Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 01:16 PM EDT

PDB ID	:	7K2N
Title	:	Kelch domain of human KEAP1 bound to Nrf2-based cyclic peptide, c[BAL-DEETGE]
Authors	:	Muellers, S.N.; Allen, K.N.
Deposited on	:	2020-09-08
Resolution	:	2.22 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:

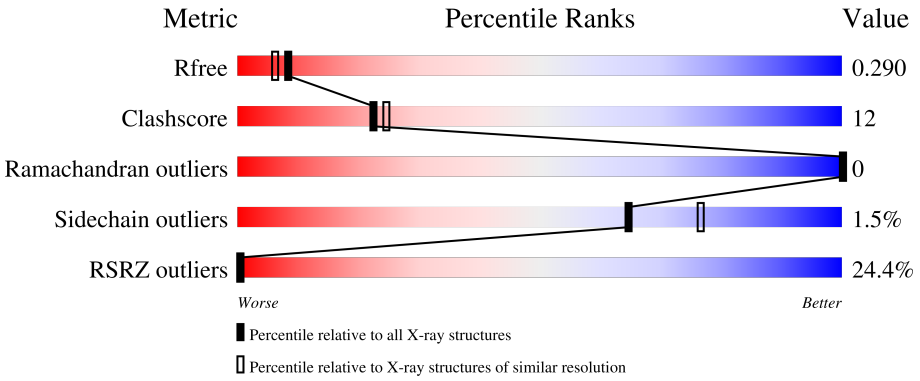
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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	39% 63% 30% · 6%
1	B	301	8% 84% 12% ·
2	P	7	57% 29% 14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4546 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	283	Total	C	N	O	S	0	0	0
			2170	1351	392	412	15			
1	B	290	Total	C	N	O	S	0	1	0
			2229	1385	405	423	16			

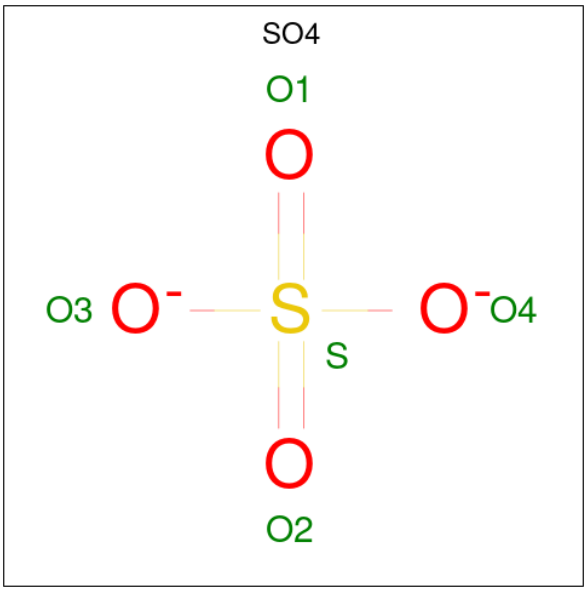
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	613	SER	CYS	conflict	UNP Q14145
B	613	SER	CYS	conflict	UNP Q14145

- Molecule 2 is a protein called (BAL)DPETGE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	7	Total	C	N	O	0	0	0
			49	28	7	14			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

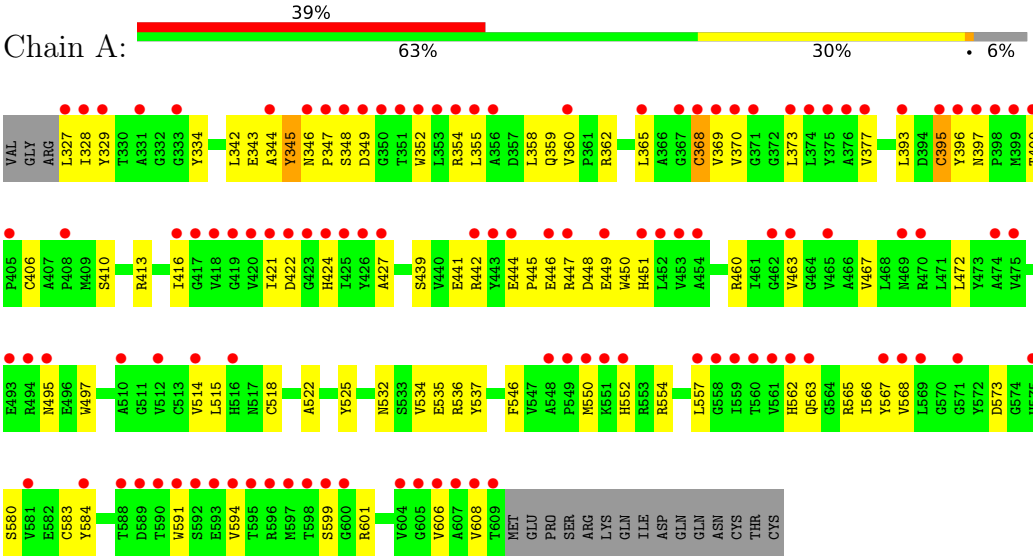
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	18	Total O 18 18	0	0
4	B	69	Total O 69 69	0	0
4	P	1	Total O 1 1	0	0

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.

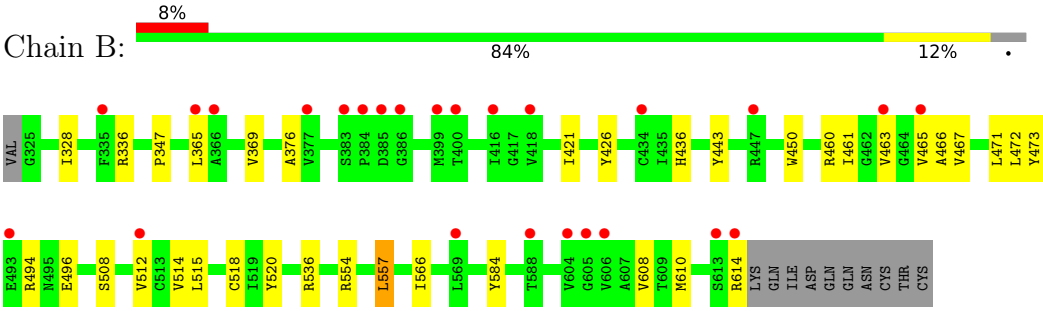
• Molecule 1: Kelch-like ECH-associated protein 1

Chain A:



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

Chain B:



• Molecule 2: (BAL)DPETGE

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	162.08Å 68.74Å 77.01Å 90.00° 117.66° 90.00°	Depositor
Resolution (Å)	29.52 – 2.22 29.52 – 2.22	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.52-2.22) 99.4 (29.52-2.22)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.247 , 0.290 0.247 , 0.290	Depositor DCC
R_{free} test set	2000 reflections (5.39%)	wwPDB-VP
Wilson B-factor (Å^2)	40.1	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 39.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.011 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4546	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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

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	0.42	1/2223 (0.0%)	0.62	1/3029 (0.0%)
1	B	0.49	0/2286	0.65	0/3112
2	P	0.57	0/44	0.83	0/59
All	All	0.46	1/4553 (0.0%)	0.64	1/6200 (0.0%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	368	CYS	CB-SG	-5.19	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	345	TYR	C-N-CA	-5.15	108.82	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	P	76	BAL	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	2170	0	2060	79	1
1	B	2229	0	2121	24	1
2	P	49	0	37	3	0
3	A	10	0	0	0	0
4	A	18	0	0	0	0
4	B	69	0	0	0	0
4	P	1	0	0	0	0
All	All	4546	0	4218	101	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 12.

All (101) 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:A:522:ALA:HB1	1:A:550:MET:HE3	1.56	0.87
1:A:397:ASN:HB3	1:A:400:THR:HB	1.58	0.83
1:A:370:VAL:HG11	1:A:445:PRO:HG2	1.61	0.81
1:A:490:TYR:OH	1:A:495:ASN:OD1	1.98	0.81
1:A:346:ASN:ND2	1:A:348:SER:OG	2.15	0.79
1:B:466:ALA:HB1	1:B:514:VAL:HG23	1.64	0.77
1:A:536:ARG:HH12	1:B:494:ARG:HH21	1.33	0.76
1:A:354:ARG:HG2	1:A:354:ARG:HH11	1.52	0.75
1:A:327:LEU:CD2	1:A:346:ASN:HB2	2.21	0.71
1:A:518:CYS:HB3	1:A:536:ARG:HB2	1.73	0.70
1:A:442:ARG:NH1	1:A:444:GLU:OE2	2.24	0.69
1:A:566:ILE:HB	1:A:584:TYR:HB3	1.74	0.68
1:A:422:ASP:HB3	1:A:424:HIS:CD2	2.30	0.66
1:A:342:LEU:O	1:A:354:ARG:HD2	1.94	0.66
1:A:557:LEU:HD23	1:A:557:LEU:H	1.60	0.66
1:A:329:TYR:CE2	1:A:344:ALA:HB2	2.31	0.65
1:A:354:ARG:HG2	1:A:354:ARG:NH1	2.10	0.65
1:A:342:LEU:O	1:A:354:ARG:CD	2.44	0.65
1:B:421:ILE:HD11	1:B:472:LEU:HB2	1.79	0.64
1:A:515:LEU:HD22	1:A:566:ILE:HG13	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:ARG:NH1	1:B:494:ARG:HH21	1.97	0.63
1:A:447:ARG:HB3	1:A:449:GLU:HG3	1.83	0.60
1:A:327:LEU:HD23	1:A:346:ASN:HB2	1.84	0.59
1:A:599:SER:OG	1:A:601:ARG:NH2	2.37	0.58
1:A:377:VAL:HG22	1:A:393:LEU:HD13	1.86	0.58
1:A:354:ARG:HD2	1:A:355:LEU:H	1.68	0.57
1:A:329:TYR:HA	1:A:343:GLU:O	2.04	0.57
1:A:534:VAL:HG21	1:A:591:TRP:CZ2	2.40	0.56
1:A:583:CYS:HB2	1:A:594:VAL:HG23	1.88	0.55
1:B:483:ARG:HG2	1:B:508[B]:SER:HB2	1.88	0.55
1:B:467:VAL:HG22	1:B:472:LEU:HD12	1.90	0.53
1:B:566:ILE:HB	1:B:584:TYR:HB3	1.90	0.53
1:A:460:ARG:HB3	1:A:463:VAL:HB	1.91	0.52
1:B:460:ARG:HB3	1:B:463:VAL:HB	1.91	0.52
1:B:483:ARG:HG2	1:B:508[A]:SER:HB3	1.90	0.52
1:A:373:LEU:HD22	1:A:397:ASN:HA	1.92	0.52
1:A:397:ASN:CB	1:A:400:THR:HB	2.36	0.51
1:A:567:TYR:HE2	1:A:594:VAL:HG21	1.74	0.51
1:A:573:ASP:HB3	1:A:578:LEU:HD11	1.92	0.51
1:B:614:ARG:NE	1:B:614:ARG:HA	2.26	0.51
1:A:416:ILE:HD11	1:A:427:ALA:HB1	1.91	0.51
1:A:365:LEU:HD23	1:A:365:LEU:H	1.75	0.50
1:A:563:GLN:OE1	1:A:567:TYR:OH	2.26	0.50
1:A:329:TYR:O	1:A:606:VAL:HG13	2.11	0.49
1:A:410:SER:HB3	1:A:441:GLU:OE2	2.12	0.49
1:B:515:LEU:HD22	1:B:566:ILE:HG13	1.94	0.48
1:A:566:ILE:O	1:A:583:CYS:HA	2.13	0.48
1:A:490:TYR:HB2	1:A:497:TRP:CH2	2.48	0.47
1:A:565:ARG:HG2	1:A:583:CYS:SG	2.55	0.47
1:A:369:VAL:HG21	1:A:608:VAL:C	2.34	0.47
1:A:535:GLU:HB3	1:A:546:PHE:CD1	2.49	0.47
1:B:494:ARG:HG3	1:B:496:GLU:HG2	1.96	0.47
1:A:346:ASN:OD1	1:A:347:PRO:HD2	2.14	0.47
1:A:327:LEU:O	1:A:608:VAL:HG22	2.14	0.47
1:B:471:LEU:HD23	1:B:492:PRO:HD3	1.97	0.47
1:B:557:LEU:H	1:B:557:LEU:HD23	1.79	0.46
1:A:489:CYS:O	1:A:497:TRP:HA	2.15	0.46
1:A:550:MET:CE	1:A:568:VAL:HG11	2.46	0.46
1:A:552:HIS:HB2	1:A:554:ARG:HH21	1.81	0.46
1:A:583:CYS:HB2	1:A:594:VAL:CG2	2.46	0.45
1:A:393:LEU:HD22	1:A:450:TRP:CZ2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:VAL:HA	1:B:520:TYR:O	2.16	0.45
1:A:562:HIS:O	1:A:563:GLN:HB2	2.17	0.45
1:A:406:CYS:HB3	1:A:448:ASP:OD1	2.17	0.44
1:A:334:TYR:CZ	2:P:82:GLU:HB2	2.52	0.44
1:A:393:LEU:HD22	1:A:450:TRP:HZ2	1.82	0.44
1:A:397:ASN:O	1:A:401:ASN:N	2.49	0.44
1:B:465:VAL:HA	1:B:473:TYR:O	2.17	0.44
1:A:328:ILE:O	1:A:345:TYR:N	2.51	0.44
1:A:413:ARG:NH2	1:A:439:SER:OG	2.51	0.44
1:A:490:TYR:HB2	1:A:497:TRP:CZ3	2.53	0.43
1:B:436:HIS:ND1	1:B:461:ILE:HD11	2.33	0.43
1:A:525:TYR:CD2	2:P:79:GLU:HG2	2.53	0.43
1:A:532:ASN:HB2	1:A:550:MET:O	2.18	0.43
1:A:334:TYR:CE1	2:P:82:GLU:HB2	2.53	0.43
1:A:354:ARG:HD2	1:A:355:LEU:N	2.32	0.43
1:A:345:TYR:HB2	1:A:352:TRP:CE3	2.54	0.43
1:A:400:THR:O	1:A:402:GLN:HG3	2.18	0.43
1:A:446:GLU:CD	1:A:447:ARG:HH21	2.22	0.43
1:B:365:LEU:HD12	1:B:376:ALA:HB1	2.01	0.43
1:A:346:ASN:HB3	1:A:349:ASP:OD2	2.19	0.42
1:A:395:CYS:O	1:A:403:TRP:HA	2.19	0.42
1:A:342:LEU:O	1:A:354:ARG:HD3	2.18	0.42
1:A:345:TYR:HB2	1:A:352:TRP:CZ3	2.54	0.42
1:B:328:ILE:HD12	1:B:347:PRO:HG3	2.02	0.42
1:B:421:ILE:HB	1:B:426:TYR:HE1	1.85	0.42
1:A:534:VAL:HG21	1:A:591:TRP:HZ2	1.81	0.42
1:A:355:LEU:HD22	1:A:396:TYR:OH	2.20	0.41
1:A:358:LEU:HD13	1:A:362:ARG:HD3	2.02	0.41
1:B:518:CYS:SG	1:B:536:ARG:HD2	2.61	0.41
1:A:467:VAL:O	1:A:514:VAL:HG21	2.21	0.41
1:A:472:LEU:HB3	1:A:490:TYR:HB3	2.03	0.41
1:A:518:CYS:HA	1:A:537:TYR:O	2.20	0.41
1:B:369:VAL:HG21	1:B:608:VAL:O	2.20	0.41
1:B:443:TYR:HB2	1:B:450:TRP:CE2	2.56	0.41
1:B:614:ARG:HA	1:B:614:ARG:HE	1.86	0.41
1:A:359:GLN:HG2	1:A:360:VAL:HG23	2.02	0.40
1:A:369:VAL:HG21	1:A:608:VAL:O	2.21	0.40
1:A:557:LEU:HD12	1:A:568:VAL:HB	2.03	0.40
1:A:421:ILE:HD11	1:A:472:LEU:HB2	2.02	0.40
1:A:584:TYR:HB2	1:A:591:TRP:CZ3	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:GLN:CG	1:B:336:ARG:NH2[1_556]	2.15	0.05

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	281/301 (93%)	265 (94%)	16 (6%)	0	100	100
1	B	289/301 (96%)	282 (98%)	7 (2%)	0	100	100
2	P	5/7 (71%)	4 (80%)	1 (20%)	0	100	100
All	All	575/609 (94%)	551 (96%)	24 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	228/247 (92%)	224 (98%)	4 (2%)	59	71
1	B	235/247 (95%)	232 (99%)	3 (1%)	69	80
2	P	5/5 (100%)	5 (100%)	0	100	100
All	All	468/499 (94%)	461 (98%)	7 (2%)	65	76

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	368	CYS
1	A	395	CYS
1	A	451	HIS
1	A	580	SER
1	B	554	ARG
1	B	557	LEU
1	B	610	MET

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	346	ASN
1	A	402	GLN

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	BAL	P	76	2	4,4,5	0.94	0	3,3,5	15.74	1 (33%)

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	BAL	P	76	2	-	0/1/2/3	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	76	BAL	CB-CA-C	27.26	151.90	111.42

There are no chirality outliers.

There are no torsion outliers.

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)

2 ligands are 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	0.13	0	6,6,6	0.20	0
3	SO4	A	702	-	4,4,4	0.18	0	6,6,6	0.42	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, 95^{th} 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	283/301 (94%)	2.02	116 (40%) 0 0	30, 66, 123, 160	0
1	B	290/301 (96%)	0.51	25 (8%) 10 9	26, 36, 56, 84	0
2	P	6/7 (85%)	0.61	0 100 100	48, 48, 54, 54	0
All	All	579/609 (95%)	1.25	141 (24%) 0 0	26, 44, 110, 160	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	353	LEU	8.8
1	A	399	MET	8.6
1	A	397	ASN	7.5
1	A	421	ILE	7.4
1	A	351	THR	7.3
1	A	348	SER	7.3
1	A	371	GLY	7.0
1	A	608	VAL	6.7
1	A	402	GLN	6.6
1	A	567	TYR	6.5
1	A	395	CYS	6.5
1	A	400	THR	6.5
1	A	346	ASN	6.3
1	A	350	GLY	6.1
1	A	405	PRO	5.9
1	A	349	ASP	5.8
1	B	385	ASP	5.8
1	A	425	ILE	5.7
1	A	559	ILE	5.7
1	A	422	ASP	5.4
1	A	452	LEU	5.4
1	A	569	LEU	5.4
1	A	374	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	368	CYS	5.2
1	A	327	LEU	5.1
1	A	398	PRO	5.0
1	A	352	TRP	4.8
1	A	596	ARG	4.7
1	A	354	ARG	4.7
1	A	563	GLN	4.7
1	A	375	TYR	4.7
1	A	561	VAL	4.7
1	A	451	HIS	4.7
1	A	604	VAL	4.6
1	A	606	VAL	4.6
1	A	373	LEU	4.6
1	A	447	ARG	4.6
1	A	377	VAL	4.5
1	B	384	PRO	4.4
1	A	416	ILE	4.2
1	A	594	VAL	4.2
1	A	376	ALA	4.1
1	A	562	HIS	4.1
1	A	557	LEU	4.1
1	A	514	VAL	4.1
1	A	329	TYR	4.0
1	B	365	LEU	4.0
1	A	423	GLY	4.0
1	A	449	GLU	4.0
1	B	366	ALA	4.0
1	A	581	VAL	3.9
1	A	446	GLU	3.9
1	A	576	THR	3.8
1	A	418	VAL	3.8
1	A	609	THR	3.8
1	A	494	ARG	3.7
1	A	493	GLU	3.7
1	A	396	TYR	3.6
1	A	365	LEU	3.5
1	A	588	THR	3.5
1	A	605	GLY	3.5
1	B	416	ILE	3.5
1	B	383	SER	3.5
1	A	510	ALA	3.4
1	A	550	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	408	PRO	3.4
1	A	551	LYS	3.3
1	A	516	HIS	3.3
1	A	370	VAL	3.3
1	A	512	VAL	3.3
1	A	558	GLY	3.3
1	B	386	GLY	3.3
1	A	491	TYR	3.2
1	A	347	PRO	3.2
1	A	575	HIS	3.2
1	A	419	GLY	3.2
1	A	549	PRO	3.1
1	B	465	VAL	3.1
1	A	443	TYR	3.1
1	A	592	SER	3.1
1	A	600	GLY	3.0
1	A	356	ALA	3.0
1	A	465	VAL	3.0
1	A	571	GLY	3.0
1	A	595	THR	3.0
1	B	605	GLY	2.9
1	A	470	ARG	2.9
1	A	607	ALA	2.9
1	A	591	TRP	2.9
1	A	584	TYR	2.9
1	A	453	VAL	2.9
1	A	469	ASN	2.9
1	A	590	THR	2.8
1	A	424	HIS	2.8
1	A	593	GLU	2.7
1	A	420	VAL	2.7
1	A	417	GLY	2.7
1	B	399	MET	2.7
1	A	568	VAL	2.6
1	B	377	VAL	2.6
1	A	548	ALA	2.5
1	B	614	ARG	2.5
1	B	493	GLU	2.5
1	B	588	THR	2.5
1	A	331	ALA	2.4
1	B	604	VAL	2.4
1	A	495	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	492	PRO	2.4
1	B	569	LEU	2.4
1	B	512	VAL	2.4
1	B	606	VAL	2.4
1	A	333	GLY	2.3
1	A	367	GLY	2.3
1	A	454	ALA	2.3
1	A	427	ALA	2.3
1	A	589	ASP	2.3
1	A	599	SER	2.3
1	B	463	VAL	2.3
1	B	400	THR	2.3
1	A	552	HIS	2.3
1	B	418	VAL	2.3
1	A	444	GLU	2.2
1	A	426	TYR	2.2
1	A	344	ALA	2.2
1	B	447	ARG	2.2
1	A	560	THR	2.2
1	A	355	LEU	2.2
1	B	613	SER	2.2
1	A	598	THR	2.2
1	B	434	CYS	2.2
1	A	369	VAL	2.1
1	A	463	VAL	2.1
1	A	360	VAL	2.1
1	A	393	LEU	2.1
1	A	475	VAL	2.1
1	A	328	ILE	2.1
1	A	597	MET	2.0
1	A	474	ALA	2.0
1	A	442	ARG	2.0
1	B	335	PHE	2.0
1	A	462	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, 95^{th} 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	BAL	P	76	5/6	0.90	0.21	51,60,63,72	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, 95^{th} 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	702	5/5	0.92	0.23	55,55,57,62	0
3	SO4	A	701	5/5	0.94	0.21	56,59,72,77	0

6.5 Other polymers (i)

There are no such residues in this entry.