



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 01:18 AM GMT

PDB ID : 1BMT
Title : HOW A PROTEIN BINDS B12: A 3.0 ANGSTROM X-RAY STRUCTURE
OF THE B12-BINDING DOMAINS OF METHIONINE SYNTHASE
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Deposited on : 1994-09-02
Resolution : 3.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

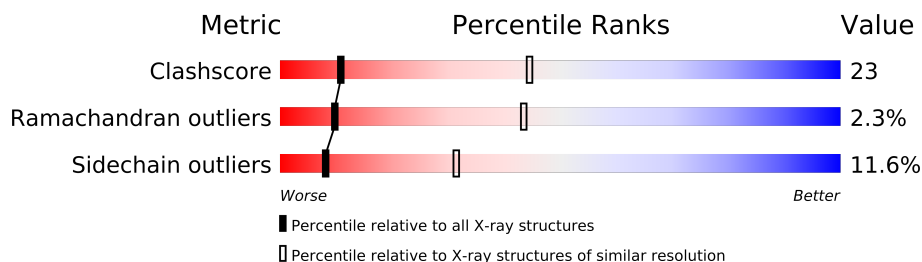
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : NOT EXECUTED
EDS : NOT EXECUTED
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.00 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))
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	246	
1	B	246	

2 Entry composition i

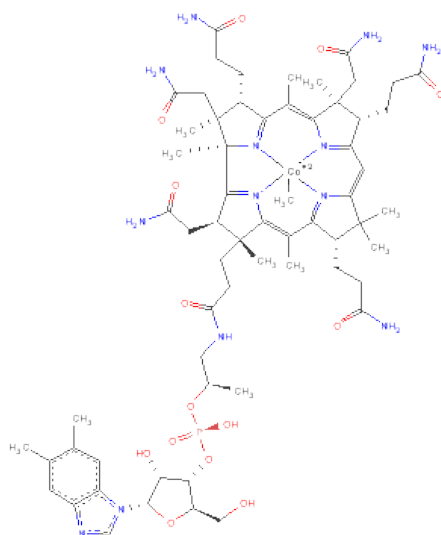
There are 3 unique types of molecules in this entry. The entry contains 4000 atoms, of which 0 are hydrogen and 0 are deuterium.

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 METHIONINE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1907	1198	332	368	9			
1	B	246	Total	C	N	O	S	0	0	0
			1907	1198	332	368	9			

- Molecule 2 is CO-METHYLCOBALAMIN (three-letter code: COB) (formula: $C_{63}H_{91}CoN_{13}O_{14}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Co	N	O	P	0
			92	63	1	13	14	1	
2	B	1	Total	C	Co	N	O	P	0
			92	63	1	13	14	1	

- Molecule 3 is water.

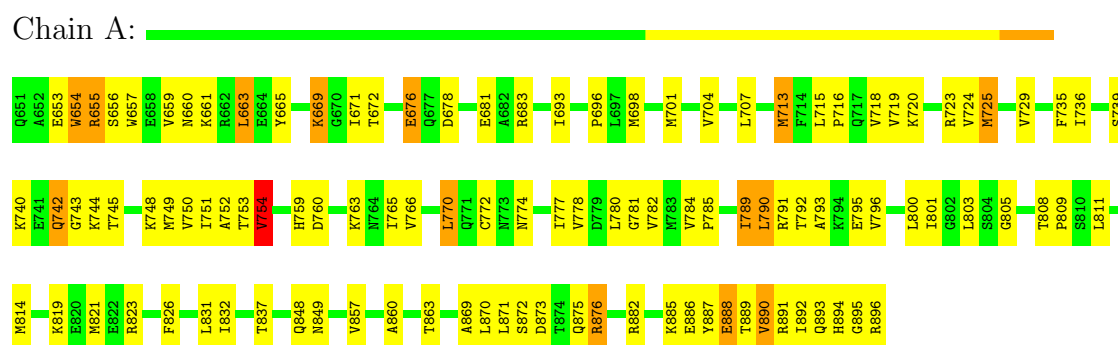
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	O 1	0	0
3	B	1	Total 1	O 1	0	0

3 Residue-property plots

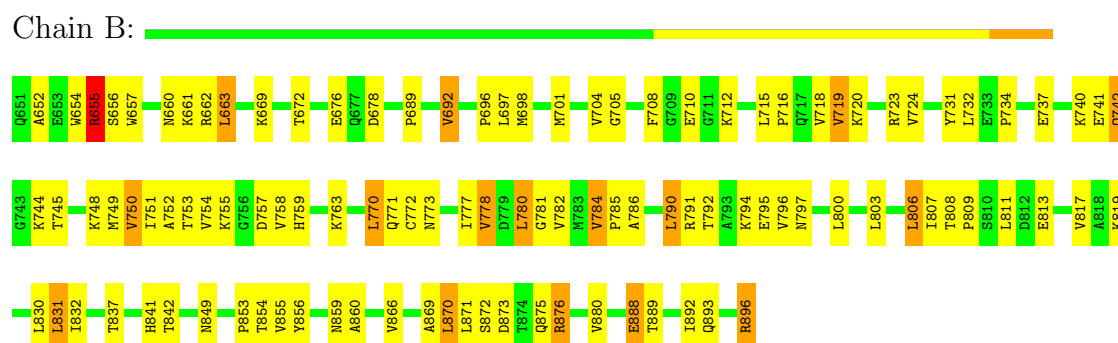
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: METHIONINE SYNTHASE



• Molecule 1: METHIONINE SYNTHASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.70Å 55.30Å 103.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.170 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4000	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.55	0/1933	0.74	0/2611
1	B	0.58	0/1933	0.75	0/2611
All	All	0.57	0/3866	0.74	0/5222

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	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
1	A	823	ARG	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1907	0	1939	82	0
1	B	1907	0	1939	84	0
2	A	92	0	78	16	0
2	B	92	0	80	22	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	4000	0	4036	183	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 23.

All (183) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:122:COB:C1	2:B:122:COB:C20	1.74	1.59
2:A:122:COB:O2	2:A:122:COB:C3R	1.65	1.42
2:B:122:COB:H362	2:B:122:COB:H351	1.59	0.84
1:B:791:ARG:O	1:B:794:LYS:HG2	1.81	0.80
1:A:752:ALA:HB1	1:A:784:VAL:HG11	1.63	0.79
1:A:748:LYS:HD3	1:A:796:VAL:HG12	1.63	0.79
1:B:752:ALA:HB1	1:B:784:VAL:CG1	2.13	0.78
2:B:122:COB:C2	2:B:122:COB:C20	2.61	0.78
1:B:748:LYS:HD3	1:B:796:VAL:HG12	1.67	0.76
1:A:808:THR:HG23	1:B:893:GLN:HG2	1.66	0.76
1:B:753:THR:HB	1:B:782:VAL:HA	1.68	0.76
1:A:869:ALA:HA	1:A:875:GLN:HE21	1.51	0.75
1:B:752:ALA:HB1	1:B:784:VAL:HG11	1.70	0.74
2:B:122:COB:N21	2:B:122:COB:C20	2.48	0.73
1:A:725:MET:O	1:A:729:VAL:HG23	1.88	0.73
1:B:794:LYS:CG	1:B:795:GLU:N	2.52	0.72
1:B:749:MET:HE3	1:B:751:ILE:HD12	1.72	0.72
2:A:122:COB:H552	2:A:122:COB:H531	1.71	0.72
1:B:808:THR:HB	1:B:809:PRO:HD3	1.71	0.71
2:A:122:COB:H351	2:A:122:COB:H362	1.72	0.71
1:B:660:ASN:OD1	1:B:696:PRO:CG	2.39	0.70
1:A:780:LEU:HD11	1:A:792:THR:HG21	1.74	0.70
1:A:698:MET:HE1	2:A:122:COB:H5R2	1.75	0.69
2:A:122:COB:C3R	2:A:122:COB:P	2.81	0.68
1:A:720:LYS:HG2	1:A:723:ARG:HH12	1.58	0.68
1:A:707:LEU:HB3	1:A:713:MET:HG3	1.76	0.68
1:B:660:ASN:OD1	1:B:696:PRO:HG3	1.93	0.68
1:B:770:LEU:HB3	1:B:777:ILE:HD11	1.76	0.67
1:A:736:ILE:O	1:A:739:SER:HB3	1.95	0.67
1:A:752:ALA:HB1	1:A:784:VAL:CG1	2.27	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:794:LYS:HG2	1:B:795:GLU:H	1.61	0.65
1:A:754:VAL:HG23	1:A:803:LEU:HD22	1.79	0.65
1:A:718:VAL:HG13	2:A:122:COB:H462	1.80	0.64
1:B:698:MET:HE1	2:B:122:COB:H5R2	1.80	0.64
1:A:753:THR:OG1	1:A:763:LYS:HD3	1.96	0.64
1:B:654:TRP:HA	1:B:657:TRP:CE2	2.32	0.63
1:A:693:ILE:HG21	1:A:765:ILE:HD13	1.81	0.63
1:B:754:VAL:HG23	1:B:803:LEU:HD22	1.79	0.63
1:B:869:ALA:HA	1:B:875:GLN:HE21	1.63	0.63
2:A:122:COB:H3	2:A:122:COB:O28	1.99	0.62
1:B:716:PRO:O	1:B:719:VAL:HG12	2.00	0.62
1:B:819:LYS:HG3	1:B:849:ASN:HB3	1.81	0.62
1:A:740:LYS:NZ	1:A:742:GLN:HB2	2.14	0.62
1:A:893:GLN:HG2	1:B:808:THR:HG23	1.83	0.61
1:A:793:ALA:CB	1:A:801:ILE:HD11	2.32	0.60
1:B:889:THR:O	1:B:892:ILE:HB	2.01	0.59
1:A:748:LYS:HD3	1:A:796:VAL:CG1	2.31	0.59
1:A:742:GLN:HB3	1:A:774:ASN:OD1	2.03	0.59
1:B:749:MET:CE	1:B:751:ILE:HD12	2.33	0.58
1:A:832:ILE:HG22	1:A:837:THR:HG21	1.86	0.58
1:B:889:THR:HA	1:B:892:ILE:HD12	1.85	0.58
1:A:654:TRP:HA	1:A:657:TRP:CE2	2.39	0.58
2:B:122:COB:C25	2:B:122:COB:C20	2.82	0.57
1:B:811:LEU:HD12	1:B:841:HIS:CE1	2.38	0.57
1:A:887:TYR:HA	1:A:890:VAL:CG1	2.34	0.57
1:A:750:VAL:CG1	1:A:801:ILE:HG12	2.35	0.57
1:B:794:LYS:NZ	1:B:795:GLU:HG3	2.19	0.57
2:B:122:COB:C19	2:B:122:COB:C20	2.74	0.56
1:A:750:VAL:HG13	1:A:801:ILE:HG12	1.87	0.56
1:A:857:VAL:HG11	1:A:863:THR:HA	1.87	0.56
2:B:122:COB:H8	2:B:122:COB:N40	2.21	0.56
1:A:693:ILE:CG2	1:A:765:ILE:HD13	2.35	0.56
1:B:832:ILE:HG22	1:B:837:THR:HG21	1.87	0.56
1:B:794:LYS:HG3	1:B:795:GLU:N	2.21	0.55
1:B:780:LEU:HD11	1:B:792:THR:HG21	1.88	0.55
1:B:698:MET:CE	2:B:122:COB:H5R2	2.36	0.55
1:B:718:VAL:HG13	2:B:122:COB:H462	1.87	0.54
1:B:853:PRO:HG3	1:B:880:VAL:HG21	1.90	0.54
1:B:698:MET:SD	2:B:122:COB:H3P2	2.48	0.54
1:A:748:LYS:CD	1:A:796:VAL:HG12	2.36	0.54
1:A:663:LEU:CD1	1:A:678:ASP:HB3	2.38	0.54
1:A:760:ASP:HB2	1:A:763:LYS:HE2	1.88	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:888:GLU:O	1:A:892:ILE:HG13	2.08	0.54
1:B:744:LYS:HD3	1:B:745:THR:HG22	1.88	0.54
1:A:753:THR:HB	1:A:782:VAL:HA	1.90	0.54
1:A:765:ILE:HD12	2:A:122:COB:H3P1	1.89	0.54
1:A:720:LYS:HG2	1:A:723:ARG:NH1	2.22	0.53
1:A:872:SER:O	1:A:876:ARG:HB2	2.08	0.53
1:A:770:LEU:HB3	1:A:777:ILE:HD11	1.90	0.53
1:A:808:THR:HB	1:A:809:PRO:HD3	1.91	0.53
1:B:786:ALA:O	1:B:790:LEU:HD22	2.09	0.53
1:B:860:ALA:H	2:B:122:COB:H5R1	1.75	0.52
1:A:791:ARG:O	1:A:795:GLU:HG3	2.09	0.52
1:A:698:MET:CE	2:A:122:COB:H5R2	2.38	0.52
1:A:869:ALA:HA	1:A:875:GLN:NE2	2.23	0.52
1:A:793:ALA:HB2	1:A:801:ILE:HD11	1.91	0.52
1:B:663:LEU:CD1	1:B:678:ASP:HB3	2.40	0.52
1:B:813:GLU:O	1:B:817:VAL:HG13	2.09	0.52
1:A:790:LEU:HG	1:A:826:PHE:CE1	2.45	0.51
2:B:122:COB:H552	2:B:122:COB:H531	1.92	0.51
2:B:122:COB:H253	2:B:122:COB:C20	2.40	0.51
2:B:122:COB:H262	2:B:122:COB:H601	1.92	0.51
2:A:122:COB:O2	2:A:122:COB:C4R	2.53	0.51
1:B:654:TRP:HZ3	1:B:662:ARG:HB3	1.76	0.51
1:B:758:VAL:HG12	2:B:122:COB:H421	1.93	0.51
1:A:886:GLU:O	1:A:890:VAL:HG12	2.12	0.50
1:A:740:LYS:HZ1	1:A:742:GLN:HB2	1.75	0.50
1:B:794:LYS:HZ2	1:B:795:GLU:HG3	1.77	0.50
1:B:704:VAL:CG1	1:B:718:VAL:HG23	2.42	0.49
1:A:716:PRO:O	1:A:719:VAL:HG12	2.12	0.49
1:A:744:LYS:HG3	1:A:745:THR:H	1.77	0.49
1:A:873:ASP:HA	1:A:876:ARG:NH1	2.27	0.49
1:A:665:TYR:HE1	1:A:671:ILE:HD11	1.77	0.49
1:B:672:THR:HG22	1:B:724:VAL:HG22	1.94	0.48
1:A:752:ALA:CB	1:A:784:VAL:HG11	2.39	0.48
1:A:657:TRP:HB3	1:A:661:LYS:HD3	1.94	0.48
1:B:873:ASP:HA	1:B:876:ARG:NH1	2.28	0.48
1:A:654:TRP:CD1	1:A:654:TRP:N	2.82	0.48
1:A:672:THR:HG22	1:A:724:VAL:HG22	1.96	0.47
1:B:660:ASN:OD1	1:B:696:PRO:HG2	2.14	0.47
1:B:842:THR:HG21	1:B:856:TYR:HB2	1.96	0.47
1:A:763:LYS:O	1:A:766:VAL:HG12	2.14	0.47
1:A:716:PRO:C	1:A:719:VAL:HG12	2.35	0.47
1:B:652:ALA:O	1:B:655:ARG:HB2	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:831:LEU:HD12	1:B:855:VAL:HB	1.95	0.47
1:B:654:TRP:CZ3	1:B:662:ARG:HB3	2.49	0.47
1:A:860:ALA:H	2:A:122:COB:H5R1	1.80	0.47
1:A:790:LEU:HD11	1:A:821:MET:HG2	1.96	0.47
1:B:784:VAL:HA	1:B:785:PRO:HD3	1.73	0.46
1:A:759:HIS:CE1	2:A:122:COB:H412	2.51	0.46
1:A:676:GLU:HG2	1:A:676:GLU:H	1.55	0.46
1:A:805:GLY:HA3	1:A:814:MET:CE	2.46	0.45
1:A:749:MET:CE	1:A:751:ILE:HD12	2.46	0.45
1:B:896:ARG:HD3	1:B:896:ARG:O	2.16	0.45
2:A:122:COB:H262	2:A:122:COB:H601	1.97	0.45
1:A:759:HIS:NE2	2:A:122:COB:H202	2.31	0.45
1:A:665:TYR:CE1	1:A:669:LYS:HG3	2.50	0.45
1:B:831:LEU:CD1	1:B:855:VAL:HB	2.47	0.45
1:B:859:ASN:HB2	2:B:122:COB:H5R1	1.99	0.45
1:B:771:GLN:C	1:B:773:ASN:H	2.20	0.45
1:B:692:VAL:CG2	1:B:732:LEU:HD11	2.46	0.45
1:A:857:VAL:HB	2:A:122:COB:HM61	1.98	0.45
1:B:866:VAL:HG12	1:B:870:LEU:HD22	1.97	0.45
1:A:659:VAL:HG21	1:A:681:GLU:HB3	1.98	0.45
1:A:660:ASN:OD1	1:A:696:PRO:CG	2.65	0.45
1:B:741:GLU:C	1:B:742:GLN:HG3	2.38	0.45
1:B:731:TYR:O	1:B:734:PRO:HD2	2.16	0.44
1:B:759:HIS:HE1	2:B:122:COB:H412	1.82	0.44
1:A:805:GLY:HA3	1:A:814:MET:HE1	1.99	0.44
1:B:753:THR:HG22	1:B:757:ASP:HB3	2.00	0.44
1:B:752:ALA:HB1	1:B:784:VAL:HG13	1.98	0.44
1:A:872:SER:HB3	1:A:875:GLN:HB2	1.98	0.44
1:B:754:VAL:HG13	1:B:755:LYS:N	2.32	0.44
1:A:660:ASN:OD1	1:A:696:PRO:HG3	2.18	0.44
2:B:122:COB:O28	2:B:122:COB:H3	2.17	0.43
1:B:720:LYS:O	1:B:723:ARG:HG2	2.18	0.43
2:B:122:COB:N62	2:B:122:COB:H252	2.34	0.43
1:A:715:LEU:O	1:A:718:VAL:HG12	2.19	0.43
1:B:796:VAL:O	1:B:797:ASN:HB2	2.19	0.43
1:A:754:VAL:CG2	1:A:803:LEU:HD22	2.48	0.43
1:A:784:VAL:HG13	1:A:789:ILE:HD11	2.01	0.43
1:B:755:LYS:HB3	1:B:813:GLU:HG3	2.01	0.43
1:B:753:THR:HG21	1:B:759:HIS:O	2.19	0.42
1:B:654:TRP:C	1:B:656:SER:H	2.22	0.42
1:A:882:ARG:HE	1:B:710:GLU:CD	2.22	0.42
1:B:830:LEU:O	1:B:854:THR:HA	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:806:LEU:HD23	2:B:122:COB:H201	2.01	0.42
1:B:888:GLU:O	1:B:892:ILE:HG13	2.19	0.42
1:A:718:VAL:CG1	2:A:122:COB:H462	2.49	0.42
1:B:763:LYS:HB3	1:B:763:LYS:HE2	1.88	0.42
1:B:692:VAL:HG21	1:B:732:LEU:HD11	2.01	0.42
1:B:712:LYS:HE2	1:B:712:LYS:HB3	1.89	0.42
1:B:750:VAL:HA	1:B:778:VAL:O	2.20	0.41
1:A:893:GLN:C	1:A:895:GLY:H	2.23	0.41
1:B:831:LEU:HD12	1:B:831:LEU:HA	1.92	0.41
1:B:763:LYS:HZ2	1:B:781:GLY:HA2	1.86	0.41
1:B:715:LEU:O	1:B:718:VAL:HG12	2.20	0.41
1:A:704:VAL:CG1	1:A:718:VAL:HG23	2.50	0.41
1:B:872:SER:HB3	1:B:875:GLN:HB2	2.03	0.41
1:A:819:LYS:HG3	1:A:849:ASN:HB3	2.02	0.41
2:B:122:COB:H541	2:B:122:COB:H602	1.98	0.41
1:A:683:ARG:NH2	1:A:735:PHE:CE1	2.88	0.41
1:B:790:LEU:N	1:B:790:LEU:HD13	2.35	0.41
1:A:889:THR:HA	1:A:892:ILE:HD12	2.02	0.40
1:A:891:ARG:HB3	1:A:896:ARG:HD2	2.03	0.40
1:B:807:ILE:HD13	1:B:807:ILE:HG21	1.82	0.40
1:A:784:VAL:HA	1:A:785:PRO:HD3	1.82	0.40
1:A:796:VAL:HG12	1:A:796:VAL:O	2.21	0.40
1:B:657:TRP:HB3	1:B:661:LYS:HD3	2.02	0.40
1:B:705:GLY:O	1:B:708:PHE:HB3	2.21	0.40
1:A:763:LYS:NZ	1:A:781:GLY:HA2	2.36	0.40
1:B:794:LYS:HZ3	1:B:795:GLU:CG	2.34	0.40
1:B:803:LEU:HD11	1:B:817:VAL:HG22	2.04	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	244/246 (99%)	225 (92%)	11 (4%)	8 (3%)	6 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	244/246 (99%)	218 (89%)	23 (9%)	3 (1%)	19	64
All	All	488/492 (99%)	443 (91%)	34 (7%)	11 (2%)	10	43

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	740	LYS
1	A	848	GLN
1	A	876	ARG
1	A	655	ARG
1	A	742	GLN
1	A	743	GLY
1	A	754	VAL
1	B	655	ARG
1	B	876	ARG
1	A	654	TRP
1	A	894	HIS

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	207/207 (100%)	184 (89%)	23 (11%)	9	34
1	B	207/207 (100%)	182 (88%)	25 (12%)	7	29
All	All	414/414 (100%)	366 (88%)	48 (12%)	8	31

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	653	GLU
1	A	655	ARG
1	A	656	SER
1	A	663	LEU
1	A	669	LYS
1	A	676	GLU
1	A	701	MET

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Mol	Chain	Res	Type
1	A	713	MET
1	A	725	MET
1	A	754	VAL
1	A	770	LEU
1	A	772	CYS
1	A	778	VAL
1	A	789	ILE
1	A	790	LEU
1	A	800	LEU
1	A	811	LEU
1	A	831	LEU
1	A	870	LEU
1	A	871	LEU
1	A	885	LYS
1	A	888	GLU
1	A	890	VAL
1	B	655	ARG
1	B	663	LEU
1	B	669	LYS
1	B	676	GLU
1	B	689	PRO
1	B	692	VAL
1	B	697	LEU
1	B	701	MET
1	B	719	VAL
1	B	737	GLU
1	B	742	GLN
1	B	750	VAL
1	B	770	LEU
1	B	772	CYS
1	B	778	VAL
1	B	780	LEU
1	B	784	VAL
1	B	790	LEU
1	B	800	LEU
1	B	806	LEU
1	B	831	LEU
1	B	870	LEU
1	B	871	LEU
1	B	888	GLU
1	B	896	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	685	GLN
1	A	771	GLN
1	A	816	ASN
1	A	841	HIS
1	A	875	GLN
1	B	685	GLN
1	B	771	GLN
1	B	774	ASN
1	B	816	ASN
1	B	841	HIS
1	B	875	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	COB	A	122	1	102,102,102	2.93	44 (43%)	149,170,170	2.28	49 (32%)
2	COB	B	122	1	102,102,102	3.15	46 (45%)	149,170,170	2.71	44 (29%)

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	COB	A	122	1	-	0/56/231/231	0/1/11/11
2	COB	B	122	1	-	0/56/231/231	0/1/11/11

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	122	COB	O6R-C1R	14.25	1.63	1.41
2	B	122	COB	C1-N21	-10.21	1.32	1.50
2	B	122	COB	CO-N21	-9.57	1.84	1.90
2	B	122	COB	C4B-C9B	9.44	1.53	1.41
2	B	122	COB	C20-C1	8.78	1.74	1.52
2	B	122	COB	O6R-C1R	7.68	1.53	1.41
2	B	122	COB	C2-C3	-7.47	1.46	1.58
2	A	122	COB	C53-C15	7.43	1.69	1.51
2	A	122	COB	C1-N21	-6.73	1.38	1.50
2	A	122	COB	O2-C3R	6.67	1.65	1.44
2	B	122	COB	C1-C19	-6.26	1.43	1.51
2	B	122	COB	O2-C3R	5.68	1.62	1.44
2	A	122	COB	C2-C3	-5.64	1.49	1.58
2	B	122	COB	C5M-C5B	-5.45	1.39	1.51
2	A	122	COB	C41-C8	-5.29	1.45	1.53
2	B	122	COB	C37-C38	-5.29	1.32	1.51
2	A	122	COB	C5M-C5B	-4.91	1.40	1.51
2	A	122	COB	C4B-C9B	4.85	1.47	1.41
2	B	122	COB	C6M-C6B	4.47	1.60	1.51
2	B	122	COB	C41-C8	-4.39	1.46	1.53
2	A	122	COB	C19-N24	4.16	1.44	1.33
2	A	122	COB	C7B-C6B	4.13	1.49	1.37
2	B	122	COB	CO-N22	-4.07	1.85	1.97
2	A	122	COB	C49-C50	-4.05	1.34	1.51
2	A	122	COB	C20-C1	4.05	1.62	1.52
2	B	122	COB	C1P-C2P	-4.02	1.40	1.51
2	A	122	COB	C48-C13	-3.97	1.47	1.53
2	A	122	COB	C50-N52	-3.79	1.20	1.32
2	B	122	COB	C13-C14	3.75	1.60	1.52
2	A	122	COB	C8-C9	-3.70	1.45	1.52
2	A	122	COB	C6M-C6B	3.59	1.58	1.51
2	B	122	COB	C11-C10	-3.57	1.34	1.41
2	A	122	COB	C1-C19	-3.56	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	122	COB	O8R-C5R	-3.54	1.26	1.42
2	B	122	COB	C56-C57	-3.54	1.44	1.51
2	A	122	COB	O6R-C4R	-3.50	1.36	1.45
2	B	122	COB	C4B-C5B	3.49	1.47	1.37
2	A	122	COB	C4B-C5B	3.43	1.47	1.37
2	B	122	COB	C17-C18	-3.41	1.49	1.55
2	B	122	COB	C42-C43	3.38	1.65	1.51
2	B	122	COB	C8-C9	-3.37	1.46	1.52
2	B	122	COB	C19-N24	3.37	1.42	1.33
2	B	122	COB	C30-C3	-3.28	1.48	1.53
2	A	122	COB	C7B-C8B	3.22	1.47	1.40
2	A	122	COB	C30-C3	-3.18	1.48	1.53
2	B	122	COB	C50-N52	-3.11	1.22	1.32
2	A	122	COB	C32-N33	-3.11	1.22	1.32
2	A	122	COB	CO-N21	3.08	1.93	1.90
2	A	122	COB	C35-C5	3.06	1.58	1.51
2	A	122	COB	C5R-C4R	-3.02	1.41	1.52
2	B	122	COB	O8R-C5R	-3.00	1.29	1.42
2	A	122	COB	C26-C27	-2.99	1.40	1.51
2	B	122	COB	P-O5	-2.98	1.41	1.55
2	B	122	COB	C5R-C4R	-2.97	1.41	1.52
2	A	122	COB	C47-C12	2.97	1.60	1.54
2	A	122	COB	C56-C57	2.95	1.57	1.51
2	A	122	COB	C43-N45	-2.93	1.23	1.32
2	B	122	COB	C43-N45	-2.92	1.23	1.32
2	A	122	COB	C4-N21	-2.89	1.23	1.31
2	B	122	COB	C7B-C8B	2.88	1.46	1.40
2	A	122	COB	C8B-C9B	2.82	1.46	1.40
2	A	122	COB	C25-C2	2.81	1.60	1.54
2	B	122	COB	C7-C6	2.78	1.59	1.52
2	B	122	COB	C35-C5	2.77	1.57	1.51
2	B	122	COB	C49-C50	-2.76	1.39	1.51
2	A	122	COB	C17-C18	-2.74	1.50	1.55
2	B	122	COB	O6R-C4R	-2.74	1.38	1.45
2	B	122	COB	C38-N40	-2.72	1.23	1.32
2	A	122	COB	C27-N29	-2.72	1.23	1.32
2	A	122	COB	C37-C38	2.66	1.61	1.51
2	A	122	COB	C61-N62	-2.61	1.24	1.32
2	B	122	COB	C12-C13	-2.57	1.47	1.55
2	A	122	COB	C11-C10	-2.54	1.36	1.41
2	B	122	COB	C41-C42	-2.51	1.44	1.52
2	A	122	COB	C16-N24	-2.48	1.26	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	122	COB	C12-C13	-2.47	1.47	1.55
2	B	122	COB	C61-N62	-2.43	1.24	1.32
2	B	122	COB	C7-C8	-2.41	1.51	1.55
2	A	122	COB	C6B-C5B	2.37	1.47	1.40
2	A	122	COB	C41-C42	-2.31	1.45	1.52
2	B	122	COB	C30-C31	-2.30	1.45	1.52
2	B	122	COB	C53-C15	2.25	1.56	1.51
2	B	122	COB	C2R-C1R	2.22	1.56	1.53
2	A	122	COB	C1-C2	2.14	1.61	1.56
2	B	122	COB	C2B-N1B	-2.10	1.33	1.36
2	A	122	COB	C12-C11	2.10	1.57	1.52
2	B	122	COB	C7B-C6B	2.09	1.43	1.37
2	B	122	COB	CO-C1A	2.07	2.08	1.98
2	B	122	COB	C9-N22	2.06	1.43	1.34
2	B	122	COB	C9-C10	-2.03	1.34	1.43

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	122	COB	O6R-C1R-N1B	14.88	122.28	108.44
2	B	122	COB	C19-C1-N21	-10.51	99.55	105.78
2	B	122	COB	O58-C57-C56	-7.81	106.39	121.92
2	A	122	COB	C35-C5-C4	-7.61	107.62	118.64
2	A	122	COB	C35-C5-C6	6.65	128.26	118.64
2	B	122	COB	C56-C57-N59	6.44	128.21	116.50
2	A	122	COB	C18-C19-N24	-6.34	94.12	109.44
2	B	122	COB	C56-C55-C17	6.10	128.40	115.47
2	A	122	COB	C54-C17-C55	-5.93	99.17	109.14
2	B	122	COB	C53-C15-C16	5.61	126.75	118.64
2	A	122	COB	C6-N22-C9	5.59	118.78	107.34
2	B	122	COB	C18-C19-N24	-5.55	96.03	109.44
2	B	122	COB	C20-C1-C19	5.53	118.89	109.51
2	A	122	COB	C2-C1-N21	-5.49	98.25	101.05
2	A	122	COB	C7-C6-N22	-5.14	99.07	110.90
2	B	122	COB	O3-C2P-C1P	-4.82	96.23	106.77
2	A	122	COB	O58-C57-C56	-4.81	112.35	121.92
2	A	122	COB	O6R-C1R-C2R	-4.72	99.53	106.77
2	B	122	COB	O39-C38-C37	-4.57	106.36	122.02
2	A	122	COB	O39-C38-C37	-4.51	106.56	122.02
2	B	122	COB	C20-C1-C2	-4.45	102.54	116.07
2	B	122	COB	C53-C15-C14	-4.44	112.20	118.64
2	B	122	COB	C4R-O6R-C1R	-4.43	104.94	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	122	COB	C9-C10-C11	-4.43	120.99	132.53
2	A	122	COB	O3-C2P-C1P	-4.37	97.21	106.77
2	B	122	COB	C7-C8-C9	-4.28	95.69	100.77
2	B	122	COB	C7-C6-N22	-4.26	101.08	110.90
2	B	122	COB	C2-C1-N21	4.22	103.20	101.05
2	A	122	COB	C4R-O6R-C1R	4.16	114.26	109.75
2	B	122	COB	C8-C7-C6	4.13	108.42	100.98
2	A	122	COB	C17-C16-N24	-4.09	101.49	110.90
2	B	122	COB	O6R-C4R-C5R	3.86	117.40	109.15
2	B	122	COB	O28-C27-C26	-3.82	108.94	122.02
2	A	122	COB	O39-C38-N40	3.75	133.48	122.47
2	A	122	COB	C2R-C1R-N1B	3.73	122.85	113.27
2	A	122	COB	O7R-C2R-C3R	-3.70	100.31	111.20
2	B	122	COB	O6R-C4R-C3R	3.63	113.13	104.88
2	A	122	COB	O2-P-O3	-3.55	94.19	104.37
2	B	122	COB	C37-C38-N40	3.54	129.05	116.58
2	A	122	COB	C1-N21-C4	3.54	123.41	111.55
2	A	122	COB	C54-C17-C18	3.51	119.06	112.01
2	B	122	COB	C17-C18-C19	3.50	108.37	103.02
2	B	122	COB	C31-C30-C3	-3.38	103.73	114.84
2	A	122	COB	C25-C2-C3	3.37	121.72	115.57
2	B	122	COB	O28-C27-N29	3.32	132.19	122.47
2	B	122	COB	O8R-C5R-C4R	-3.27	100.11	111.36
2	A	122	COB	C9-C10-C11	-3.24	124.09	132.53
2	B	122	COB	O51-C50-C49	-3.23	111.61	121.06
2	A	122	COB	C17-C18-C19	3.22	107.94	103.02
2	A	122	COB	C20-C1-C2	-3.16	106.45	116.07
2	B	122	COB	C20-C1-N21	-3.15	107.43	110.47
2	B	122	COB	C60-C61-N62	-3.11	108.38	116.10
2	B	122	COB	O44-C43-N45	-3.10	113.40	122.47
2	B	122	COB	C17-C16-N24	-3.09	103.79	110.90
2	A	122	COB	C20-C1-C19	-3.02	104.40	109.51
2	A	122	COB	C8-C7-C6	2.93	106.26	100.98
2	B	122	COB	C49-C48-C13	-2.86	105.43	114.84
2	A	122	COB	C1-C2-C3	2.71	105.27	101.58
2	B	122	COB	C54-C17-C18	2.70	117.45	112.01
2	A	122	COB	C56-C57-N59	2.68	121.38	116.50
2	A	122	COB	C19-C1-N21	2.68	107.37	105.78
2	A	122	COB	C1R-N1B-C8B	-2.60	121.67	125.85
2	B	122	COB	C5B-C4B-C9B	-2.56	116.61	120.91
2	A	122	COB	C25-C2-C26	-2.54	104.24	109.59
2	A	122	COB	C36-C7-C8	2.53	117.05	112.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	122	COB	O63-C61-C60	-2.52	114.75	120.88
2	A	122	COB	O8R-C5R-C4R	-2.49	102.78	111.36
2	A	122	COB	C7-C8-C9	-2.48	97.83	100.77
2	B	122	COB	C35-C5-C4	-2.44	115.11	118.64
2	A	122	COB	C20-C1-N21	2.43	112.82	110.47
2	A	122	COB	C13-C14-C15	-2.39	122.49	131.83
2	A	122	COB	C15-C14-N23	2.39	129.07	124.77
2	A	122	COB	C53-C15-C16	2.36	122.05	118.64
2	A	122	COB	C10-C9-N22	2.35	129.45	123.43
2	A	122	COB	C3P-C2P-C1P	-2.34	106.21	111.28
2	A	122	COB	C14-N23-C11	2.34	112.13	107.34
2	B	122	COB	C42-C43-N45	2.30	123.90	116.51
2	A	122	COB	C5-C6-N22	2.29	129.45	124.99
2	A	122	COB	O6R-C1R-N1B	2.28	110.56	108.44
2	A	122	COB	C41-C8-C7	2.27	120.72	114.23
2	B	122	COB	C7-C6-C5	2.26	132.56	125.07
2	A	122	COB	C2P-C1P-N59	2.24	116.53	112.98
2	B	122	COB	C6M-C6B-C5B	2.22	125.88	120.74
2	B	122	COB	C3-C4-C5	-2.18	123.31	131.83
2	A	122	COB	C3R-C2R-C1R	2.18	105.17	99.98
2	A	122	COB	C60-C18-C17	-2.16	112.58	118.73
2	B	122	COB	O51-C50-N52	2.12	128.69	122.47
2	B	122	COB	C2-C26-C27	2.10	121.43	115.21
2	A	122	COB	C2B-N1B-C1R	2.09	130.50	126.38
2	B	122	COB	C41-C42-C43	-2.08	105.59	112.60
2	A	122	COB	C3-C4-C5	-2.08	123.72	131.83
2	B	122	COB	P-O3-C2P	2.02	127.48	119.41
2	B	122	COB	C60-C18-C17	-2.01	113.03	118.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.