



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:59 AM UTC

PDB ID : 1OBL / pdb_00001obl
Title : crystal structure of the S133A mutant of Malonamidase E2 complexed with malonate from Bradyrhizobium japonicum
Authors : Shin, S.; Oh, B.-H.
Deposited on : 2003-01-31
Resolution : 2.00 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
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

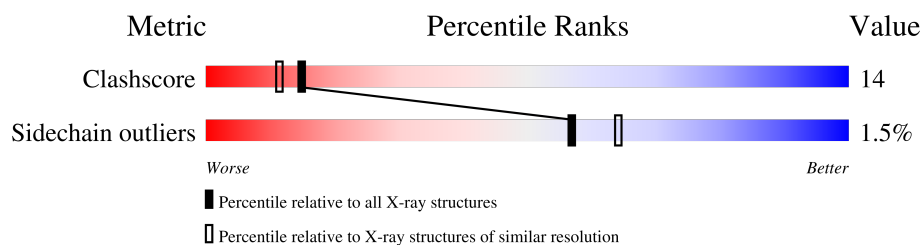
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	190562	11152 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 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	414	
1	B	414	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7049 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.

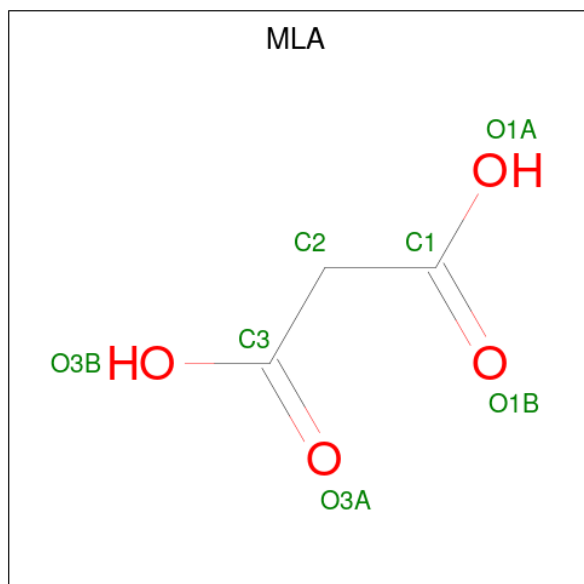
- Molecule 1 is a protein called MALONAMIDASE E2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	S	0	0	0
			3061	1919	562	567	13			
1	B	412	Total	C	N	O	S	0	0	0
			3061	1919	562	567	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	133	ALA	SER	engineered mutation	UNP Q9ZIV5
B	133	ALA	SER	engineered mutation	UNP Q9ZIV5

- Molecule 2 is MALONIC ACID (CCD ID: MLA) (formula: $C_3H_4O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	3	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			7	3	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	427	Total	O	0	0
			427	427		
3	B	486	Total	O	0	0
			486	486		

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.63Å 95.22Å 74.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.00 – 2.00	Depositor
% Data completeness (in resolution range)	92.1 (52.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.188 , 0.245	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7049	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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: MLA

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	0.37	0/3125	0.98	20/4246 (0.5%)
1	B	0.38	0/3125	0.99	20/4246 (0.5%)
All	All	0.38	0/6250	0.98	40/8492 (0.5%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	64	ILE	N-CA-C	-11.57	101.79	112.43
1	A	64	ILE	N-CA-C	-8.90	104.47	113.10
1	B	113	ARG	N-CA-C	8.82	122.05	111.82
1	B	40	VAL	N-CA-C	-8.74	101.47	111.00
1	A	297	ALA	CA-C-N	7.70	129.47	119.84
1	A	297	ALA	C-N-CA	7.70	129.47	119.84
1	A	183	TYR	N-CA-C	-7.66	101.64	112.13
1	B	152	THR	N-CA-C	-6.94	105.35	113.88
1	A	113	ARG	N-CA-C	6.58	121.06	112.89
1	A	152	THR	N-CA-C	-6.49	105.38	113.55
1	B	63	ASP	N-CA-C	6.22	124.05	110.80
1	A	224	ILE	N-CA-C	6.19	116.84	108.17
1	B	183	TYR	N-CA-C	-6.17	104.83	112.72
1	B	157	ILE	N-CA-C	6.00	116.18	110.42
1	B	297	ALA	CA-C-N	5.97	127.31	119.84
1	B	297	ALA	C-N-CA	5.97	127.31	119.84
1	B	66	ASP	N-CA-C	5.96	118.97	110.10
1	A	36	VAL	N-CA-C	5.89	116.88	111.81
1	B	363	ARG	N-CA-C	5.80	118.35	111.33
1	A	73	GLU	N-CA-C	5.78	120.32	113.16
1	A	363	ARG	N-CA-C	5.76	118.03	111.11
1	A	108	THR	N-CA-C	-5.72	102.98	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	128	PRO	N-CA-C	-5.62	106.83	114.80
1	A	63	ASP	N-CA-C	5.58	122.70	110.80
1	B	120	ASN	CA-C-N	5.56	125.40	119.28
1	B	120	ASN	C-N-CA	5.56	125.40	119.28
1	B	31	ALA	N-CA-C	5.54	117.32	111.28
1	A	120	ASN	CA-C-N	5.52	125.18	119.05
1	A	120	ASN	C-N-CA	5.52	125.18	119.05
1	A	17	SER	CA-C-N	5.48	124.94	119.24
1	A	17	SER	C-N-CA	5.48	124.94	119.24
1	A	40	VAL	N-CA-C	-5.46	105.05	111.00
1	B	383	LEU	CA-C-N	5.32	125.26	119.78
1	B	383	LEU	C-N-CA	5.32	125.26	119.78
1	A	169	LYS	N-CA-C	-5.27	99.04	109.10
1	B	169	LYS	N-CA-C	-5.24	98.17	109.01
1	B	108	THR	N-CA-C	-5.21	103.65	110.53
1	A	66	ASP	N-CA-C	5.20	117.77	110.23
1	A	155	SER	N-CA-C	5.19	119.36	113.19
1	B	133	ALA	N-CA-C	5.13	116.56	110.97

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	3061	0	3073	86	0
1	B	3061	0	3073	87	0
2	A	7	0	2	0	0
2	B	7	0	2	0	0
3	A	427	0	0	17	0
3	B	486	0	0	14	0
All	All	7049	0	6150	170	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 14.

All (170) 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:392:ARG:HB2	1:B:392:ARG:NH1	1.78	0.98
1:A:119:LEU:HD13	1:A:124:THR:HG23	1.52	0.89
1:B:337:ASP:HB3	1:B:398:HIS:NE2	1.92	0.84
1:A:375:VAL:HG11	1:A:406:LEU:HD22	1.58	0.84
1:A:412:LYS:HA	1:A:412:LYS:HE2	1.61	0.82
1:B:217:VAL:HG13	1:B:218:PRO:HD2	1.64	0.79
1:A:320:ARG:HB3	1:A:324:ARG:HH12	1.49	0.75
1:B:392:ARG:HB2	1:B:392:ARG:HH11	1.46	0.74
1:B:216:ILE:HB	3:B:2312:HOH:O	1.89	0.73
1:A:267:HIS:HB3	3:A:2303:HOH:O	1.88	0.72
1:B:32:ARG:HH11	1:B:32:ARG:HB3	1.55	0.71
1:B:252:ARG:HH21	1:B:412:LYS:HD2	1.57	0.70
1:B:403:ALA:O	1:B:407:GLU:HG3	1.92	0.69
1:B:32:ARG:HB3	1:B:32:ARG:NH1	2.08	0.69
1:B:242:GLY:HA2	1:B:378:LEU:HD11	1.75	0.69
1:A:210:ARG:HB3	1:A:212:GLU:OE2	1.94	0.67
1:A:337:ASP:HB3	1:A:398:HIS:CE1	2.30	0.66
1:B:273:HIS:HB3	1:B:274:PRO:HD3	1.78	0.66
1:B:152:THR:HG22	1:B:277:GLN:HE21	1.60	0.66
1:A:320:ARG:HG2	1:A:323:ARG:HH21	1.60	0.65
1:A:218:PRO:HG3	1:A:404:TRP:CD1	2.32	0.64
1:A:320:ARG:HG2	1:A:323:ARG:NH2	2.13	0.64
1:A:232:ALA:O	1:A:360:ARG:HD2	1.98	0.64
1:B:252:ARG:NH2	1:B:412:LYS:HD2	2.12	0.63
1:B:392:ARG:HH11	1:B:392:ARG:CB	2.11	0.62
1:B:217:VAL:CG1	1:B:218:PRO:HD2	2.30	0.62
1:A:70:MET:HE1	1:A:101:ILE:HG22	1.82	0.62
1:B:372:CYS:HB3	1:B:388:GLN:HE21	1.66	0.61
1:A:230:GLU:H	1:A:230:GLU:CD	2.07	0.61
1:B:152:THR:CG2	1:B:277:GLN:HE21	2.14	0.61
1:A:403:ALA:O	1:A:407:GLU:HG3	2.01	0.61
1:A:406:LEU:HD23	1:A:406:LEU:O	2.01	0.60
1:A:324:ARG:HB3	3:A:2370:HOH:O	2.02	0.60
1:B:169:LYS:HE2	3:B:2287:HOH:O	2.02	0.59
1:A:412:LYS:HE2	1:A:412:LYS:CA	2.30	0.59
1:A:273:HIS:HB3	1:A:274:PRO:HD3	1.84	0.59
1:B:77:GLU:HG2	3:B:2155:HOH:O	2.03	0.59
1:B:225:GLY:N	1:B:336:VAL:HG11	2.17	0.59
1:A:172:PHE:CD2	1:A:173:ARG:HG3	2.37	0.59
1:A:142:GLY:HA2	3:A:2198:HOH:O	2.01	0.58
1:B:283:ARG:NH2	3:B:2376:HOH:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ARG:HD2	3:A:2248:HOH:O	2.04	0.57
1:A:304:LEU:HD23	3:A:2343:HOH:O	2.03	0.57
1:B:146:LEU:HD12	1:B:193:PHE:O	2.03	0.57
1:A:161:ALA:HB2	1:A:374:ASN:ND2	2.20	0.57
1:B:34:LYS:HB2	3:B:2083:HOH:O	2.04	0.56
1:B:392:ARG:HB2	1:B:392:ARG:CZ	2.35	0.56
1:A:112:SER:HB3	3:A:2170:HOH:O	2.05	0.56
1:A:119:LEU:HD13	1:A:124:THR:CG2	2.32	0.55
1:A:210:ARG:NH2	1:B:316:ASP:OD2	2.39	0.55
1:B:221:ALA:N	1:B:222:PRO:HD3	2.21	0.55
1:B:70:MET:C	1:B:83:GLN:HE22	2.13	0.55
1:B:208:THR:HB	1:B:210:ARG:HG3	1.88	0.55
1:B:235:VAL:HG22	1:B:345:PRO:O	2.07	0.55
1:B:218:PRO:HG3	1:B:404:TRP:CD1	2.42	0.54
1:A:47:ARG:HD2	3:A:2072:HOH:O	2.07	0.54
1:B:41:ARG:HG2	1:B:41:ARG:HH11	1.71	0.54
1:A:324:ARG:HD3	3:A:2370:HOH:O	2.08	0.53
1:A:77:GLU:HG3	3:A:2115:HOH:O	2.08	0.53
1:A:42:HIS:CE1	1:A:44:LYS:HE3	2.43	0.52
1:B:331:GLU:O	1:B:334:GLU:HG3	2.09	0.52
1:B:92:MET:SD	1:B:95:LYS:HE2	2.50	0.52
1:A:80:ARG:NH2	3:A:2119:HOH:O	2.43	0.52
1:A:337:ASP:HB3	1:A:398:HIS:HE1	1.72	0.51
1:B:151:GLN:HA	1:B:155:SER:HB2	1.92	0.51
1:A:16:LEU:HD12	1:A:17:SER:H	1.75	0.51
1:A:217:VAL:CG2	1:A:218:PRO:HD2	2.39	0.51
1:B:22:ILE:CG1	1:B:48:ALA:HB2	2.40	0.51
1:A:173:ARG:HD3	3:A:2208:HOH:O	2.10	0.51
1:A:272:ILE:C	1:A:272:ILE:HD12	2.35	0.51
1:A:338:VAL:HG21	1:A:402:THR:HG21	1.92	0.51
1:B:230:GLU:H	1:B:230:GLU:CD	2.19	0.51
1:B:220:LYS:O	1:B:221:ALA:C	2.53	0.50
1:A:247:ILE:HD12	3:A:2264:HOH:O	2.10	0.50
1:B:11:ILE:HA	1:B:16:LEU:O	2.10	0.50
1:A:218:PRO:HG3	1:A:404:TRP:CG	2.47	0.50
1:A:221:ALA:N	1:A:222:PRO:HD3	2.26	0.50
1:A:124:THR:HG21	3:A:2051:HOH:O	2.11	0.50
1:B:218:PRO:HG3	1:B:404:TRP:CG	2.47	0.50
1:B:276:ILE:O	1:B:280:GLU:HG3	2.12	0.50
1:B:338:VAL:HG21	1:B:402:THR:HG21	1.95	0.49
1:B:32:ARG:NH1	1:B:35:GLU:OE1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:LEU:HB3	1:B:199:ASP:HB3	1.95	0.49
1:B:212:GLU:HG2	3:B:2311:HOH:O	2.11	0.49
1:A:117:ALA:HB1	3:A:2054:HOH:O	2.11	0.48
1:A:217:VAL:HG22	1:A:218:PRO:HD2	1.94	0.48
1:B:45:SER:O	1:B:47:ARG:HG3	2.13	0.48
1:B:122:HIS:CD2	1:B:384:PRO:HG2	2.47	0.48
1:A:55:ARG:HH11	1:A:55:ARG:HG2	1.79	0.48
1:A:4:LEU:HD23	1:A:4:LEU:C	2.39	0.48
1:A:114:ASP:OD1	1:A:299:MET:HG3	2.14	0.47
1:B:41:ARG:HG2	1:B:41:ARG:NH1	2.29	0.47
1:B:201:ALA:HB1	3:B:2312:HOH:O	2.13	0.47
1:A:236:GLU:HB2	1:A:345:PRO:O	2.15	0.47
1:B:64:ILE:HB	1:B:181:LYS:HB3	1.96	0.47
1:B:377:VAL:HG12	1:B:378:LEU:HD12	1.97	0.46
1:A:210:ARG:HH22	1:B:316:ASP:CG	2.23	0.46
1:B:22:ILE:HG13	1:B:48:ALA:HB2	1.96	0.46
1:A:231:PHE:CE1	1:A:262:LEU:HD12	2.50	0.46
1:B:47:ARG:HD2	3:B:2114:HOH:O	2.16	0.46
1:A:208:THR:HB	1:A:210:ARG:HG3	1.97	0.46
1:B:377:VAL:HG21	1:B:387:VAL:HG13	1.98	0.46
1:B:312:PRO:HD2	3:B:2408:HOH:O	2.14	0.46
1:A:227:VAL:O	1:A:227:VAL:HG23	2.15	0.45
1:A:410:LEU:C	1:A:412:LYS:H	2.24	0.45
1:A:406:LEU:HD23	1:A:406:LEU:C	2.40	0.45
1:B:170:PRO:HD2	1:B:190:VAL:O	2.16	0.45
1:B:392:ARG:HG3	3:B:2476:HOH:O	2.17	0.45
1:B:229:GLN:HA	1:B:231:PHE:CE1	2.52	0.45
1:A:208:THR:CB	1:A:210:ARG:HG3	2.46	0.45
1:B:120:ASN:HA	1:B:121:PRO:HD3	1.86	0.45
1:A:231:PHE:HE1	1:A:262:LEU:HD12	1.82	0.44
1:B:223:ARG:HD2	3:B:2320:HOH:O	2.17	0.44
1:A:18:PRO:HG2	3:A:2078:HOH:O	2.16	0.44
1:B:7:LEU:O	1:B:11:ILE:HG13	2.16	0.44
1:B:196:ARG:HD3	3:B:2291:HOH:O	2.17	0.44
1:B:372:CYS:CB	1:B:388:GLN:HE21	2.30	0.44
1:B:244:GLN:HG2	3:B:2346:HOH:O	2.17	0.44
1:A:297:ALA:HA	1:A:298:PRO:HD3	1.86	0.44
1:A:61:ILE:HD12	1:A:148:LEU:HD12	2.00	0.44
1:A:144:ILE:HD12	1:A:146:LEU:O	2.18	0.44
1:B:383:LEU:HD22	1:B:383:LEU:N	2.32	0.44
1:B:273:HIS:N	1:B:274:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ASN:HA	1:A:121:PRO:HD3	1.88	0.43
1:A:272:ILE:HG21	1:A:321:ILE:HD12	2.00	0.43
1:A:378:LEU:C	1:A:378:LEU:HD12	2.43	0.43
1:B:220:LYS:C	1:B:222:PRO:HD3	2.44	0.43
1:B:333:PHE:CD1	1:B:392:ARG:HB3	2.54	0.43
1:A:181:LYS:HD2	3:A:2222:HOH:O	2.17	0.43
1:B:272:ILE:C	1:B:272:ILE:HD12	2.44	0.43
1:B:227:VAL:O	1:B:227:VAL:HG23	2.17	0.43
1:B:108:THR:OG1	1:B:131:SER:HB2	2.18	0.43
1:B:217:VAL:CG1	1:B:218:PRO:CD	2.96	0.43
1:A:41:ARG:HD2	1:A:70:MET:HB3	2.00	0.43
1:A:191:GLY:C	1:A:192:LEU:HD12	2.44	0.43
1:B:155:SER:O	1:B:159:PRO:HG3	2.19	0.43
1:B:282:HIS:CE1	1:B:308:VAL:HG22	2.54	0.42
1:A:316:ASP:O	1:A:320:ARG:HG3	2.19	0.42
1:A:222:PRO:HG2	1:A:405:PHE:CD2	2.54	0.42
1:A:273:HIS:N	1:A:274:PRO:CD	2.82	0.42
1:B:316:ASP:HB2	3:B:2409:HOH:O	2.19	0.42
1:A:22:ILE:HG13	1:A:48:ALA:HB2	2.01	0.42
1:A:348:ALA:HA	1:A:349:PRO:HD3	1.82	0.42
1:A:131:SER:H	1:A:155:SER:CB	2.32	0.42
1:A:383:LEU:HD22	1:A:383:LEU:N	2.35	0.42
1:B:358:ASP:HA	1:B:359:PRO:HD3	1.85	0.42
1:A:212:GLU:H	1:A:212:GLU:CD	2.28	0.41
1:A:377:VAL:HG21	1:A:387:VAL:HG13	2.01	0.41
1:B:114:ASP:HA	1:B:115:PRO:HD3	1.93	0.41
1:A:243:LEU:O	1:A:247:ILE:HG13	2.20	0.41
1:A:320:ARG:HA	1:A:323:ARG:HH21	1.85	0.41
1:A:368:MET:HA	1:A:368:MET:HE2	2.01	0.41
1:B:8:GLN:OE1	1:B:202:ARG:HD3	2.20	0.41
1:A:170:PRO:HD2	1:A:190:VAL:O	2.20	0.41
1:B:33:GLU:OE2	1:B:33:GLU:HA	2.21	0.41
1:A:138:ALA:O	1:A:143:MET:HB2	2.19	0.41
1:A:372:CYS:HB3	1:A:388:GLN:HE21	1.85	0.41
1:B:183:TYR:HE1	1:B:277:GLN:HG2	1.85	0.41
1:A:20:ALA:O	1:A:24:GLN:HG3	2.20	0.41
1:B:208:THR:CB	1:B:210:ARG:HG3	2.51	0.41
1:A:262:LEU:O	1:A:267:HIS:NE2	2.53	0.41
1:B:349:PRO:HB3	1:B:353:LEU:HD12	2.03	0.41
1:A:300:LEU:HA	3:A:2177:HOH:O	2.21	0.41
1:A:89:PRO:HD2	1:A:178:VAL:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:TRP:CE3	1:B:86:SER:HB3	2.56	0.40
1:B:239:ALA:HB2	1:B:346:GLY:HA2	2.03	0.40
1:B:235:VAL:HG23	1:B:345:PRO:HA	2.03	0.40
1:B:70:MET:HE1	1:B:101:ILE:HG22	2.03	0.40
1:A:124:THR:O	1:A:124:THR:HG22	2.20	0.40
1:B:236:GLU:HB2	1:B:345:PRO:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	297/305 (97%)	294 (99%)	3 (1%)	68	75
1	B	304/305 (100%)	298 (98%)	6 (2%)	48	54
All	All	601/610 (98%)	592 (98%)	9 (2%)	57	64

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	PRO
1	A	212	GLU
1	A	283	ARG
1	B	24	GLN
1	B	30	GLU
1	B	32	ARG
1	B	378	LEU

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Mol	Chain	Res	Type
1	B	392	ARG
1	B	406	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	37	HIS
1	A	83	GLN
1	A	277	GLN
1	A	362	ASN
1	A	374	ASN
1	A	388	GLN
1	A	398	HIS
1	B	24	GLN
1	B	83	GLN
1	B	277	GLN
1	B	388	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 ⓘ

There are no oligosaccharides 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	MLA	A	501	-	6,6,6	2.25	2 (33%)	7,7,7	2.07	2 (28%)
2	MLA	B	501	-	6,6,6	2.33	2 (33%)	7,7,7	1.99	2 (28%)

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	MLA	A	501	-	-	2/4/4/4	-
2	MLA	B	501	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	MLA	O1B-C1	3.89	1.34	1.22
2	A	501	MLA	O1B-C1	3.80	1.34	1.22
2	B	501	MLA	O1A-C1	-3.40	1.19	1.30
2	A	501	MLA	O1A-C1	-3.21	1.20	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	MLA	O1B-C1-C2	-3.74	111.45	122.11
2	A	501	MLA	O1A-C1-C2	3.68	125.92	114.51
2	B	501	MLA	O1B-C1-C2	-3.56	111.96	122.11
2	B	501	MLA	O1A-C1-C2	3.55	125.50	114.51

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	MLA	C1-C2-C3-O3A
2	A	501	MLA	C1-C2-C3-O3B
2	B	501	MLA	C1-C2-C3-O3A
2	B	501	MLA	C1-C2-C3-O3B

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

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.