU	N-CA-C	5.18	116.97	108.52
1	A	560	THR	N-CA-C	5.11	116.07	108.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	P	76	B3A	Peptide

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	2101	0	1943	79	0
1	B	2225	0	2124	41	1
2	P	50	0	35	1	0
3	A	5	0	0	0	0
4	A	18	0	0	0	0
4	B	91	0	0	1	0
4	P	6	0	0	0	0
All	All	4496	0	4102	111	1

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 13.

All (111) 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:338:SER:O	1:B:361:PRO:HB3	1.53	1.07
1:B:471:LEU:CD2	1:A:517:ASN:ND2	2.21	1.03
1:B:471:LEU:HD21	1:A:517:ASN:ND2	1.76	0.99
1:B:471:LEU:HG	1:A:517:ASN:HD21	1.27	0.97
1:A:550:MET:HG2	1:A:591:TRP:CZ3	1.99	0.97
1:A:584:TYR:HB2	1:A:591:TRP:CE2	2.00	0.96
1:A:584:TYR:CD1	1:A:591:TRP:NE1	2.38	0.90
1:B:471:LEU:HG	1:A:517:ASN:ND2	1.86	0.90
1:A:554:ARG:HG3	1:A:557:LEU:HD22	1.52	0.89
1:B:471:LEU:CG	1:A:517:ASN:ND2	2.36	0.88
1:A:584:TYR:HD1	1:A:591:TRP:CD1	1.92	0.86
1:A:550:MET:HG2	1:A:591:TRP:CE3	2.11	0.86
1:A:548:ALA:HB2	1:A:589:ASP:OD1	1.74	0.86
1:B:338:SER:O	1:B:361:PRO:CB	2.24	0.85
1:A:559:ILE:HG13	1:A:568:VAL:HG12	1.64	0.80
1:B:613:SER:HB3	1:B:614:ARG:HH11	1.45	0.79
1:A:518:CYS:HG	1:A:538:ASP:HA	1.49	0.77
1:B:471:LEU:CD2	1:A:517:ASN:HD22	1.98	0.75
1:B:471:LEU:HD21	1:A:517:ASN:HD22	1.49	0.75
1:A:548:ALA:CB	1:A:589:ASP:OD1	2.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:ALA:HB3	1:A:584:TYR:HE1	1.52	0.74
1:A:584:TYR:HD1	1:A:591:TRP:NE1	1.82	0.74
1:A:518:CYS:SG	1:A:538:ASP:HA	2.28	0.74
1:A:548:ALA:HB2	1:A:589:ASP:CG	2.12	0.72
1:A:569:LEU:HD12	1:A:569:LEU:N	2.05	0.71
1:B:494:ARG:HG2	1:B:496:GLU:OE2	1.91	0.71
1:A:566:ILE:HD12	1:A:566:ILE:O	1.91	0.71
1:A:490:TYR:OH	1:A:495:ASN:ND2	2.23	0.70
1:B:466:ALA:HB1	1:B:514:VAL:HG23	1.74	0.70
1:A:393:LEU:HD22	1:A:450:TRP:HZ2	1.57	0.69
1:A:442:ARG:HB3	1:A:442:ARG:NH1	2.08	0.69
1:A:472:LEU:HB3	1:A:490:TYR:HB3	1.75	0.68
1:A:548:ALA:HB3	1:A:584:TYR:CE1	2.29	0.68
1:A:551:LYS:HE3	1:A:591:TRP:O	1.94	0.66
1:A:442:ARG:HB3	1:A:442:ARG:CZ	2.26	0.65
1:B:515:LEU:HD22	1:B:566:ILE:HG13	1.79	0.64
1:A:548:ALA:N	1:A:589:ASP:OD1	2.30	0.64
1:A:329:TYR:HA	1:A:344:ALA:HA	1.80	0.62
1:A:568:VAL:O	1:A:568:VAL:HG23	2.01	0.60
1:A:393:LEU:HD22	1:A:450:TRP:CZ2	2.35	0.60
1:A:338:SER:HB3	1:A:361:PRO:HB2	1.84	0.60
1:A:584:TYR:CD1	1:A:591:TRP:CD1	2.81	0.60
1:A:338:SER:OG	1:A:381:ASN:HA	2.00	0.60
1:A:365:LEU:HD23	1:A:365:LEU:H	1.68	0.58
1:A:355:LEU:HD23	1:A:396:TYR:OH	2.03	0.58
1:B:557:LEU:H	1:B:557:LEU:HD23	1.69	0.57
1:B:537:TYR:HD1	1:B:544:TRP:CD1	2.24	0.56
1:B:494:ARG:HG2	1:B:496:GLU:CD	2.31	0.56
1:A:584:TYR:HB2	1:A:591:TRP:NE1	2.21	0.56
1:A:487:ALA:HB3	1:A:500:ILE:HD11	1.87	0.55
1:A:342:LEU:HD22	1:A:403:TRP:CZ2	2.41	0.55
1:A:328:ILE:HG12	1:A:608:VAL:HG22	1.89	0.55
1:A:566:ILE:HD11	1:A:584:TYR:HB3	1.88	0.54
1:B:537:TYR:CD1	1:B:544:TRP:NE1	2.77	0.53
1:A:342:LEU:HD22	1:A:403:TRP:HZ2	1.74	0.53
1:A:569:LEU:N	1:A:569:LEU:CD1	2.72	0.52
1:B:365:LEU:HD12	1:B:376:ALA:HB1	1.92	0.52
1:B:421:ILE:HD11	1:B:472:LEU:HB2	1.90	0.52
1:A:361:PRO:O	1:A:362:ARG:HG3	2.10	0.52
1:B:537:TYR:CD1	1:B:544:TRP:CD1	2.98	0.51
1:A:345:TYR:HB2	1:A:352:TRP:CZ3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:VAL:HB	1:A:495:ASN:HD21	1.76	0.50
1:A:518:CYS:SG	1:A:537:TYR:O	2.70	0.50
1:B:471:LEU:CG	1:A:517:ASN:HD21	2.03	0.50
1:A:447:ARG:CG	1:A:447:ARG:HH11	2.24	0.50
1:A:338:SER:HB2	1:A:381:ASN:OD1	2.12	0.50
1:A:424:HIS:ND1	1:A:442:ARG:HD2	2.26	0.50
1:A:519:ILE:O	1:A:536:ARG:HA	2.12	0.49
1:B:415:ARG:NE	4:B:701:HOH:O	2.39	0.48
1:B:471:LEU:HD21	1:A:517:ASN:CG	2.37	0.48
1:B:566:ILE:HB	1:B:584:TYR:HB3	1.95	0.48
1:B:472:LEU:HB3	1:B:490:TYR:HB3	1.94	0.48
1:A:407:ALA:HB2	1:A:448:ASP:OD2	2.14	0.48
1:B:380:ARG:NH2	1:B:387:ASN:HB3	2.29	0.47
1:A:354:ARG:HE	1:A:354:ARG:HB3	1.58	0.47
1:B:519:ILE:O	1:B:536:ARG:HA	2.15	0.47
1:A:443:TYR:CE1	1:A:448:ASP:HA	2.49	0.46
1:A:466:ALA:HB1	1:A:514:VAL:HG23	1.96	0.46
1:A:334:TYR:HE2	1:A:382:ASN:HB3	1.81	0.46
1:A:460:ARG:HB3	1:A:463:VAL:HB	1.98	0.46
1:A:490:TYR:HB2	1:A:497:TRP:CH2	2.51	0.45
1:B:338:SER:HB3	1:B:361:PRO:C	2.42	0.44
1:A:455:PRO:O	1:A:497:TRP:CD1	2.71	0.44
1:A:335:PHE:CB	1:A:339:LEU:HD11	2.48	0.44
1:B:613:SER:HB3	1:B:614:ARG:NH1	2.23	0.43
1:A:550:MET:CG	1:A:591:TRP:CZ3	2.87	0.43
1:A:581:VAL:HG12	1:A:594:VAL:CG1	2.48	0.43
1:B:332:GLY:O	1:B:604:VAL:HG12	2.19	0.43
1:B:537:TYR:HB2	1:B:544:TRP:CE2	2.54	0.42
1:A:416:ILE:HD11	1:A:427:ALA:HB1	2.01	0.42
1:A:443:TYR:HB2	1:A:450:TRP:CE2	2.54	0.42
1:A:400:THR:HG22	1:A:402:GLN:HB2	2.01	0.42
1:A:442:ARG:CZ	1:A:442:ARG:CB	2.94	0.42
1:B:353:LEU:HD12	1:B:353:LEU:HA	1.91	0.42
1:B:512:VAL:HA	1:B:520:TYR:O	2.20	0.42
1:A:584:TYR:HB2	1:A:591:TRP:CZ2	2.51	0.42
1:B:515:LEU:HB3	1:B:520:TYR:CE1	2.54	0.42
1:B:343:GLU:HA	1:B:353:LEU:O	2.20	0.41
1:A:396:TYR:HB2	1:A:403:TRP:CE3	2.55	0.41
1:B:483:ARG:HG2	1:B:508:SER:HB3	2.01	0.41
1:B:494:ARG:O	1:B:494:ARG:HG3	2.20	0.41
1:A:397:ASN:HA	1:A:398:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:TYR:CZ	1:B:336:ARG:HA	2.56	0.41
1:B:377:VAL:HG22	1:B:393:LEU:CD1	2.51	0.41
1:A:581:VAL:HG12	1:A:594:VAL:HG13	2.03	0.41
1:B:490:TYR:CE2	1:B:492:PRO:HA	2.56	0.41
1:A:550:MET:HE3	1:A:550:MET:HB2	1.88	0.41
1:A:584:TYR:CE2	1:A:586:PRO:HA	2.56	0.41
1:A:334:TYR:CD1	2:P:82:GLU:HG2	2.56	0.40
1:B:334:TYR:HB2	1:B:363:SER:CB	2.52	0.40
1:A:447:ARG:CG	1:A:447:ARG:NH1	2.80	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:PRO:O	1:B:596:ARG:NH1[4_556]	2.08	0.12

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	283/290 (98%)	266 (94%)	16 (6%)	1 (0%)	30	28
1	B	288/290 (99%)	276 (96%)	12 (4%)	0	100	100
2	P	5/7 (71%)	4 (80%)	1 (20%)	0	100	100
All	All	576/587 (98%)	546 (95%)	29 (5%)	1 (0%)	43	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	516	HIS

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	209/234 (89%)	198 (95%)	11 (5%)	20	19
1	B	235/234 (100%)	233 (99%)	2 (1%)	70	78
2	P	5/5 (100%)	5 (100%)	0	100	100
All	All	449/473 (95%)	436 (97%)	13 (3%)	37	42

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	336	ARG
1	B	337	GLN
1	A	338	SER
1	A	442	ARG
1	A	447	ARG
1	A	517	ASN
1	A	518	CYS
1	A	552	HIS
1	A	557	LEU
1	A	559	ILE
1	A	569	LEU
1	A	576	THR
1	A	594	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	469	ASN
1	A	432	HIS
1	A	469	ASN
1	A	482	ASN
1	A	495	ASN
1	A	517	ASN

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	B3A	P	76	2	5,5,6	1.08	0	5,5,7	1.20	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	B3A	P	76	2	-	1/3/3/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	76	B3A	O-C-CB-CA

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand 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	$\# Z > 2$
3	SO4	A	701	-	4,4,4	0.22	0	6,6,6	0.20	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	284/290 (97%)	2.68	159 (55%) 0 0	28, 60, 106, 128	1 (0%)
1	B	289/290 (99%)	0.25	15 (5%) 33 35	25, 33, 54, 83	1 (0%)
2	P	6/7 (85%)	0.25	0 100 100	37, 38, 39, 41	0
All	All	579/587 (98%)	1.44	174 (30%) 1 1	25, 41, 101, 128	2 (0%)

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	445	PRO	8.3
1	A	518	CYS	8.1
1	A	328	ILE	7.8
1	A	517	ASN	7.6
1	A	591	TRP	7.6
1	A	335	PHE	7.6
1	A	353	LEU	7.2
1	A	590	THR	7.2
1	A	423	GLY	7.2
1	A	584	TYR	7.1
1	B	338	SER	7.0
1	A	371	GLY	7.0
1	A	370	VAL	7.0
1	B	337	GLN	6.9
1	A	566	ILE	6.8
1	A	514	VAL	6.8
1	A	344	ALA	6.6
1	A	421	ILE	6.6
1	A	420	VAL	6.6
1	A	609	THR	6.5
1	A	345	TYR	6.4
1	A	327	LEU	6.4
1	A	348	SER	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	373	LEU	6.4
1	A	374	LEU	6.3
1	A	586	PRO	6.2
1	B	336	ARG	6.2
1	A	342	LEU	6.1
1	A	515	LEU	6.1
1	A	355	LEU	6.0
1	A	369	VAL	6.0
1	A	338	SER	5.9
1	A	565	ARG	5.8
1	A	352	TRP	5.8
1	A	567	TYR	5.7
1	A	595	THR	5.6
1	A	516	HIS	5.6
1	A	347	PRO	5.6
1	A	356	ALA	5.6
1	A	399	MET	5.5
1	A	564	GLY	5.5
1	A	608	VAL	5.5
1	A	329	TYR	5.4
1	A	596	ARG	5.4
1	A	346	ASN	5.3
1	A	419	GLY	5.3
1	A	594	VAL	5.3
1	A	581	VAL	5.3
1	A	592	SER	5.2
1	A	585	ASP	5.2
1	A	425	ILE	5.0
1	A	444	GLU	5.0
1	A	607	ALA	4.8
1	A	396	TYR	4.8
1	A	398	PRO	4.8
1	A	349	ASP	4.7
1	A	442	ARG	4.7
1	A	549	PRO	4.7
1	A	443	TYR	4.6
1	A	368	CYS	4.5
1	A	407	ALA	4.5
1	A	403	TRP	4.5
1	A	326	ARG	4.5
1	A	351	THR	4.4
1	A	400	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	548	ALA	4.3
1	A	568	VAL	4.3
1	A	606	VAL	4.3
1	A	547	VAL	4.3
1	A	587	ASP	4.3
1	A	334	TYR	4.3
1	A	562	HIS	4.2
1	A	367	GLY	4.2
1	A	583	CYS	4.2
1	A	451	HIS	4.1
1	A	397	ASN	4.1
1	A	401	ASN	4.1
1	A	491	TYR	4.1
1	A	337	GLN	4.1
1	A	563	GLN	4.1
1	A	375	TYR	4.1
1	A	598	THR	4.1
1	A	372	GLY	4.0
1	A	424	HIS	4.0
1	A	330	THR	4.0
1	A	453	VAL	3.9
1	A	350	GLY	3.9
1	A	404	SER	3.8
1	A	599	SER	3.7
1	A	468	LEU	3.7
1	A	597	MET	3.7
1	A	519	ILE	3.7
1	A	589	ASP	3.7
1	A	601	ARG	3.6
1	A	450	TRP	3.6
1	A	470	ARG	3.6
1	A	605	GLY	3.5
1	A	395	CYS	3.5
1	A	446	GLU	3.5
1	A	561	VAL	3.5
1	A	343	GLU	3.4
1	A	449	GLU	3.4
1	A	552	HIS	3.4
1	A	588	THR	3.4
1	A	394	ASP	3.4
1	A	600	GLY	3.4
1	A	454	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	452	LEU	3.3
1	A	546	PHE	3.3
1	A	406	CYS	3.2
1	A	492	PRO	3.2
1	A	540	ALA	3.2
1	B	494	ARG	3.2
1	A	422	ASP	3.1
1	A	471	LEU	3.1
1	A	513	CYS	3.1
1	A	575	HIS	3.1
1	A	405	PRO	3.1
1	A	500	ILE	3.1
1	A	576	THR	3.0
1	A	360	VAL	3.0
1	A	467	VAL	3.0
1	A	336	ARG	3.0
1	A	426	TYR	3.0
1	A	580	SER	3.0
1	A	376	ALA	2.9
1	A	490	TYR	2.9
1	A	570	GLY	2.9
1	A	354	ARG	2.8
1	A	331	ALA	2.8
1	A	582	GLU	2.8
1	A	393	LEU	2.8
1	A	560	THR	2.7
1	A	341	TYR	2.7
1	B	516	HIS	2.7
1	A	551	LYS	2.6
1	B	544	TRP	2.6
1	A	472	LEU	2.6
1	A	569	LEU	2.6
1	B	371	GLY	2.5
1	A	469	ASN	2.5
1	A	578	LEU	2.5
1	A	520	TYR	2.5
1	A	447	ARG	2.5
1	B	493	GLU	2.4
1	B	384	PRO	2.4
1	B	387	ASN	2.4
1	A	534	VAL	2.4
1	B	614	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	408	PRO	2.4
1	A	358	LEU	2.4
1	A	579	ASP	2.4
1	A	498	ARG	2.4
1	A	473	TYR	2.3
1	A	532	ASN	2.3
1	B	372	GLY	2.3
1	A	536	ARG	2.3
1	B	613	SER	2.3
1	A	493	GLU	2.3
1	A	489	CYS	2.3
1	A	494	ARG	2.2
1	B	386	GLY	2.2
1	A	392	ALA	2.2
1	A	340	SER	2.2
1	A	554	ARG	2.2
1	A	559	ILE	2.2
1	A	366	ALA	2.2
1	A	402	GLN	2.1
1	A	418	VAL	2.1
1	B	434[A]	CYS	2.1
1	A	574	GLY	2.1
1	A	550	MET	2.0
1	A	593	GLU	2.0
1	A	558	GLY	2.0

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

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($\text{\AA}^2$)	Q<0.9
2	B3A	P	76	6/7	0.93	0.10	36,39,42,44	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

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
3	SO4	A	701	5/5	0.93	0.14	60,61,64,64	0

6.5 Other polymers

There are no such residues in this entry.