



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 03:54 AM EST

PDB ID : 7K2R
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

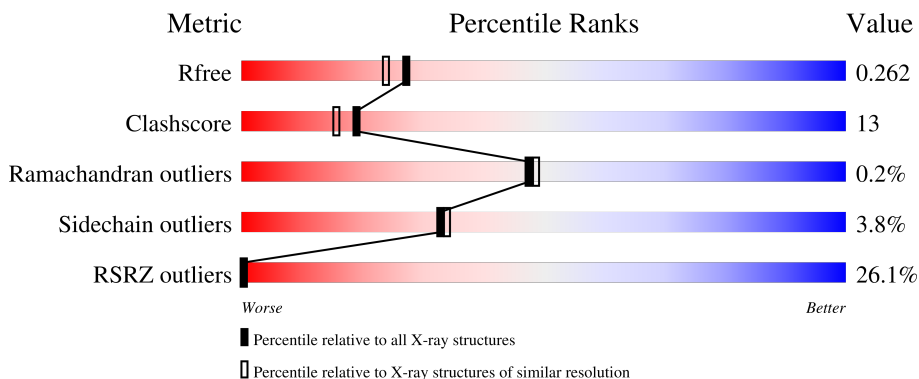
1 Overall quality at a glance

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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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	
1	B	290	
2	P	7	

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
			Total	C	N	O	S			
1	B	289	2225	1383	404	421	17	0	1	0
1	A	284	2101	1306	378	402	15	0	1	0

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
			Total	C	N	O			
2	P	7	50	29	7	14	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

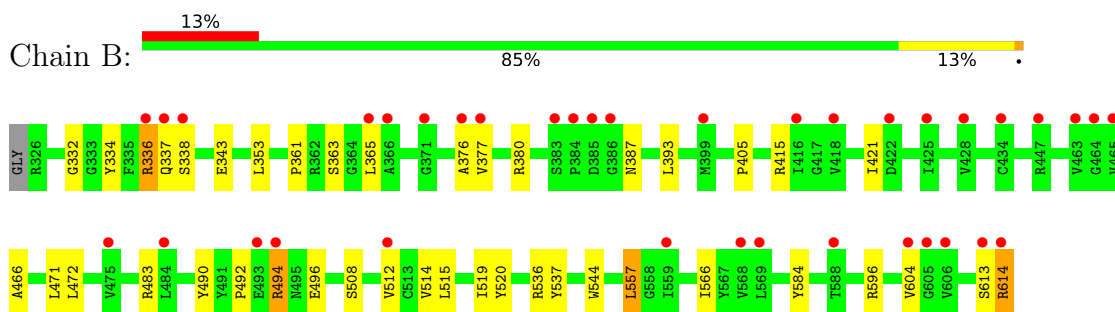
- Molecule 4 is water.

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		

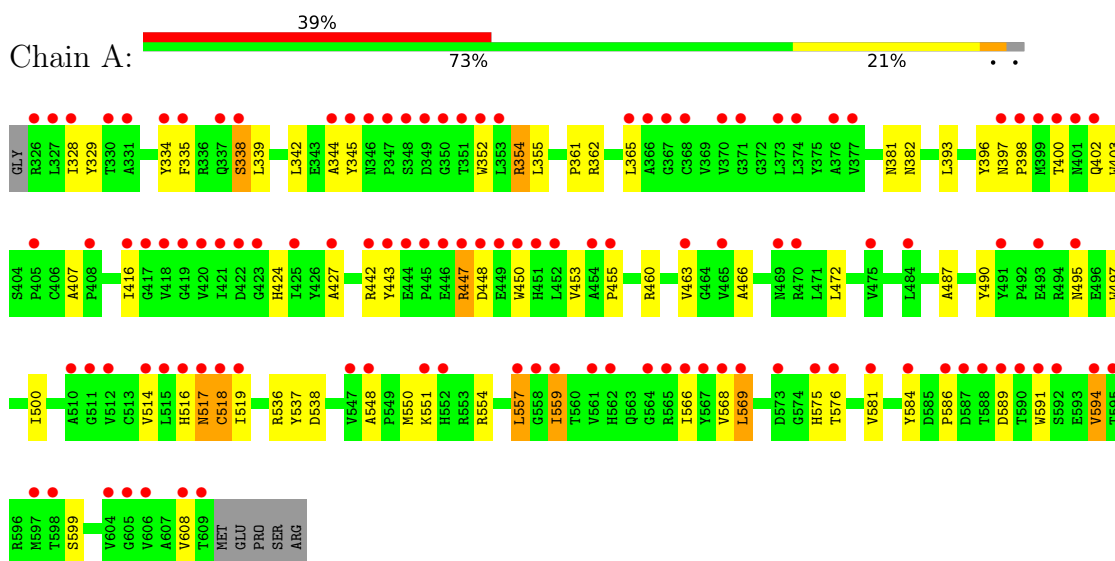
3 Residue-property plots [i](#)

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.

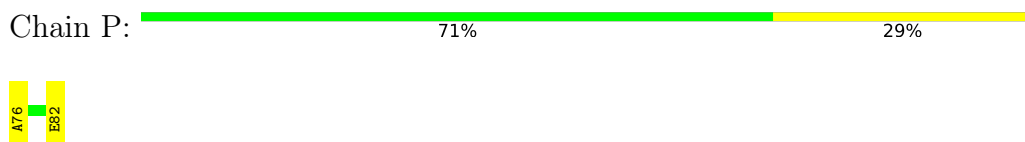
- Molecule 1: Kelch-like ECH-associated protein 1



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



- Molecule 2: B3A-ASP-PRO-GLU-THR-GLY-GLU



4 Data and refinement statistics i

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) 99.6 (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)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.240 , 0.262 0.240 , 0.262	Depositor DCC
R_{free} test set	2001 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtrriage
Anisotropy	0.479	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.010 for -h-2*1,-k,l	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.45	0/2152	0.62	0/2938
1	B	0.49	0/2282	0.63	0/3107
2	P	0.40	0/44	0.55	0/59
All	All	0.47	0/4478	0.62	0/6104

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.

There are no bond angle outliers.

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 [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	2101	0	1943	79	0
1	B	2225	0	2124	40	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	110	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 (110) 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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HB2	1:A:589:ASP:CG	2.12	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: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:494:ARG:HG2	1:B:496:GLU:CD	2.31	0.51
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:ARG:NE	4:B:701:HOH:O	2.39	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:A:455:PRO:O	1:A:497:TRP:CD1	2.71	0.44
1:B:471:LEU:HD21	1:A:517:ASN:CG	2.37	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:338:SER:HG	1:A:381:ASN:HA	1.82	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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	283/290 (98%)	266 (94%)	16 (6%)	1 (0%)	34	32
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%)	47	49

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%)	197 (94%)	12 (6%)	20	18
1	B	235/234 (100%)	230 (98%)	5 (2%)	53	59
2	P	5/5 (100%)	5 (100%)	0	100	100
All	All	449/473 (95%)	432 (96%)	17 (4%)	33	34

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	336	ARG
1	B	337	GLN
1	B	494	ARG
1	B	557	LEU
1	B	614	ARG
1	A	338	SER
1	A	354	ARG
1	A	447	ARG
1	A	517	ASN
1	A	518	CYS
1	A	557	LEU
1	A	559	ILE
1	A	569	LEU
1	A	575	HIS
1	A	576	THR
1	A	594	VAL
1	A	599	SER

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	495	ASN
1	A	517	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	1.12	0	5,5,7	1.27	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 [i](#)

There are no monosaccharides 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	0.14	0	6,6,6	0.22	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%)	1.96	114 (40%) 0 0	28, 60, 106, 128	0
1	B	289/290 (99%)	0.72	37 (12%) 3 4	25, 33, 54, 83	0
2	P	6/7 (85%)	0.07	0 100 100	37, 38, 39, 41	0
All	All	579/587 (98%)	1.32	151 (26%) 0 0	25, 41, 101, 128	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	349	ASP	9.1
1	A	518	CYS	8.2
1	A	399	MET	8.2
1	A	517	ASN	7.9
1	A	423	GLY	7.6
1	A	371	GLY	7.2
1	A	591	TRP	7.2
1	A	348	SER	7.2
1	A	370	VAL	6.4
1	A	516	HIS	6.2
1	A	588	THR	6.2
1	A	335	PHE	6.0
1	A	400	THR	6.0
1	B	385	ASP	5.9
1	A	351	THR	5.9
1	A	445	PRO	5.9
1	A	422	ASP	5.8
1	A	346	ASN	5.7
1	A	449	GLU	5.6
1	A	353	LEU	5.5
1	A	328	ILE	5.5
1	A	592	SER	5.2
1	A	402	GLN	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	608	VAL	5.1
1	B	337	GLN	4.9
1	A	575	HIS	4.9
1	A	421	ILE	4.9
1	B	336	ARG	4.8
1	A	347	PRO	4.6
1	A	447	ARG	4.6
1	B	384	PRO	4.6
1	A	446	GLU	4.6
1	B	614	ARG	4.6
1	B	365	LEU	4.5
1	A	374	LEU	4.5
1	A	425	ILE	4.5
1	A	448	ASP	4.5
1	A	367	GLY	4.5
1	A	352	TRP	4.5
1	A	595	THR	4.3
1	B	366	ALA	4.2
1	A	604	VAL	4.2
1	A	590	THR	4.1
1	A	416	ILE	4.1
1	A	598	THR	4.1
1	A	548	ALA	4.0
1	B	416	ILE	3.9
1	A	401	ASN	3.8
1	A	567	TYR	3.8
1	B	613	SER	3.8
1	A	559	ILE	3.8
1	A	470	ARG	3.8
1	A	365	LEU	3.8
1	A	594	VAL	3.8
1	A	366	ALA	3.8
1	A	373	LEU	3.7
1	B	465	VAL	3.6
1	A	606	VAL	3.6
1	A	442	ARG	3.6
1	A	584	TYR	3.5
1	B	512	VAL	3.5
1	A	576	THR	3.5
1	A	566	ILE	3.5
1	A	397	ASN	3.5
1	B	338	SER	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	350	GLY	3.4
1	B	606	VAL	3.4
1	A	491	TYR	3.4
1	B	399	MET	3.3
1	A	568	VAL	3.3
1	A	327	LEU	3.3
1	A	569	LEU	3.3
1	A	597	MET	3.3
1	A	609	THR	3.2
1	A	557	LEU	3.2
1	A	475	VAL	3.2
1	A	418	VAL	3.2
1	A	514	VAL	3.2
1	A	589	ASP	3.2
1	B	605	GLY	3.1
1	A	515	LEU	3.1
1	A	547	VAL	3.1
1	A	581	VAL	3.1
1	B	383	SER	3.1
1	A	465	VAL	3.1
1	A	377	VAL	3.1
1	A	605	GLY	3.0
1	A	587	ASP	3.0
1	A	452	LEU	3.0
1	A	463	VAL	3.0
1	A	326	ARG	3.0
1	A	398	PRO	3.0
1	A	443	TYR	2.9
1	B	493	GLU	2.8
1	A	552	HIS	2.8
1	A	455	PRO	2.8
1	A	561	VAL	2.8
1	A	408	PRO	2.7
1	A	420	VAL	2.7
1	B	376	ALA	2.7
1	A	338	SER	2.7
1	A	586	PRO	2.7
1	B	386	GLY	2.7
1	A	405	PRO	2.7
1	B	484	LEU	2.7
1	B	422	ASP	2.6
1	B	494	ARG	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	444	GLU	2.6
1	B	434[A]	CYS	2.6
1	A	376	ALA	2.6
1	B	588	THR	2.6
1	A	562	HIS	2.6
1	A	368	CYS	2.6
1	A	551	LYS	2.6
1	A	419	GLY	2.6
1	A	451	HIS	2.6
1	B	559	ILE	2.6
1	B	464	GLY	2.5
1	B	447	ARG	2.5
1	A	512	VAL	2.5
1	A	565	ARG	2.5
1	A	519	ILE	2.5
1	B	604	VAL	2.5
1	A	558	GLY	2.5
1	A	493	GLU	2.5
1	A	454	ALA	2.5
1	A	330	THR	2.5
1	A	469	ASN	2.5
1	B	569	LEU	2.4
1	A	450	TRP	2.4
1	B	377	VAL	2.4
1	B	371	GLY	2.4
1	A	337	GLN	2.4
1	A	334	TYR	2.3
1	B	568	VAL	2.3
1	A	510	ALA	2.3
1	A	484	LEU	2.2
1	B	425	ILE	2.2
1	A	345	TYR	2.2
1	B	418	VAL	2.2
1	A	427	ALA	2.2
1	A	573	ASP	2.2
1	A	564	GLY	2.2
1	B	463	VAL	2.2
1	A	495	ASN	2.2
1	A	331	ALA	2.1
1	B	428	VAL	2.1
1	B	475	VAL	2.1
1	A	344	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	511	GLY	2.1
1	A	417	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	B3A	P	76	6/7	0.90	0.16	36,39,42,44	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [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
3	SO4	A	701	5/5	0.96	0.14	60,61,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.