



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:35 PM UTC

PDB ID : 1N8W / pdb_00001n8w
Title : Biochemical and Structural Studies of Malate Synthase from Mycobacterium tuberculosis
Authors : Smith, C.V.; Huang, C.C.; Miczak, A.; Russell, D.G.; Sacchettini, J.C.; Honer zu Bentrup, K.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2002-11-21
Resolution : 2.70 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

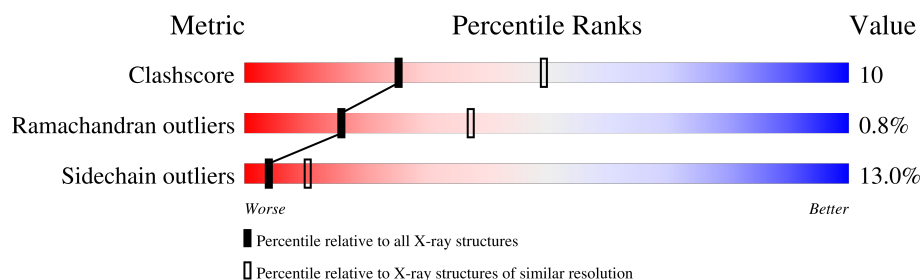
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	741	
1	B	741	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MLT	A	901	X	-	X	-
4	MLT	A	902	X	-	-	-
4	MLT	B	1902	X	-	-	-
6	GLV	B	1901	-	X	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 11696 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 Probable malate synthase G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	718	Total	C	N	O	S	0	0	0
			5486	3448	964	1052	22			
1	B	715	Total	C	N	O	S	0	0	0
			5474	3441	964	1047	22			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

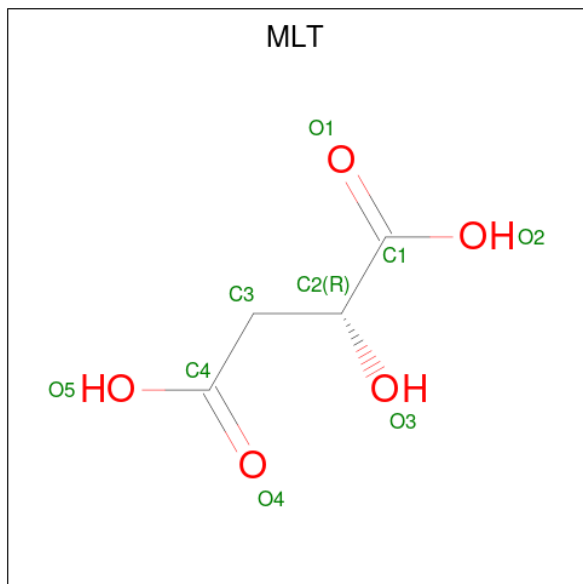
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



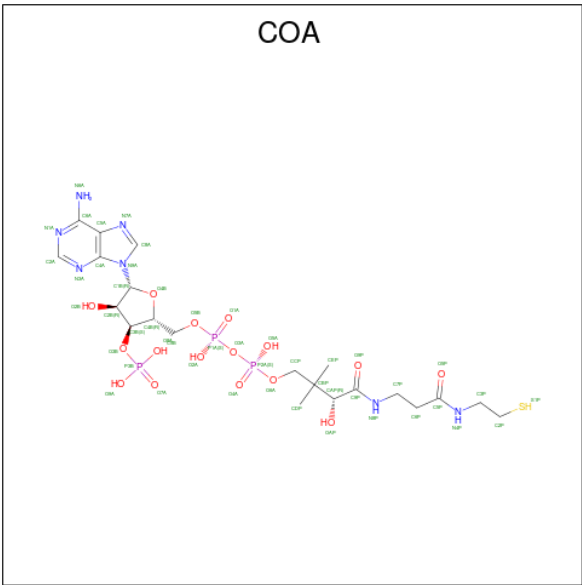
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is D-MALATE (CCD ID: MLT) (formula: $C_4H_6O_5$).



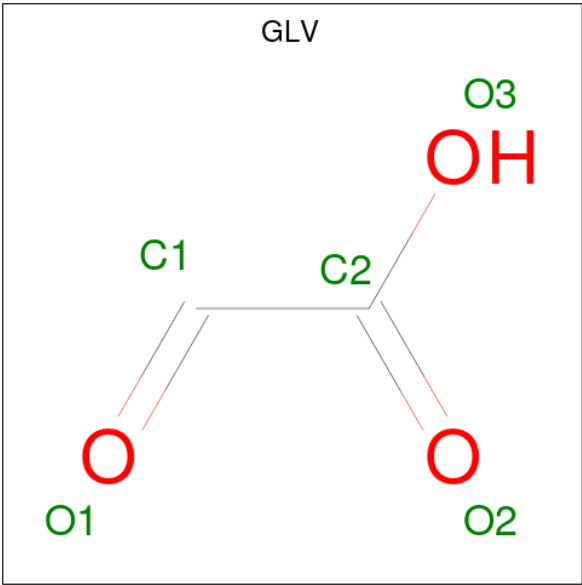
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			9	4	5		
4	A	1	Total	C	O	0	0
			9	4	5		
4	B	1	Total	C	O	0	0
			9	4	5		

- Molecule 5 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 6 is GLYOXYLIC ACID (CCD ID: GLV) (formula: C₂H₂O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			5	2	3		

- Molecule 7 is water.

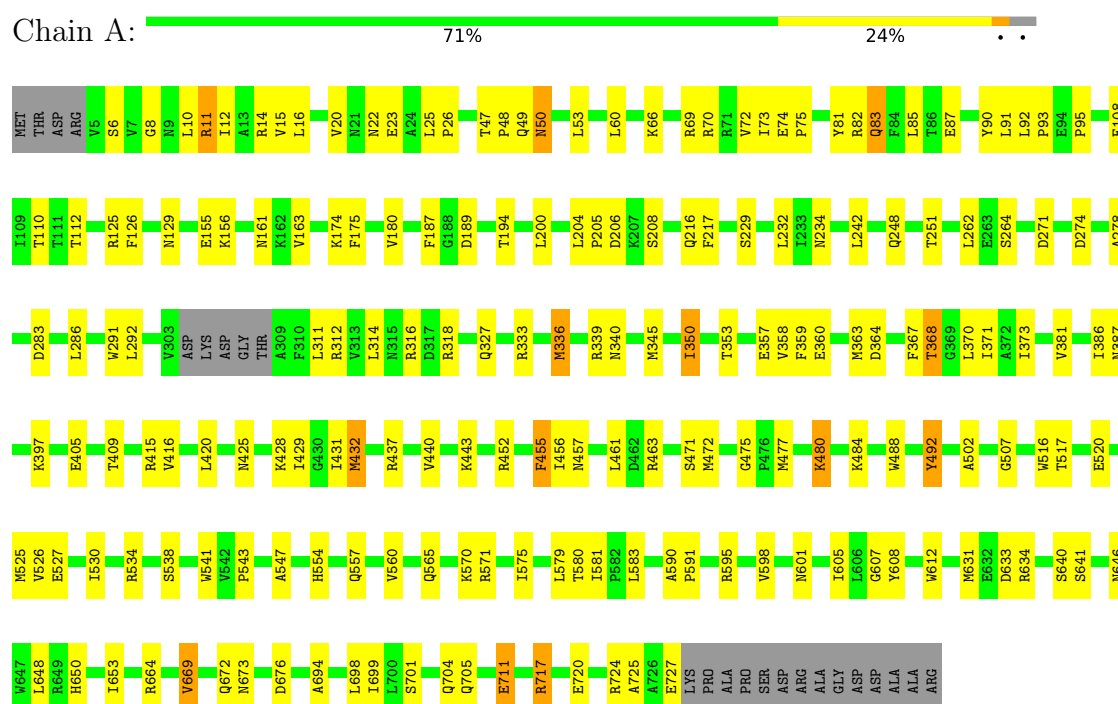
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	348	Total 348	O 348	0	0
7	B	291	Total 291	O 291	0	0

3 Residue-property plots

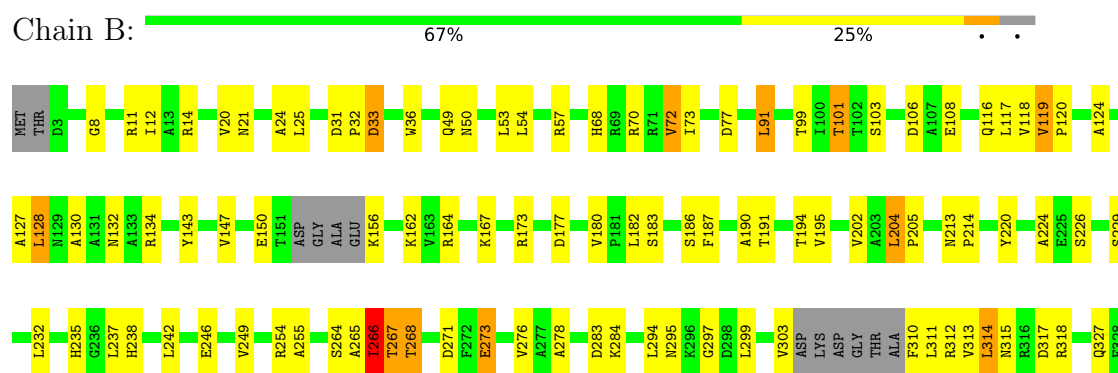
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

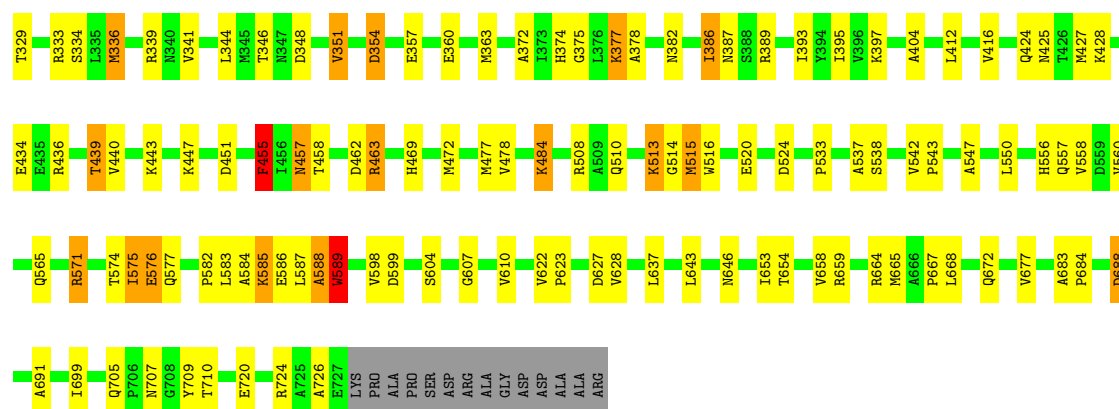
Note EDS was not executed.

• Molecule 1: Probable malate synthase G



• Molecule 1: Probable malate synthase G





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	120.98Å 120.98Å 232.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.36 – 2.70	Depositor
% Data completeness (in resolution range)	94.3 (29.36-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.190 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11696	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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: COA, MG, SO4, MLT, GLV

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	0.56	2/5591 (0.0%)	0.94	1/7606 (0.0%)
1	B	0.55	2/5578 (0.0%)	1.00	9/7586 (0.1%)
All	All	0.56	4/11169 (0.0%)	0.97	10/15192 (0.1%)

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	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	588	ALA	C-N	-9.72	1.20	1.33
1	B	515	MET	SD-CE	-5.93	1.64	1.79
1	A	336	MET	SD-CE	-5.66	1.65	1.79
1	A	432	MET	SD-CE	-5.33	1.66	1.79

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	589	TRP	O-C-N	-10.20	109.03	122.59
1	B	589	TRP	CA-C-N	7.30	130.86	120.49
1	B	589	TRP	C-N-CA	7.30	130.86	120.49
1	B	266	ILE	CA-C-N	6.76	133.86	121.70
1	B	266	ILE	C-N-CA	6.76	133.86	121.70
1	B	266	ILE	N-CA-C	6.67	123.21	109.34
1	A	271	ASP	N-CA-C	5.48	117.67	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	514	GLY	N-CA-C	5.45	120.85	112.51
1	B	276	VAL	N-CA-C	5.27	117.64	108.95
1	B	455	PHE	N-CA-C	5.10	116.59	108.79

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	266	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	5486	0	5433	90	0
1	B	5474	0	5426	118	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
4	A	18	0	7	4	0
4	B	9	0	4	0	0
5	A	48	0	32	6	0
6	B	5	0	1	0	0
7	A	348	0	0	11	0
7	B	291	0	0	11	0
All	All	11696	0	10903	210	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 10.

All (210) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:ARG:HH11	1:B:571:ARG:HG2	1.22	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ASP:HB3	7:A:1138:HOH:O	1.62	0.97
1:B:425:ASN:O	1:B:428:LYS:HE2	1.65	0.96
1:B:533:PRO:HB2	1:B:558:VAL:HG11	1.47	0.96
1:A:340:ASN:HD21	1:A:368:THR:HG21	1.31	0.93
1:B:101:THR:HG22	1:B:451:ASP:HB3	1.51	0.90
1:B:267:THR:HG21	1:B:510:GLN:HE22	1.37	0.89
1:A:415:ARG:HD3	7:A:1221:HOH:O	1.78	0.82
1:B:132:ASN:HD21	1:B:315:ASN:H	1.29	0.80
1:A:416:VAL:O	1:A:420:LEU:HG	1.84	0.77
1:B:439:THR:HG21	1:B:463:ARG:HE	1.49	0.77
1:B:91:LEU:HD11	1:B:575:ILE:HD13	1.67	0.77
1:B:664:ARG:HB3	1:B:665:MET:HE2	1.70	0.74
1:B:101:THR:HG22	1:B:451:ASP:CB	2.19	0.72
1:B:571:ARG:HG2	1:B:571:ARG:NH1	1.95	0.72
1:B:436:ARG:HA	1:B:439:THR:HG23	1.71	0.72
1:A:11:ARG:HD2	1:A:11:ARG:O	1.92	0.70
1:B:543:PRO:HD2	1:B:547:ALA:CB	2.22	0.70
1:A:694:ALA:HB2	1:A:717:ARG:HG2	1.74	0.69
1:B:204:LEU:HB3	1:B:205:PRO:HD2	1.74	0.69
1:A:204:LEU:HB3	1:A:205:PRO:HD2	1.75	0.68
1:B:515:MET:HE1	1:B:542:VAL:C	2.17	0.68
1:A:425:ASN:O	1:A:428:LYS:NZ	2.24	0.68
1:A:640:SER:OG	7:A:1027:HOH:O	2.11	0.67
1:B:434:GLU:OE2	7:B:1140:HOH:O	2.12	0.66
1:B:108:GLU:HB3	1:B:266:ILE:HG22	1.76	0.66
1:B:515:MET:HE1	1:B:543:PRO:N	2.11	0.65
1:B:49:GLN:HG3	7:B:1229:HOH:O	1.97	0.65
1:B:515:MET:HE3	1:B:516:TRP:H	1.61	0.64
1:B:317:ASP:HB3	1:B:329:THR:CG2	2.28	0.64
1:B:132:ASN:ND2	1:B:315:ASN:H	1.96	0.64
1:B:439:THR:HG21	1:B:463:ARG:NE	2.13	0.63
1:A:350:ILE:HG23	1:A:363:MET:SD	2.38	0.63
1:B:278:ALA:HA	1:B:283:ASP:HB3	1.79	0.63
1:A:336:MET:HE3	1:A:387:ASN:ND2	2.14	0.62
1:B:533:PRO:HB2	1:B:558:VAL:CG1	2.27	0.61
1:B:436:ARG:HA	1:B:439:THR:CG2	2.30	0.61
1:B:599:ASP:OD1	1:B:664:ARG:NH1	2.34	0.61
1:A:10:LEU:HD22	1:A:350:ILE:HD11	1.83	0.60
1:B:472:MET:SD	1:B:646:ASN:HA	2.41	0.60
1:B:346:THR:HB	1:B:357:GLU:HB3	1.84	0.59
1:A:83:GLN:HG2	7:A:1123:HOH:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:GLN:HE21	1:B:267:THR:HB	1.67	0.59
1:A:126:PHE:CE2	5:A:903:COA:H2B	2.38	0.58
1:A:25:LEU:N	1:A:26:PRO:HD2	2.19	0.58
1:B:31:ASP:C	1:B:33:ASP:H	2.11	0.57
1:A:461:LEU:HB2	4:A:901:MLT:O1	2.04	0.57
1:A:475:GLY:HA2	1:A:650:HIS:CD2	2.40	0.57
1:B:11:ARG:HB2	1:B:351:VAL:HG12	1.86	0.57
1:B:377:LYS:HD2	1:B:378:ALA:H	1.69	0.57
1:B:297:GLY:HA2	1:B:314:LEU:HD23	1.88	0.56
1:A:95:PRO:HG2	1:A:443:LYS:HG2	1.88	0.56
1:B:128:LEU:HD22	1:B:314:LEU:HD13	1.87	0.56
1:B:106:ASP:HB3	1:B:108:GLU:OE1	2.06	0.56
1:B:119:VAL:HG22	1:B:120:PRO:HD2	1.87	0.55
1:B:478:VAL:HG12	1:B:584:ALA:HA	1.89	0.55
1:B:515:MET:HE3	1:B:516:TRP:N	2.21	0.55
1:B:20:VAL:HA	1:B:24:ALA:HB3	1.89	0.55
1:B:637:LEU:HG	1:B:710:THR:HG21	1.88	0.55
1:A:605:ILE:HD13	1:A:699:ILE:HD11	1.88	0.54
1:A:339:ARG:HH12	4:A:901:MLT:H31	1.72	0.54
1:A:314:LEU:HB3	1:A:333:ARG:HD3	1.89	0.54
1:B:455:PHE:C	1:B:455:PHE:CD1	2.86	0.54
1:B:372:ALA:HB1	1:B:393:ILE:HG12	1.90	0.54
1:A:364:ASP:O	1:A:368:THR:HB	2.08	0.54
1:B:295:ASN:HD22	1:B:375:GLY:HA3	1.73	0.53
1:B:571:ARG:HH11	1:B:571:ARG:CG	2.06	0.53
1:B:610:VAL:HA	1:B:691:ALA:HB1	1.89	0.53
1:A:472:MET:O	1:A:650:HIS:HE1	1.90	0.53
1:B:134:ARG:HD3	1:B:333:ARG:O	2.09	0.53
1:A:608:TYR:CE1	1:A:633:ASP:HA	2.44	0.52
1:B:317:ASP:HB3	1:B:329:THR:HG23	1.91	0.52
1:A:180:VAL:HG21	1:A:232:LEU:HD13	1.91	0.52
1:A:429:ILE:HG22	1:A:452:ARG:HB3	1.91	0.52
1:B:377:LYS:HA	1:B:386:ILE:HD11	1.92	0.52
1:B:101:THR:CG2	1:B:451:ASP:HB3	2.33	0.52
1:B:294:LEU:HG	1:B:299:LEU:HD22	1.92	0.52
1:B:462:ASP:OD1	7:B:1140:HOH:O	2.19	0.52
1:B:515:MET:HE2	1:B:516:TRP:O	2.09	0.51
1:A:292:LEU:HA	1:A:371:ILE:HG23	1.93	0.51
1:A:631:MET:HE1	5:A:903:COA:H22	1.92	0.51
1:B:273:GLU:HG3	1:B:341:VAL:HA	1.92	0.51
1:B:237:LEU:HB2	1:B:556:HIS:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ASN:OD1	1:A:163:VAL:N	2.44	0.50
1:A:291:TRP:CD1	1:A:371:ILE:HG21	2.47	0.50
1:B:127:ALA:HB1	1:B:294:LEU:HD11	1.93	0.50
1:B:130:ALA:HB1	1:B:268:THR:HG21	1.93	0.50
1:B:705:GLN:HG3	7:B:1202:HOH:O	2.12	0.50
1:A:129:ASN:ND2	1:A:312:ARG:HD3	2.26	0.50
1:B:12:ILE:HG12	1:B:36:TRP:CZ3	2.47	0.49
1:A:455:PHE:C	1:A:455:PHE:CD1	2.89	0.49
1:B:180:VAL:HG11	1:B:232:LEU:HD22	1.94	0.49
1:A:641:SER:HB2	1:A:698:LEU:O	2.11	0.49
1:B:336:MET:HB2	1:B:387:ASN:OD1	2.13	0.49
1:A:22:ASN:O	1:A:26:PRO:HG3	2.13	0.49
1:B:143:TYR:O	1:B:164:ARG:NH2	2.44	0.49
1:B:688:ASP:OD2	1:B:688:ASP:N	2.46	0.49
1:A:12:ILE:HG23	1:A:16:LEU:HD23	1.94	0.48
1:A:291:TRP:CD1	1:A:371:ILE:CG2	2.96	0.48
1:B:664:ARG:O	1:B:667:PRO:HD2	2.13	0.48
1:B:469:HIS:CD2	1:B:707:ASN:HA	2.48	0.48
1:A:125:ARG:CZ	5:A:903:COA:O9A	2.61	0.48
1:B:404:ALA:HB3	7:B:1395:HOH:O	2.13	0.48
1:A:161:ASN:OD1	1:A:161:ASN:C	2.57	0.48
1:B:191:THR:O	1:B:255:ALA:HA	2.14	0.48
1:A:350:ILE:HG12	1:A:358:VAL:HG21	1.96	0.48
1:B:354:ASP:HB3	7:B:1386:HOH:O	2.13	0.48
1:B:576:GLU:HG2	7:B:1527:HOH:O	2.13	0.48
1:A:11:ARG:HD2	1:A:11:ARG:C	2.38	0.47
1:B:455:PHE:C	1:B:455:PHE:HD1	2.21	0.47
1:B:21:ASN:HD22	1:B:25:LEU:HD12	1.79	0.47
1:A:125:ARG:HD2	7:A:1543:HOH:O	2.14	0.47
1:B:586:GLU:HG3	1:B:588:ALA:HB3	1.96	0.47
1:B:424:GLN:O	1:B:425:ASN:HB2	2.15	0.47
1:B:477:MET:HE2	1:B:646:ASN:ND2	2.29	0.47
1:A:543:PRO:HD2	1:A:547:ALA:CB	2.44	0.47
1:B:173:ARG:HD2	1:B:187:PHE:HB3	1.96	0.47
1:A:345:MET:HE2	1:A:711:GLU:HB3	1.96	0.46
1:A:530:ILE:HG12	1:A:534:ARG:HD2	1.97	0.46
1:A:92:LEU:HB3	1:A:93:PRO:HD2	1.96	0.46
1:B:377:LYS:HD2	1:B:378:ALA:N	2.31	0.46
1:B:607:GLY:HA3	1:B:622:VAL:HG11	1.96	0.46
1:A:367:PHE:O	1:A:371:ILE:HD12	2.16	0.46
1:A:53:LEU:HD22	1:A:405:GLU:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:MET:HG2	1:A:646:ASN:OD1	2.16	0.45
1:B:271:ASP:OD2	1:B:339:ARG:NH2	2.42	0.45
1:B:623:PRO:HA	1:B:628:VAL:O	2.16	0.45
1:B:372:ALA:CB	1:B:393:ILE:HG12	2.45	0.45
1:A:180:VAL:HG12	1:A:216:GLN:NE2	2.31	0.45
1:B:264:SER:O	1:B:266:ILE:HG12	2.17	0.45
1:B:412:LEU:O	1:B:416:VAL:HG23	2.16	0.45
1:B:134:ARG:HA	1:B:265:ALA:O	2.15	0.45
1:A:432:MET:HE2	1:A:455:PHE:HE1	1.82	0.45
1:A:595:ARG:NH2	7:A:1014:HOH:O	2.49	0.45
1:B:513:LYS:HD3	1:B:537:ALA:HB2	1.98	0.45
1:A:480:LYS:HD3	1:A:601:ASN:OD1	2.17	0.45
1:A:125:ARG:HD3	7:A:1517:HOH:O	2.17	0.44
1:A:60:LEU:HD22	1:A:90:TYR:HB2	1.98	0.44
1:A:81:TYR:CE2	1:A:85:LEU:HD11	2.52	0.44
1:B:588:ALA:O	1:B:589:TRP:HB2	2.17	0.44
1:B:658:VAL:HG11	1:B:699:ILE:HG21	2.00	0.44
1:B:333:ARG:HH11	1:B:333:ARG:HG3	1.82	0.44
1:B:124:ALA:O	1:B:128:LEU:HB2	2.17	0.44
1:B:20:VAL:HG12	1:B:25:LEU:HG	1.99	0.44
1:B:147:VAL:HG21	1:B:550:LEU:HD13	1.99	0.44
1:A:516:TRP:CE2	1:A:525:MET:HB2	2.53	0.44
1:A:336:MET:H	1:A:387:ASN:HD21	1.64	0.44
1:B:68:HIS:O	1:B:72:VAL:HG22	2.18	0.43
1:A:311:LEU:HB2	1:B:313:VAL:HG11	2.00	0.43
1:A:541:TRP:HZ3	4:A:901:MLT:H32	1.82	0.43
1:A:360:GLU:HA	1:A:363:MET:HE3	1.99	0.43
1:B:57:ARG:NH1	1:B:709:TYR:HE1	2.16	0.43
1:B:213:ASN:HA	1:B:214:PRO:HD2	1.80	0.43
1:A:180:VAL:HG12	1:A:216:GLN:CD	2.44	0.43
1:A:47:THR:N	1:A:48:PRO:CD	2.81	0.43
1:A:397:LYS:HG2	1:A:409:THR:HG21	1.99	0.43
1:B:190:ALA:O	1:B:255:ALA:HB2	2.18	0.43
1:A:463:ARG:HG3	1:A:488:TRP:HZ3	1.84	0.43
1:B:177:ASP:OD2	1:B:186:SER:HB2	2.18	0.43
1:A:607:GLY:HA2	1:A:669:VAL:HG11	2.00	0.43
1:A:590:ALA:HB1	1:A:591:PRO:HD2	2.01	0.42
1:B:574:THR:OG1	1:B:577:GLN:HG3	2.19	0.42
1:A:538:SER:HA	1:A:560:VAL:HG11	1.99	0.42
1:B:443:LYS:HD2	7:B:1279:HOH:O	2.18	0.42
1:A:216:GLN:NE2	1:A:234:ASN:HD22	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:VAL:HG11	1:A:579:LEU:HD21	2.01	0.42
1:B:213:ASN:CG	1:B:213:ASN:O	2.61	0.42
1:B:386:ILE:HB	7:B:1630:HOH:O	2.18	0.42
1:A:274:ASP:CG	1:A:634:ARG:HB2	2.45	0.42
1:B:598:VAL:HG21	1:B:653:ILE:HG21	2.00	0.42
1:B:538:SER:HA	1:B:560:VAL:HG11	2.02	0.42
1:B:436:ARG:O	1:B:440:VAL:HG22	2.20	0.42
1:A:125:ARG:NH1	7:A:1391:HOH:O	2.51	0.42
5:A:903:COA:OAP	7:A:1343:HOH:O	2.22	0.42
1:A:16:LEU:HD21	1:A:367:PHE:CZ	2.55	0.42
1:B:49:GLN:O	1:B:53:LEU:HG	2.21	0.41
1:A:200:LEU:HB2	1:A:217:PHE:CD1	2.56	0.41
1:A:526:VAL:O	1:A:554:HIS:NE2	2.43	0.41
1:A:581:ILE:HG22	1:A:583:LEU:HG	2.03	0.41
1:B:119:VAL:HG22	1:B:120:PRO:CD	2.50	0.41
1:A:180:VAL:HG21	1:A:232:LEU:CD1	2.50	0.41
1:A:432:MET:HE2	1:A:455:PHE:CE1	2.54	0.41
1:B:103:SER:O	1:B:428:LYS:NZ	2.54	0.41
1:B:508:ARG:HA	7:B:1433:HOH:O	2.20	0.41
1:B:344:LEU:HD22	1:B:709:TYR:CD1	2.56	0.41
1:A:415:ARG:NH1	1:A:415:ARG:HB3	2.34	0.41
4:A:901:MLT:O5	5:A:903:COA:S1P	2.76	0.41
1:B:195:VAL:HB	1:B:224:ALA:HB1	2.02	0.41
1:A:431:ILE:O	1:A:456:ILE:HA	2.20	0.41
1:B:374:HIS:HD2	1:B:382:ASN:HD22	1.69	0.41
1:A:278:ALA:HA	1:A:283:ASP:HB3	2.03	0.41
1:A:598:VAL:HG21	1:A:653:ILE:HG21	2.03	0.41
1:B:478:VAL:HG13	1:B:582:PRO:O	2.21	0.41
1:B:508:ARG:HG2	7:B:1433:HOH:O	2.21	0.41
1:B:683:ALA:HA	1:B:684:PRO:HA	1.81	0.41
1:A:50:ASN:HB3	1:A:359:PHE:CE1	2.56	0.41
1:A:187:PHE:C	1:A:189:ASP:H	2.29	0.41
1:A:488:TRP:HB3	1:A:580:THR:O	2.21	0.41
1:B:220:TYR:HB2	1:B:229:SER:O	2.20	0.41
1:B:232:LEU:O	1:B:238:HIS:HA	2.21	0.41
1:A:16:LEU:O	1:A:20:VAL:HG23	2.21	0.40
1:A:455:PHE:C	1:A:455:PHE:HD1	2.29	0.40
1:A:463:ARG:HG2	1:A:492:TYR:CE1	2.57	0.40
1:B:360:GLU:HA	1:B:363:MET:HE3	2.03	0.40
1:A:502:ALA:HB1	7:A:1534:HOH:O	2.21	0.40
1:B:543:PRO:HD2	1:B:547:ALA:HB1	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:THR:HB	1:A:507:GLY:O	2.20	0.40
1:A:175:PHE:CE2	1:A:262:LEU:HD21	2.56	0.40
5:A:903:COA:H131	7:A:1357:HOH:O	2.20	0.40
1:B:457:ASN:C	1:B:457:ASN:HD22	2.30	0.40

There are no symmetry-related clashes.

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	714/741 (96%)	667 (93%)	43 (6%)	4 (1%)	21	44
1	B	709/741 (96%)	656 (92%)	45 (6%)	8 (1%)	11	29
All	All	1423/1482 (96%)	1323 (93%)	88 (6%)	12 (1%)	16	37

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	ILE
1	B	585	LYS
1	B	589	TRP
1	B	267	THR
1	B	726	ALA
1	A	725	ALA
1	B	32	PRO
1	B	484	LYS
1	B	235	HIS
1	B	8	GLY
1	A	8	GLY
1	A	75	PRO

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	577/594 (97%)	507 (88%)	70 (12%)	5	12
1	B	577/594 (97%)	497 (86%)	80 (14%)	3	9
All	All	1154/1188 (97%)	1004 (87%)	150 (13%)	4	10

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	11	ARG
1	A	14	ARG
1	A	15	VAL
1	A	23	GLU
1	A	49	GLN
1	A	50	ASN
1	A	66	LYS
1	A	69	ARG
1	A	70	ARG
1	A	72	VAL
1	A	74	GLU
1	A	82	ARG
1	A	83	GLN
1	A	87	GLU
1	A	91	LEU
1	A	108	GLU
1	A	112	THR
1	A	155	GLU
1	A	156	LYS
1	A	174	LYS
1	A	194	THR
1	A	208	SER
1	A	229	SER
1	A	242	LEU
1	A	248	GLN
1	A	251	THR

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Mol	Chain	Res	Type
1	A	264	SER
1	A	286	LEU
1	A	316	ARG
1	A	318	ARG
1	A	327	GLN
1	A	350	ILE
1	A	353	THR
1	A	357	GLU
1	A	368	THR
1	A	370	LEU
1	A	373	ILE
1	A	381	VAL
1	A	386	ILE
1	A	437	ARG
1	A	455	PHE
1	A	457	ASN
1	A	471	SER
1	A	480	LYS
1	A	484	LYS
1	A	492	TYR
1	A	517	THR
1	A	520	GLU
1	A	527	GLU
1	A	557	GLN
1	A	565	GLN
1	A	570	LYS
1	A	571	ARG
1	A	575	ILE
1	A	612	TRP
1	A	648	LEU
1	A	664	ARG
1	A	669	VAL
1	A	672	GLN
1	A	673	ASN
1	A	676	ASP
1	A	701	SER
1	A	704	GLN
1	A	705	GLN
1	A	711	GLU
1	A	717	ARG
1	A	720	GLU
1	A	724	ARG

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Mol	Chain	Res	Type
1	A	727	GLU
1	B	14	ARG
1	B	33	ASP
1	B	50	ASN
1	B	54	LEU
1	B	70	ARG
1	B	72	VAL
1	B	73	ILE
1	B	77	ASP
1	B	91	LEU
1	B	99	THR
1	B	101	THR
1	B	117	LEU
1	B	118	VAL
1	B	119	VAL
1	B	128	LEU
1	B	150	GLU
1	B	156	LYS
1	B	162	LYS
1	B	167	LYS
1	B	182	LEU
1	B	183	SER
1	B	194	THR
1	B	202	VAL
1	B	204	LEU
1	B	226	SER
1	B	242	LEU
1	B	246	GLU
1	B	249	VAL
1	B	254	ARG
1	B	268	THR
1	B	273	GLU
1	B	284	LYS
1	B	303	VAL
1	B	310	PHE
1	B	311	LEU
1	B	312	ARG
1	B	314	LEU
1	B	318	ARG
1	B	327	GLN
1	B	334	SER
1	B	336	MET

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Mol	Chain	Res	Type
1	B	348	ASP
1	B	351	VAL
1	B	354	ASP
1	B	377	LYS
1	B	386	ILE
1	B	389	ARG
1	B	395	ILE
1	B	397	LYS
1	B	427	MET
1	B	439	THR
1	B	447	LYS
1	B	455	PHE
1	B	457	ASN
1	B	458	THR
1	B	463	ARG
1	B	484	LYS
1	B	513	LYS
1	B	520	GLU
1	B	524	ASP
1	B	557	GLN
1	B	565	GLN
1	B	571	ARG
1	B	575	ILE
1	B	576	GLU
1	B	583	LEU
1	B	585	LYS
1	B	587	LEU
1	B	589	TRP
1	B	604	SER
1	B	627	ASP
1	B	643	LEU
1	B	654	THR
1	B	659	ARG
1	B	668	LEU
1	B	672	GLN
1	B	677	VAL
1	B	688	ASP
1	B	720	GLU
1	B	724	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	63	GLN
1	A	129	ASN
1	A	196	GLN
1	A	213	ASN
1	A	234	ASN
1	A	248	GLN
1	A	290	ASN
1	A	340	ASN
1	A	382	ASN
1	A	387	ASN
1	A	425	ASN
1	A	457	ASN
1	A	642	GLN
1	A	650	HIS
1	A	672	GLN
1	A	707	ASN
1	B	21	ASN
1	B	49	GLN
1	B	63	GLN
1	B	132	ASN
1	B	196	GLN
1	B	199	GLN
1	B	234	ASN
1	B	290	ASN
1	B	295	ASN
1	B	327	GLN
1	B	340	ASN
1	B	374	HIS
1	B	457	ASN
1	B	495	HIS
1	B	510	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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	1800	-	4,4,4	0.23	0	6,6,6	0.25	0
4	MLT	A	902	-	8,8,8	1.93	3 (37%)	10,10,10	1.43	1 (10%)
3	SO4	B	1803	-	4,4,4	0.25	0	6,6,6	0.18	0
5	COA	A	903	-	47,50,50	1.77	7 (14%)	69,75,75	1.45	10 (14%)
6	GLV	B	1901	2	4,4,4	5.34	2 (50%)	3,4,4	2.21	2 (66%)
4	MLT	A	901	2	8,8,8	1.73	2 (25%)	10,10,10	2.04	2 (20%)
4	MLT	B	1902	-	8,8,8	1.64	2 (25%)	10,10,10	1.67	2 (20%)
3	SO4	A	1802	-	4,4,4	0.23	0	6,6,6	0.12	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MLT	A	902	-	1/1/3/3	6/8/8/8	-
6	GLV	B	1901	2	-	0/0/2/2	-
4	MLT	A	901	2	1/1/3/3	2/8/8/8	-
4	MLT	B	1902	-	1/1/3/3	4/8/8/8	-
5	COA	A	903	-	-	19/48/64/64	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	903	COA	O9P-C9P	9.67	1.41	1.23
6	B	1901	GLV	O1-C1	9.58	1.43	1.22
6	B	1901	GLV	C1-C2	4.51	1.53	1.44
4	A	902	MLT	O1-C1	3.34	1.32	1.22
4	A	901	MLT	O4-C4	3.31	1.32	1.22
4	B	1902	MLT	O1-C1	3.18	1.31	1.22
4	B	1902	MLT	O4-C4	3.17	1.32	1.22
4	A	902	MLT	O4-C4	3.12	1.32	1.22
5	A	903	COA	C2A-N1A	2.92	1.39	1.33
4	A	901	MLT	O1-C1	2.84	1.30	1.22
5	A	903	COA	C2A-N3A	2.74	1.38	1.33
4	A	902	MLT	C2-C1	-2.62	1.48	1.52
5	A	903	COA	P2A-O3A	2.56	1.62	1.59
5	A	903	COA	C8A-N7A	2.54	1.36	1.31
5	A	903	COA	P3B-O3B	2.37	1.63	1.59
5	A	903	COA	P1A-O3A	2.05	1.61	1.59

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	903	COA	N3A-C2A-N1A	-5.56	120.17	128.58
4	A	901	MLT	O2-C1-C2	4.70	122.68	112.74
5	A	903	COA	C5A-C4A-N3A	-4.30	120.80	126.72
4	B	1902	MLT	O2-C1-C2	3.79	120.75	112.74
5	A	903	COA	C2A-N3A-C4A	3.29	119.87	111.83
5	A	903	COA	C5A-N7A-C8A	3.19	108.47	103.45
4	A	901	MLT	O1-C1-C2	-3.08	116.45	122.60
5	A	903	COA	N9A-C8A-N7A	-3.08	109.57	113.94
6	B	1901	GLV	O3-C2-C1	2.98	122.22	113.42
5	A	903	COA	C4A-C5A-N7A	-2.94	107.22	110.58
4	A	902	MLT	O2-C1-C2	2.79	118.64	112.74
5	A	903	COA	C3B-C2B-C1B	2.56	105.51	99.89
4	B	1902	MLT	O2-C1-O1	-2.38	118.67	124.08
5	A	903	COA	C5A-C4A-N9A	2.26	108.27	105.81
5	A	903	COA	N3A-C4A-N9A	2.21	130.93	127.17
5	A	903	COA	O4B-C1B-N9A	2.17	112.25	108.09
6	B	1901	GLV	O2-C2-C1	-2.09	117.56	123.96

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	901	MLT	C2
4	A	902	MLT	C2

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Mol	Chain	Res	Type	Atom
4	B	1902	MLT	C2

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	MLT	O3-C2-C3-C4
4	A	902	MLT	O1-C1-C2-O3
4	A	902	MLT	O2-C1-C2-O3
4	A	902	MLT	C1-C2-C3-C4
4	A	902	MLT	O3-C2-C3-C4
5	A	903	COA	C4B-C5B-O5B-P1A
5	A	903	COA	C5B-O5B-P1A-O1A
5	A	903	COA	C5B-O5B-P1A-O3A
5	A	903	COA	OAP-CAP-CBP-CCP
5	A	903	COA	C9P-CAP-CBP-CCP
5	A	903	COA	OAP-CAP-CBP-CDP
5	A	903	COA	C9P-CAP-CBP-CDP
5	A	903	COA	OAP-CAP-CBP-CEP
5	A	903	COA	C9P-CAP-CBP-CEP
5	A	903	COA	CAP-C9P-N8P-C7P
5	A	903	COA	O9P-C9P-N8P-C7P
5	A	903	COA	C5P-C6P-C7P-N8P
5	A	903	COA	O4B-C4B-C5B-O5B
5	A	903	COA	C6P-C5P-N4P-C3P
5	A	903	COA	O5P-C5P-N4P-C3P
5	A	903	COA	C3B-C4B-C5B-O5B
4	B	1902	MLT	O2-C1-C2-C3
4	A	902	MLT	O1-C1-C2-C3
4	A	902	MLT	O2-C1-C2-C3
4	B	1902	MLT	O1-C1-C2-C3
4	A	901	MLT	C1-C2-C3-C4
5	A	903	COA	C3B-O3B-P3B-O7A
4	B	1902	MLT	O2-C1-C2-O3
5	A	903	COA	C3B-O3B-P3B-O8A
5	A	903	COA	C3B-O3B-P3B-O9A
4	B	1902	MLT	O1-C1-C2-O3

There are no ring outliers.

2 monomers are involved in 9 short contacts:

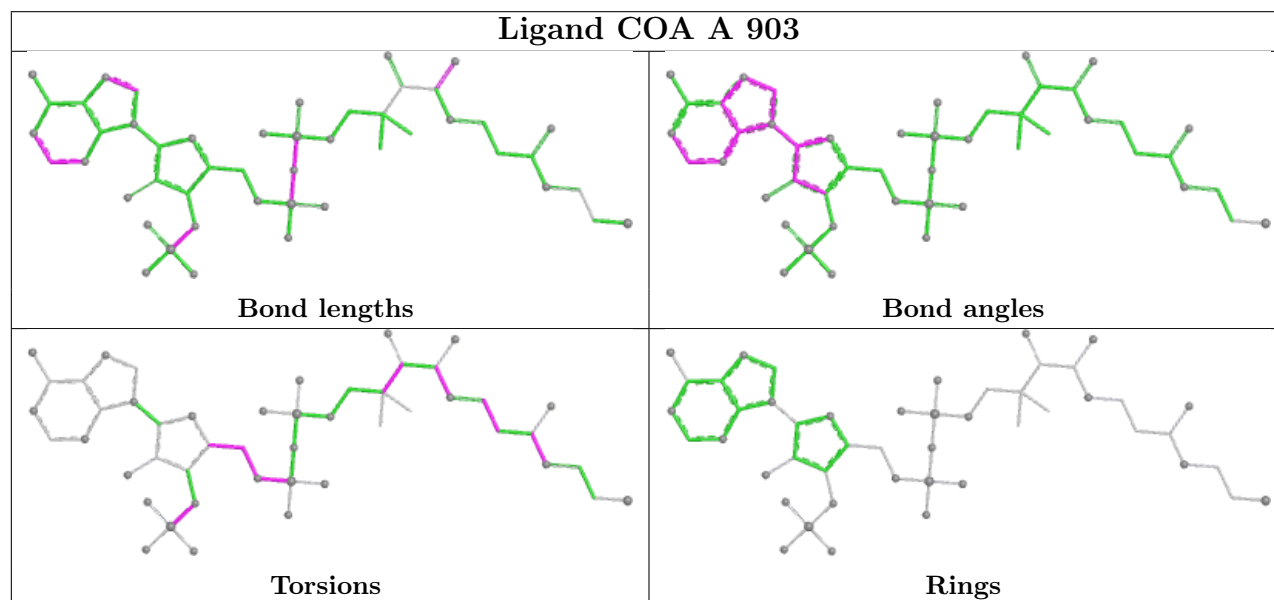
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	903	COA	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	MLT	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	588:ALA	C	589:TRP	N	1.20

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.