



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:12 PM UTC

PDB ID : 7K2C / pdb_00007k2c
Title : Kelch domain of human KEAP1 bound to Nrf2 peptide, ADEETGEAA
Authors : Muellers, S.N.; Allen, K.N.
Deposited on : 2020-09-08
Resolution : 2.11 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

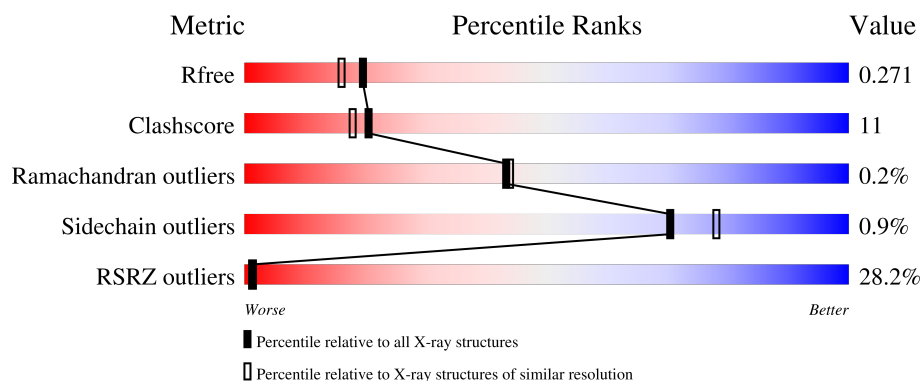
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	50% 71% 26% ..
1	B	290	6% 87% 13%
2	P	11	18% 82% 18%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4502 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
			2107	1312	381	400	14			
1	B	290	Total	C	N	O	S	0	1	0
			2214	1378	399	421	16			

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 peptide,ADEETGEAA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	11	Total	C	N	O	0	0	1
			65	36	10	19			

- 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		

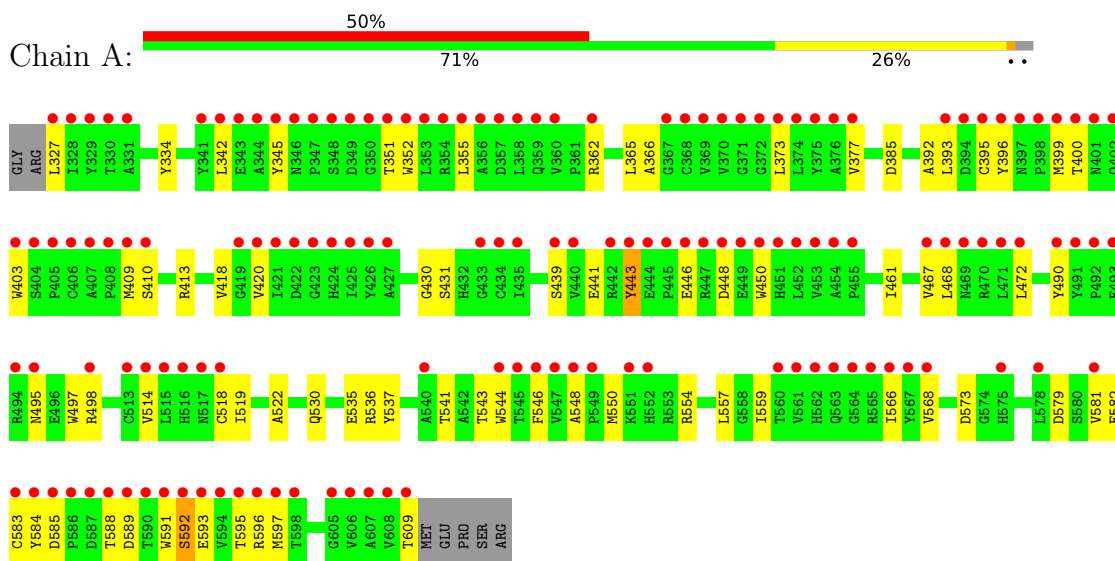
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	19	Total	O	0	0
			19	19		
4	B	89	Total	O	0	0
			89	89		
4	P	3	Total	O	0	0
			3	3		

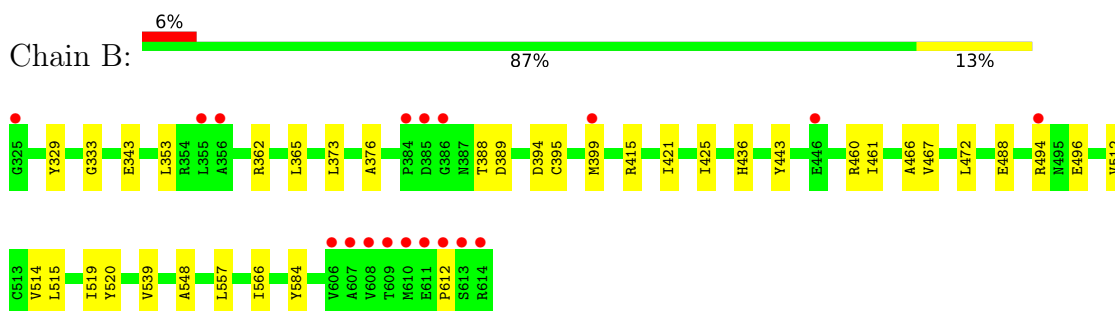
3 Residue-property plots [i](#)

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.

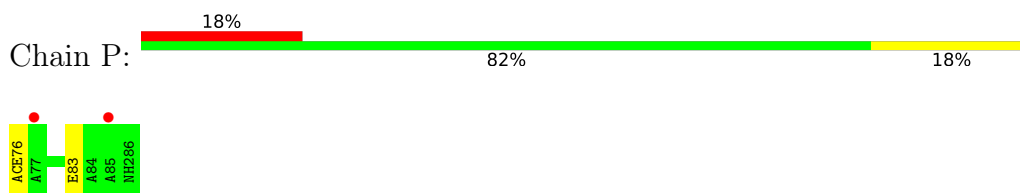
• Molecule 1: Kelch-like ECH-associated protein 1



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



• Molecule 2: Nrf2 peptide, ADEETGEAA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.62Å 68.88Å 77.44Å 90.00° 117.82° 90.00°	Depositor
Resolution (Å)	29.38 – 2.11 29.38 – 2.11	Depositor EDS
% Data completeness (in resolution range)	98.0 (29.38-2.11) 98.3 (29.38-2.11)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.237 , 0.271 0.238 , 0.271	Depositor DCC
R_{free} test set	1997 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.008 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4502	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% 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: ACE, NH2, 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	0/2158	0.66	1/2946 (0.0%)
1	B	0.60	2/2271 (0.1%)	0.65	1/3094 (0.0%)
2	P	0.73	1/61 (1.6%)	0.86	1/82 (1.2%)
All	All	0.57	3/4490 (0.1%)	0.66	3/6122 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	333	GLY	C-O	-5.29	1.18	1.23
1	B	548	ALA	C-O	-5.20	1.17	1.24
2	P	76	ACE	C-N	5.03	1.43	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	76	ACE	C-N-CA	-6.91	100.97	121.70
1	A	399	MET	N-CA-C	-6.16	104.48	112.68
1	B	539	VAL	N-CA-C	5.59	116.32	110.62

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	2107	0	1957	72	1
1	B	2214	0	2103	23	1
2	P	65	0	50	1	0
3	A	5	0	0	0	0
4	A	19	0	0	0	0
4	B	89	0	0	0	0
4	P	3	0	0	0	0
All	All	4502	0	4110	95	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 11.

All (95) 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:355:LEU:HD23	1:A:396:TYR:OH	1.63	0.98
1:A:393:LEU:HD21	1:A:443:TYR:CE2	1.99	0.96
1:A:584:TYR:CD1	1:A:591:TRP:NE1	2.41	0.89
1:A:584:TYR:HB2	1:A:591:TRP:CE2	2.11	0.86
1:A:581:VAL:HB	1:A:595:THR:O	1.75	0.85
1:A:550:MET:CE	1:A:568:VAL:HG11	2.11	0.79
1:A:355:LEU:HD23	1:A:396:TYR:HH	1.46	0.79
1:A:355:LEU:CD2	1:A:396:TYR:OH	2.33	0.77
1:B:466:ALA:HB1	1:B:514:VAL:HG23	1.66	0.76
1:A:584:TYR:HD1	1:A:591:TRP:CD1	2.05	0.73
1:A:550:MET:HE1	1:A:568:VAL:HG11	1.71	0.72
1:A:550:MET:HE2	1:A:568:VAL:HG21	1.72	0.71
1:A:584:TYR:HB2	1:A:591:TRP:CD2	2.24	0.71
1:A:554:ARG:HG3	1:A:557:LEU:HD22	1.78	0.65
1:B:494:ARG:HG3	1:B:496:GLU:HG2	1.79	0.65
1:A:584:TYR:HD1	1:A:591:TRP:NE1	1.91	0.64
1:A:584:TYR:HB2	1:A:591:TRP:CZ2	2.34	0.63
1:A:537:TYR:CD1	1:A:544:TRP:NE1	2.67	0.62
1:B:557:LEU:H	1:B:557:LEU:HD23	1.65	0.62
1:A:351:THR:HG22	1:A:352:TRP:H	1.62	0.62
1:A:362:ARG:HH21	1:A:392:ALA:HB3	1.65	0.61
1:A:393:LEU:CD2	1:A:443:TYR:CE2	2.81	0.61
1:A:362:ARG:NH2	1:A:392:ALA:HB3	2.16	0.60
1:A:420:VAL:O	1:A:467:VAL:HG21	2.02	0.59
1:B:436:HIS:HB3	1:B:461:ILE:HD11	1.84	0.58
1:B:515:LEU:HD22	1:B:566:ILE:HG13	1.83	0.58
1:A:559:ILE:HG13	1:A:568:VAL:HG12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:ARG:HH22	1:A:439:SER:HB2	1.71	0.55
1:A:584:TYR:CD1	1:A:591:TRP:CE2	2.94	0.55
1:A:365:LEU:HD23	1:A:365:LEU:H	1.71	0.55
1:B:329:TYR:OH	1:B:612:PRO:HD3	2.07	0.55
1:A:583:CYS:N	1:A:592:SER:O	2.30	0.55
1:B:514:VAL:HG22	1:B:519:ILE:HD13	1.90	0.53
1:A:541:THR:O	1:A:543:THR:HG23	2.09	0.53
1:A:582:GLU:HA	1:A:593:GLU:HA	1.91	0.53
1:A:548:ALA:HB2	1:A:589:ASP:OD2	2.10	0.52
1:A:518:CYS:SG	1:A:536:ARG:HD2	2.50	0.52
1:A:584:TYR:CD1	1:A:591:TRP:CD1	2.89	0.52
1:A:585:ASP:HB3	1:A:588:THR:HG22	1.93	0.51
1:A:373:LEU:HB3	1:A:395:CYS:SG	2.52	0.50
1:A:537:TYR:HD1	1:A:544:TRP:CD1	2.29	0.50
1:A:327:LEU:N	1:A:609:THR:O	2.44	0.50
1:B:421:ILE:HD11	1:B:472:LEU:HB2	1.94	0.50
1:A:522:ALA:HB1	1:A:550:MET:HE3	1.94	0.50
1:A:537:TYR:HB2	1:A:544:TRP:CZ2	2.48	0.49
1:A:548:ALA:HB2	1:A:589:ASP:CG	2.37	0.49
1:A:342:LEU:HD22	1:A:403:TRP:HZ2	1.78	0.48
1:A:366:ALA:HB1	1:A:418:VAL:HG22	1.95	0.48
1:B:365:LEU:H	1:B:365:LEU:HD23	1.77	0.48
1:B:467:VAL:O	1:B:514:VAL:HG21	2.13	0.48
1:A:550:MET:CE	1:A:568:VAL:HG21	2.41	0.48
1:A:537:TYR:CD1	1:A:544:TRP:CD1	3.01	0.48
1:B:362:ARG:NH1	1:B:394:ASP:OD2	2.45	0.47
1:A:467:VAL:O	1:A:514:VAL:HG21	2.15	0.47
1:A:396:TYR:CD2	1:A:396:TYR:O	2.69	0.46
1:A:537:TYR:HB2	1:A:544:TRP:CE2	2.51	0.45
1:A:566:ILE:HG21	1:A:591:TRP:CH2	2.51	0.45
1:A:377:VAL:HG22	1:A:393:LEU:CD1	2.46	0.45
1:A:498:ARG:HA	1:A:498:ARG:HD3	1.72	0.45
1:A:579:ASP:O	1:A:597:MET:HG3	2.15	0.45
1:B:494:ARG:NE	1:B:494:ARG:HA	2.32	0.45
1:A:472:LEU:HB3	1:A:490:TYR:HB3	1.98	0.44
1:A:566:ILE:HG21	1:A:591:TRP:HH2	1.82	0.44
1:B:399:MET:HB2	1:B:399:MET:HE2	1.80	0.44
1:A:345:TYR:HB2	1:A:352:TRP:CE3	2.52	0.44
1:A:410:SER:HB3	1:A:441:GLU:OE2	2.17	0.44
1:B:460:ARG:HH21	1:B:488:GLU:HG2	1.81	0.44
1:A:448:ASP:N	1:A:448:ASP:OD1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:TYR:CD1	1:A:544:TRP:CE2	3.05	0.44
1:B:566:ILE:HB	1:B:584:TYR:HB3	1.99	0.44
1:A:490:TYR:OH	1:A:495:ASN:OD1	2.28	0.44
1:B:388:THR:HG22	1:B:389:ASP:O	2.18	0.44
1:B:343:GLU:HA	1:B:353:LEU:O	2.18	0.44
1:A:443:TYR:O	1:A:443:TYR:CD2	2.70	0.43
1:A:535:GLU:HB3	1:A:546:PHE:CD1	2.53	0.43
1:A:584:TYR:HB2	1:A:591:TRP:CE3	2.54	0.43
1:A:490:TYR:HB2	1:A:497:TRP:CH2	2.54	0.43
1:A:530:GLN:HG2	1:A:573:ASP:HA	1.99	0.43
1:A:334:TYR:CE1	2:P:83:GLU:HA	2.54	0.43
1:B:373:LEU:HB3	1:B:395:CYS:SG	2.59	0.42
1:B:365:LEU:HD12	1:B:376:ALA:HB1	2.02	0.42
1:A:431:SER:HB3	1:A:461:ILE:HG21	2.02	0.42
1:A:430:GLY:C	1:A:461:ILE:HG22	2.45	0.41
1:A:393:LEU:HD22	1:A:450:TRP:HZ2	1.86	0.41
1:A:395:CYS:SG	1:A:396:TYR:N	2.93	0.41
1:B:494:ARG:HG3	1:B:496:GLU:CG	2.49	0.41
1:B:512:VAL:HA	1:B:520:TYR:O	2.20	0.41
1:A:518:CYS:HB3	1:A:536:ARG:HB2	2.02	0.41
1:A:468:LEU:HD13	1:A:514:VAL:HG11	2.02	0.41
1:A:519:ILE:O	1:A:536:ARG:HA	2.20	0.41
1:B:467:VAL:HG22	1:B:472:LEU:HD12	2.02	0.41
1:B:425:ILE:HB	1:B:443:TYR:HB3	2.03	0.41
1:A:537:TYR:HB2	1:A:544:TRP:CH2	2.56	0.41
1:A:409:MET:HE1	1:A:413:ARG:HB2	2.03	0.40
1:A:585:ASP:OD1	1:A:588:THR:HG22	2.21	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:A:385:ASP:OD2	1:B:415:ARG:NH2[1_556]	2.18	0.02

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	281/290 (97%)	267 (95%)	13 (5%)	1 (0%)	30	28
1	B	289/290 (100%)	278 (96%)	11 (4%)	0	100	100
2	P	9/11 (82%)	9 (100%)	0	0	100	100
All	All	579/591 (98%)	554 (96%)	24 (4%)	1 (0%)	43	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	446	GLU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	211/234 (90%)	207 (98%)	4 (2%)	50	57
1	B	232/234 (99%)	232 (100%)	0	100	100
2	P	5/5 (100%)	5 (100%)	0	100	100
All	All	448/473 (95%)	444 (99%)	4 (1%)	70	78

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	400	THR
1	A	443	TYR
1	A	592	SER
1	A	596	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	387	ASN
1	A	401	ASN
1	A	414	ASN
1	A	469	ASN
1	A	482	ASN
1	A	552	HIS
1	B	432	HIS
1	B	469	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	0.27	0	6,6,6	0.07	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

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	283/290 (97%)	2.34	144 (50%) 0 0	24, 56, 101, 122	0
1	B	290/290 (100%)	0.32	18 (6%) 26 29	18, 33, 62, 106	1 (0%)
2	P	9/11 (81%)	1.05	2 (22%) 2 2	35, 38, 58, 61	0
All	All	582/591 (98%)	1.32	164 (28%) 1 1	18, 40, 94, 122	1 (0%)

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	591	TRP	8.4
1	A	423	GLY	7.6
1	A	373	LEU	7.6
1	A	594	VAL	7.3
1	A	327	LEU	7.2
1	B	607	ALA	7.0
1	B	612	PRO	6.8
1	A	419	GLY	6.7
1	B	608	VAL	6.6
1	A	445	PRO	6.5
1	A	353	LEU	6.4
1	A	421	ILE	6.3
1	A	420	VAL	6.3
1	A	595	THR	6.1
1	A	356	ALA	6.1
1	A	443	TYR	6.0
1	A	329	TYR	6.0
1	B	609	THR	6.0
1	A	344	ALA	5.9
1	A	608	VAL	5.8
1	A	516	HIS	5.7
1	A	566	ILE	5.6
1	A	374	LEU	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	567	TYR	5.5
1	A	407	ALA	5.4
1	B	614	ARG	5.3
1	A	446	GLU	5.3
1	A	355	LEU	5.3
1	A	348	SER	5.3
1	A	590	THR	5.3
1	A	442	ARG	5.1
1	A	369	VAL	5.1
1	A	399	MET	5.1
1	A	609	THR	5.0
1	A	395	CYS	5.0
1	A	584	TYR	5.0
1	A	349	ASP	4.9
1	A	328	ILE	4.9
1	A	493	GLU	4.9
1	A	398	PRO	4.9
1	A	345	TYR	4.8
1	A	371	GLY	4.8
1	A	351	THR	4.8
1	A	425	ILE	4.7
1	A	375	TYR	4.7
1	B	610	MET	4.7
1	A	607	ALA	4.7
1	A	342	LEU	4.7
1	A	453	VAL	4.6
2	P	85	ALA	4.6
1	A	396	TYR	4.6
1	A	547	VAL	4.5
1	A	368	CYS	4.5
1	A	561	VAL	4.5
1	A	424	HIS	4.5
1	A	447	ARG	4.4
1	A	563	GLN	4.3
1	A	491	TYR	4.2
1	A	372	GLY	4.2
1	A	397	ASN	4.2
1	A	403	TRP	4.2
1	A	588	THR	4.2
1	A	587	ASP	4.1
1	A	451	HIS	4.1
1	A	402	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	546	PHE	4.1
1	A	581	VAL	4.1
1	A	352	TRP	4.0
1	A	592	SER	4.0
1	A	564	GLY	4.0
1	B	611	GLU	3.9
1	A	470	ARG	3.9
1	A	408	PRO	3.9
1	B	356	ALA	3.9
1	A	406	CYS	3.8
1	A	370	VAL	3.8
1	A	346	ASN	3.8
1	A	400	THR	3.7
1	A	354	ARG	3.7
1	A	549	PRO	3.7
1	A	401	ASN	3.7
1	B	325	GLY	3.7
1	A	515	LEU	3.6
1	A	347	PRO	3.6
1	A	450	TRP	3.6
1	A	468	LEU	3.6
1	A	586	PRO	3.6
1	A	426	TYR	3.6
1	A	492	PRO	3.6
1	A	404	SER	3.6
1	B	613	SER	3.6
1	A	422	ASP	3.5
1	A	545	THR	3.5
1	A	471	LEU	3.5
1	A	518	CYS	3.5
1	A	562	HIS	3.5
1	A	376	ALA	3.4
1	A	585	ASP	3.4
1	A	367	GLY	3.4
1	A	565	ARG	3.4
1	A	467	VAL	3.4
1	A	410	SER	3.4
1	A	405	PRO	3.3
1	A	605	GLY	3.3
1	A	444	GLU	3.3
1	A	330	THR	3.2
1	A	540	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	350	GLY	3.2
1	A	360	VAL	3.1
1	A	494	ARG	3.1
1	A	343	GLU	3.1
1	A	490	TYR	3.1
1	A	514	VAL	3.1
1	B	606	VAL	3.1
1	A	393	LEU	3.1
1	A	331	ALA	3.0
1	A	548	ALA	3.0
1	A	448	ASP	3.0
1	A	435	ILE	2.9
1	A	598	THR	2.9
1	A	452	LEU	2.9
1	A	377	VAL	2.9
1	B	385	ASP	2.9
1	A	544	TRP	2.9
1	A	596	ARG	2.8
1	A	454	ALA	2.8
1	A	552	HIS	2.8
1	A	359	GLN	2.8
1	A	551	LYS	2.8
1	A	394	ASP	2.7
1	B	355	LEU	2.7
1	A	517	ASN	2.7
1	A	498	ARG	2.7
1	A	589	ASP	2.7
1	A	593	GLU	2.7
1	A	357	ASP	2.7
1	A	583	CYS	2.7
1	A	409	MET	2.6
1	A	472	LEU	2.6
1	B	399	MET	2.5
1	A	469	ASN	2.5
1	A	341	TYR	2.5
1	A	513	CYS	2.5
1	A	439	SER	2.5
1	A	455	PRO	2.4
1	A	597	MET	2.4
1	B	494	ARG	2.4
1	A	568	VAL	2.3
1	A	575	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	495	ASN	2.3
2	P	77	ALA	2.3
1	A	606	VAL	2.2
1	B	384	PRO	2.2
1	A	449	GLU	2.2
1	A	427	ALA	2.2
1	A	434	CYS	2.2
1	A	433	GLY	2.1
1	A	358	LEU	2.1
1	A	578	LEU	2.1
1	A	440	VAL	2.0
1	B	446	GLU	2.0
1	A	362	ARG	2.0
1	A	560	THR	2.0
1	B	386	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	SO4	A	701	5/5	0.86	0.12	74,82,94,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.