



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:47 AM EDT

PDB ID : 2IYE / pdb_00002iye
Title : Structure of catalytic CPx-ATPase domain CopB-B
Authors : Luebben, M.; Gueldenhaupt, J.; Deigweiher, K.; Haebel, P.; Scheidig, A.J.
Deposited on : 2006-07-15
Resolution : 2.60 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

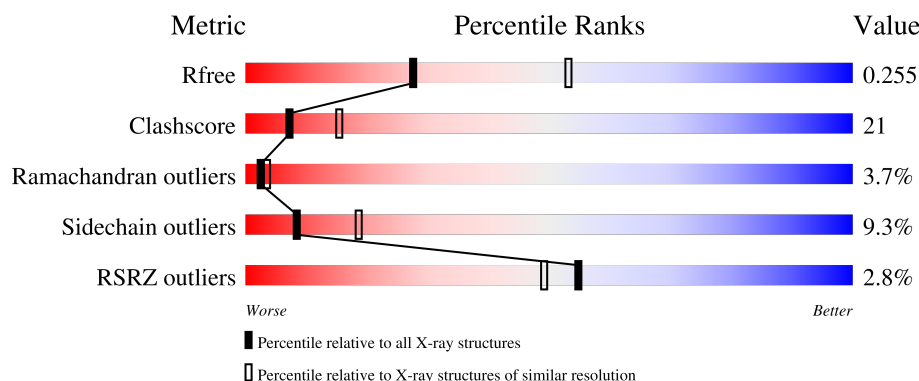
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

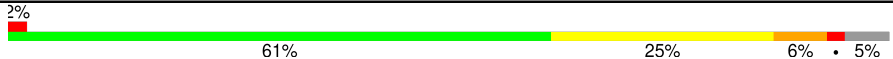
The reported resolution of this entry is 2.60 Å.

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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	263	
1	C	263	

2 Entry composition [i](#)

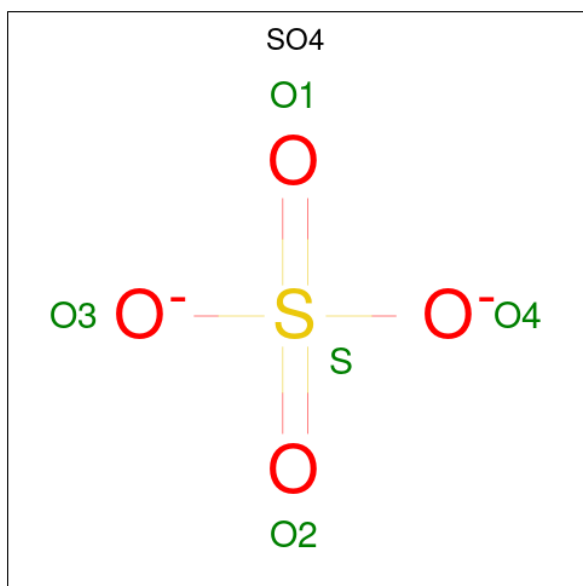
There are 3 unique types of molecules in this entry. The entry contains 3878 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 COPPER-TRANSPORTING ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1902	1213	313	372	4			
1	C	249	Total	C	N	O	S	0	0	0
			1902	1213	313	372	4			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

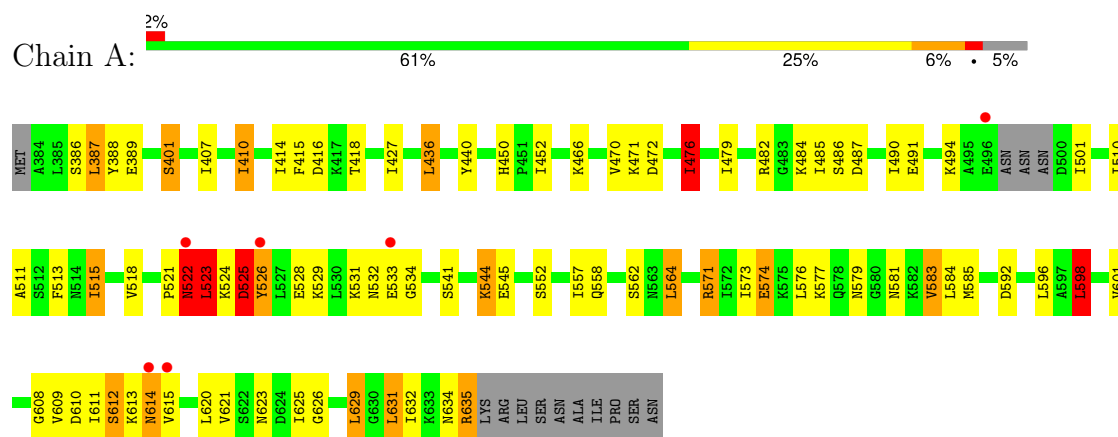
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	32	Total 32	O 32	0	0
3	C	32	Total 32	O 32	0	0

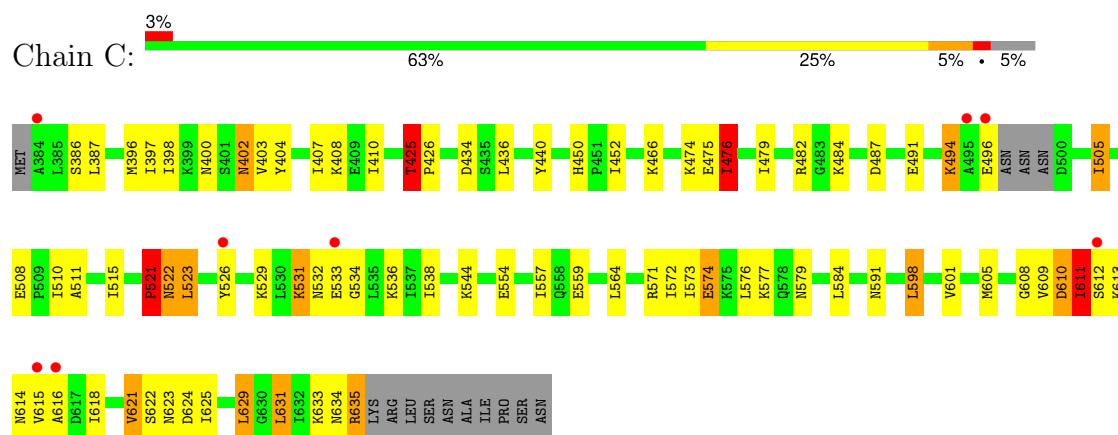
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: COPPER-TRANSPORTING ATPASE



• Molecule 1: COPPER-TRANSPORTING ATPASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.53Å 53.80Å 73.96Å 90.00° 97.08° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60 40.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-2.60) 99.7 (40.00-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.03 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.220 , 0.256 0.221 , 0.255	Depositor DCC
R_{free} test set	1739 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.036 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3878	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.84% 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: 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	1.07	1/1921 (0.1%)	1.21	11/2583 (0.4%)
1	C	1.06	1/1921 (0.1%)	1.16	6/2583 (0.2%)
All	All	1.07	2/3842 (0.1%)	1.18	17/5166 (0.3%)

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
1	A	0	3
1	C	0	3
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	476	ILE	CA-CB	5.09	1.61	1.54
1	C	505	ILE	CA-CB	5.05	1.60	1.54

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	518	VAL	N-CA-C	7.78	115.62	107.76
1	A	541	SER	N-CA-C	6.22	117.98	108.52
1	C	591	ASN	N-CA-C	6.07	120.00	112.47
1	C	425	THR	CA-C-N	6.05	125.96	119.85
1	C	425	THR	C-N-CA	6.05	125.96	119.85
1	C	402	ASN	N-CA-C	-5.99	105.46	112.89
1	A	621	VAL	CB-CA-C	-5.75	103.66	112.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	418	THR	N-CA-C	5.53	117.72	109.59
1	A	545	GLU	N-CA-C	5.44	117.64	111.11
1	A	623	ASN	N-CA-C	-5.44	105.95	112.58
1	C	508	GLU	N-CA-C	5.37	116.43	109.72
1	A	515	ILE	N-CA-C	5.32	117.04	108.85
1	C	621	VAL	CB-CA-C	-5.30	104.30	112.05
1	A	598	LEU	N-CA-C	5.22	116.97	111.28
1	A	583	VAL	N-CA-C	5.17	115.40	108.17
1	A	552	SER	N-CA-C	5.14	116.88	111.28
1	A	558	GLN	N-CA-C	5.10	116.65	111.14

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	521	PRO	Peptide
1	A	611	ILE	Peptide
1	A	612	SER	Peptide
1	C	521	PRO	Peptide
1	C	610	ASP	Peptide
1	C	611	ILE	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	1902	0	1987	85	0
1	C	1902	0	1987	81	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0
3	A	32	0	0	1	0
3	C	32	0	0	3	0
All	All	3878	0	3974	161	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (161) 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:632:ILE:HA	1:A:635:ARG:NH2	1.55	1.22
1:C:523:LEU:HD23	1:C:523:LEU:O	1.51	1.10
1:A:632:ILE:HA	1:A:635:ARG:HH22	1.03	1.08
1:C:529:LYS:NZ	1:C:629:LEU:HD12	1.83	0.93
1:A:632:ILE:CA	1:A:635:ARG:HH22	1.83	0.90
1:A:523:LEU:O	1:A:523:LEU:HD23	1.73	0.89
1:C:611:ILE:C	1:C:613:LYS:H	1.87	0.81
1:A:523:LEU:O	1:A:526:TYR:HB2	1.82	0.80
1:A:526:TYR:CE2	1:A:557:ILE:HD11	2.16	0.80
1:C:523:LEU:O	1:C:523:LEU:CD2	2.30	0.79
1:A:523:LEU:CD2	1:A:523:LEU:C	2.56	0.79
1:A:523:LEU:HD23	1:A:523:LEU:C	2.07	0.78
1:A:523:LEU:O	1:A:526:TYR:N	2.17	0.78
1:A:407:ILE:HG22	1:A:635:ARG:HE	1.47	0.78
1:C:523:LEU:HD23	1:C:523:LEU:C	2.09	0.78
1:C:523:LEU:CD2	1:C:523:LEU:C	2.58	0.76
1:A:522:ASN:O	1:A:523:LEU:HB2	1.86	0.75
1:C:452:ILE:HD12	1:C:515:ILE:HD12	1.68	0.75
1:A:631:LEU:HD23	1:A:631:LEU:O	1.86	0.74
1:C:529:LYS:HZ1	1:C:629:LEU:HD12	1.51	0.74
1:C:611:ILE:C	1:C:613:LYS:N	2.43	0.74
1:C:611:ILE:O	1:C:614:ASN:CG	2.30	0.74
1:A:450:HIS:CE1	1:A:452:ILE:HG12	2.23	0.73
1:A:522:ASN:O	1:A:523:LEU:CB	2.37	0.73
1:A:482:ARG:HG3	1:A:491:GLU:HG2	1.69	0.72
1:A:526:TYR:HE2	1:A:557:ILE:HD11	1.54	0.72
1:C:529:LYS:HZ2	1:C:629:LEU:HD12	1.51	0.71
1:C:532:ASN:C	1:C:534:GLY:H	2.00	0.70
1:A:523:LEU:O	1:A:526:TYR:CB	2.40	0.70
1:A:410:ILE:HD12	1:A:584:LEU:HB2	1.73	0.69
1:C:532:ASN:O	1:C:534:GLY:N	2.28	0.67
1:C:529:LYS:HZ1	1:C:629:LEU:HA	1.60	0.66
1:C:476:ILE:HG13	1:C:479:ILE:HB	1.78	0.66
1:C:523:LEU:O	1:C:526:TYR:HB2	1.96	0.65
1:A:571:ARG:HH12	1:C:615:VAL:HG11	1.61	0.65
1:A:525:ASP:O	1:A:529:LYS:HG2	1.97	0.65
1:A:407:ILE:CG2	1:A:635:ARG:HE	2.09	0.65
1:C:608:GLY:O	1:C:610:ASP:N	2.30	0.65
1:A:608:GLY:O	1:A:610:ASP:N	2.30	0.64
1:C:611:ILE:O	1:C:614:ASN:ND2	2.30	0.64
1:C:584:LEU:HD12	1:C:601:VAL:HG11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:SER:O	1:A:389:GLU:N	2.30	0.63
1:C:408:LYS:HA	1:C:635:ARG:HD2	1.81	0.63
1:A:634:ASN:C	1:A:635:ARG:HH11	2.08	0.62
1:C:479:ILE:O	1:C:494:LYS:HE3	2.00	0.61
1:C:482:ARG:HG3	1:C:491:GLU:HG2	1.82	0.61
1:A:452:ILE:HD12	1:A:515:ILE:CD1	2.30	0.60
1:A:532:ASN:O	1:A:534:GLY:N	2.35	0.60
1:A:386:SER:O	1:A:387:LEU:C	2.45	0.60
1:A:532:ASN:C	1:A:534:GLY:H	2.11	0.59
1:C:452:ILE:HD12	1:C:515:ILE:CD1	2.33	0.57
1:C:532:ASN:C	1:C:534:GLY:N	2.63	0.57
1:C:624:ASP:HA	3:C:2031:HOH:O	2.04	0.57
1:A:407:ILE:HG21	1:A:635:ARG:HH21	1.68	0.57
1:C:521:PRO:O	1:C:522:ASN:ND2	2.37	0.57
1:C:474:LYS:HD2	3:C:2011:HOH:O	2.05	0.57
1:A:573:ILE:O	1:A:577:LYS:HG3	2.05	0.57
1:C:635:ARG:CZ	1:C:635:ARG:HA	2.35	0.56
1:C:536:LYS:HE3	1:C:538:ILE:HD11	1.88	0.56
1:A:510:ILE:HD12	1:A:511:ALA:N	2.21	0.56
1:C:611:ILE:N	1:C:613:LYS:H	2.04	0.55
1:A:524:LYS:C	1:A:526:TYR:N	2.64	0.55
1:A:415:PHE:CE2	1:A:526:TYR:HE1	2.24	0.54
1:A:584:LEU:HG	1:A:601:VAL:HG13	1.89	0.54
1:C:397:ILE:HG13	1:C:621:VAL:HG13	1.90	0.54
1:C:526:TYR:CE2	1:C:557:ILE:HD11	2.42	0.54
1:A:631:LEU:O	1:A:635:ARG:NH1	2.39	0.53
1:A:613:LYS:C	1:A:615:VAL:H	2.16	0.53
1:C:400:ASN:HD21	1:C:402:ASN:CB	2.21	0.53
1:C:484:LYS:HE2	1:C:487:ASP:HA	1.89	0.53
1:C:559:GLU:CD	3:C:2023:HOH:O	2.51	0.53
1:A:414:ILE:HD12	1:A:583:VAL:HG11	1.92	0.52
1:A:574:GLU:HG2	1:C:598:LEU:HD21	1.91	0.52
1:A:524:LYS:C	1:A:526:TYR:H	2.17	0.51
1:C:521:PRO:O	1:C:522:ASN:CG	2.53	0.51
1:A:526:TYR:HE2	1:A:557:ILE:CD1	2.22	0.51
1:C:476:ILE:HD11	1:C:479:ILE:HD12	1.92	0.51
1:C:400:ASN:HD21	1:C:402:ASN:HB3	1.77	0.50
1:A:598:LEU:HD21	1:C:574:GLU:HG2	1.93	0.50
1:C:631:LEU:HA	1:C:634:ASN:HD22	1.77	0.50
1:A:416:ASP:OD2	1:A:592:ASP:OD2	2.30	0.50
1:C:584:LEU:HG	1:C:601:VAL:HG13	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:PHE:CE2	1:A:526:TYR:CE1	3.01	0.49
1:A:631:LEU:O	1:A:631:LEU:CD2	2.59	0.49
1:A:484:LYS:HE2	1:A:487:ASP:HA	1.95	0.48
1:A:631:LEU:CD2	1:A:631:LEU:C	2.86	0.48
1:A:579:ASN:HD22	1:A:581:ASN:ND2	2.12	0.48
1:C:584:LEU:HD12	1:C:601:VAL:CG1	2.42	0.48
1:A:485:ILE:HD12	1:A:490:ILE:HD13	1.96	0.48
1:C:611:ILE:O	1:C:613:LYS:N	2.46	0.47
1:A:452:ILE:HD12	1:A:515:ILE:HD11	1.96	0.47
1:A:634:ASN:C	1:A:635:ARG:NH1	2.72	0.47
1:A:635:ARG:NH1	1:A:635:ARG:HB2	2.30	0.47
1:C:434:ASP:C	1:C:434:ASP:OD1	2.58	0.47
1:C:529:LYS:HA	1:C:532:ASN:HB3	1.98	0.46
1:A:470:VAL:HG12	1:A:471:LYS:N	2.30	0.46
1:C:531:LYS:O	1:C:534:GLY:N	2.46	0.46
1:A:626:GLY:O	1:A:629:LEU:HB2	2.15	0.46
1:A:524:LYS:O	1:A:526:TYR:N	2.48	0.46
1:A:632:ILE:CA	1:A:635:ARG:NH2	2.48	0.46
1:A:529:LYS:HZ1	1:A:629:LEU:HA	1.80	0.46
1:C:523:LEU:O	1:C:526:TYR:CB	2.63	0.46
1:A:510:ILE:HD12	1:A:510:ILE:C	2.41	0.46
1:C:625:ILE:HG22	1:C:629:LEU:HD22	1.98	0.46
1:C:450:HIS:CE1	1:C:452:ILE:HG12	2.51	0.45
1:A:525:ASP:HA	1:A:528:GLU:HG3	1.99	0.45
1:A:532:ASN:C	1:A:534:GLY:N	2.68	0.45
1:C:408:LYS:HA	1:C:635:ARG:CD	2.45	0.45
1:A:585:MET:HG2	1:A:596:LEU:HD23	1.99	0.45
1:C:398:ILE:HG23	1:C:403:VAL:HG11	1.98	0.45
1:A:414:ILE:HD12	1:A:583:VAL:CG1	2.46	0.45
1:C:510:ILE:HD12	1:C:510:ILE:C	2.41	0.45
1:A:523:LEU:O	1:A:524:LYS:C	2.61	0.44
1:C:521:PRO:O	1:C:522:ASN:CB	2.65	0.44
1:C:605:MET:SD	1:C:625:ILE:HD11	2.57	0.44
1:A:522:ASN:HD22	1:A:522:ASN:HA	1.56	0.44
1:A:525:ASP:HB2	1:A:629:LEU:HD23	2.00	0.44
1:C:436:LEU:HD11	1:C:440:TYR:CE2	2.53	0.43
1:C:505:ILE:HD12	1:C:510:ILE:HG12	2.00	0.43
1:C:634:ASN:O	1:C:635:ARG:HG2	2.18	0.43
1:C:521:PRO:C	1:C:522:ASN:HD22	2.27	0.43
1:C:631:LEU:HA	1:C:634:ASN:ND2	2.33	0.43
1:A:486:SER:O	1:A:487:ASP:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:THR:HA	1:C:426:PRO:HD2	1.77	0.42
1:C:529:LYS:HZ2	1:C:629:LEU:CD1	2.25	0.42
1:C:475:GLU:HG2	1:C:476:ILE:N	2.34	0.42
1:C:531:LYS:O	1:C:532:ASN:C	2.62	0.42
1:C:572:ILE:O	1:C:576:LEU:HD13	2.18	0.42
1:C:611:ILE:O	1:C:614:ASN:OD1	2.37	0.42
1:A:386:SER:O	1:A:388:TYR:N	2.51	0.42
1:A:470:VAL:CG1	1:A:471:LYS:N	2.83	0.42
1:A:436:LEU:HD11	1:A:440:TYR:CE2	2.54	0.42
1:A:471:LYS:O	1:A:472:ASP:C	2.63	0.42
1:A:631:LEU:HD23	1:A:631:LEU:C	2.43	0.42
1:C:398:ILE:HD13	1:C:618:ILE:HG12	2.01	0.42
1:A:526:TYR:HE2	1:A:557:ILE:CG1	2.33	0.41
1:C:400:ASN:C	1:C:402:ASN:H	2.28	0.41
1:A:523:LEU:C	1:A:523:LEU:HD22	2.44	0.41
1:C:387:LEU:HG	1:C:404:TYR:OH	2.21	0.41
1:C:510:ILE:HD12	1:C:511:ALA:N	2.34	0.41
1:C:521:PRO:C	1:C:522:ASN:ND2	2.78	0.41
1:C:615:VAL:O	1:C:616:ALA:HB2	2.21	0.41
1:C:482:ARG:HG3	1:C:491:GLU:CG	2.48	0.41
1:A:476:ILE:HG13	1:A:479:ILE:HB	2.03	0.41
1:A:574:GLU:HG2	1:C:598:LEU:CD2	2.51	0.41
1:A:620:LEU:HD23	1:A:620:LEU:HA	1.75	0.41
1:C:573:ILE:O	1:C:577:LYS:HG3	2.21	0.41
1:A:523:LEU:O	1:A:526:TYR:CA	2.68	0.41
1:A:501:ILE:HB	1:A:513:PHE:HB2	2.03	0.41
1:C:410:ILE:HD12	1:C:584:LEU:HB2	2.01	0.41
1:A:450:HIS:HE1	1:A:452:ILE:HG12	1.80	0.41
1:A:482:ARG:HG3	1:A:491:GLU:CG	2.47	0.41
1:A:544:LYS:HE3	1:A:544:LYS:HA	2.02	0.41
1:A:562:SER:O	1:A:564:LEU:HD13	2.20	0.41
1:A:625:ILE:O	1:A:629:LEU:HD22	2.21	0.41
1:A:466:LYS:NZ	3:A:2010:HOH:O	2.54	0.41
1:A:522:ASN:HB3	1:A:523:LEU:H	1.51	0.41
1:C:396:MET:HE1	1:C:631:LEU:HD12	2.02	0.40
1:A:571:ARG:HH12	1:C:615:VAL:CG1	2.30	0.40
1:C:622:SER:O	1:C:623:ASN:HB2	2.21	0.40
1:C:400:ASN:HD21	1:C:402:ASN:HB2	1.85	0.40

There are no symmetry-related clashes.

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	245/263 (93%)	219 (89%)	17 (7%)	9 (4%)	2	3
1	C	245/263 (93%)	217 (89%)	19 (8%)	9 (4%)	2	3
All	All	490/526 (93%)	436 (89%)	36 (7%)	18 (4%)	2	3

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	387	LEU
1	A	533	GLU
1	A	612	SER
1	C	533	GLU
1	C	609	VAL
1	C	612	SER
1	A	523	LEU
1	A	525	ASP
1	A	609	VAL
1	C	386	SER
1	C	522	ASN
1	C	611	ILE
1	A	522	ASN
1	A	614	ASN
1	C	521	PRO
1	C	579	ASN
1	A	401	SER
1	C	476	ILE

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	210/226 (93%)	189 (90%)	21 (10%)	7	16
1	C	210/226 (93%)	192 (91%)	18 (9%)	10	22
All	All	420/452 (93%)	381 (91%)	39 (9%)	8	18

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	401	SER
1	A	410	ILE
1	A	427	ILE
1	A	436	LEU
1	A	476	ILE
1	A	494	LYS
1	A	522	ASN
1	A	523	LEU
1	A	525	ASP
1	A	526	TYR
1	A	531	LYS
1	A	544	LYS
1	A	564	LEU
1	A	571	ARG
1	A	574	GLU
1	A	576	LEU
1	A	598	LEU
1	A	614	ASN
1	A	629	LEU
1	A	631	LEU
1	A	635	ARG
1	C	407	ILE
1	C	425	THR
1	C	466	LYS
1	C	476	ILE
1	C	494	LYS
1	C	496	GLU
1	C	523	LEU
1	C	531	LYS
1	C	544	LYS
1	C	554	GLU
1	C	564	LEU
1	C	571	ARG

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Mol	Chain	Res	Type
1	C	574	GLU
1	C	598	LEU
1	C	629	LEU
1	C	631	LEU
1	C	633	LYS
1	C	635	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	400	ASN
1	A	402	ASN
1	A	522	ASN
1	A	558	GLN
1	A	563	ASN
1	A	581	ASN
1	C	400	ASN
1	C	402	ASN
1	C	522	ASN
1	C	558	GLN
1	C	563	ASN
1	C	581	ASN
1	C	634	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](#)

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	$\# Z > 2$
2	SO4	A	1636	-	4,4,4	0.29	0	6,6,6	0.52	0
2	SO4	C	1636	-	4,4,4	0.17	0	6,6,6	0.48	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	249/263 (94%)	-0.06	6 (2%) 59 54	34, 52, 73, 84	0
1	C	249/263 (94%)	-0.02	8 (3%) 50 44	31, 52, 74, 83	0
All	All	498/526 (94%)	-0.04	14 (2%) 55 49	31, 52, 74, 84	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	526	TYR	3.7
1	C	615	VAL	3.5
1	C	526	TYR	3.5
1	C	612	SER	3.0
1	A	522	ASN	3.0
1	A	615	VAL	2.6
1	A	533	GLU	2.5
1	C	533	GLU	2.5
1	A	496	GLU	2.4
1	C	496	GLU	2.3
1	C	616	ALA	2.2
1	C	384	ALA	2.2
1	C	495	ALA	2.2
1	A	614	ASN	2.1

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
2	SO4	A	1636	5/5	0.97	0.11	47,48,52,54	0
2	SO4	C	1636	5/5	0.98	0.10	48,48,52,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.