



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 03:40 PM EDT

PDB ID : 8OZ7 / pdb_00008oz7
Title : Abortive infection DNA polymerase AbiA from *Lactococcus lactis*
Authors : Gapinska, M.A.; Nowotny, M.
Deposited on : 2023-05-08
Resolution : 2.75 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
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

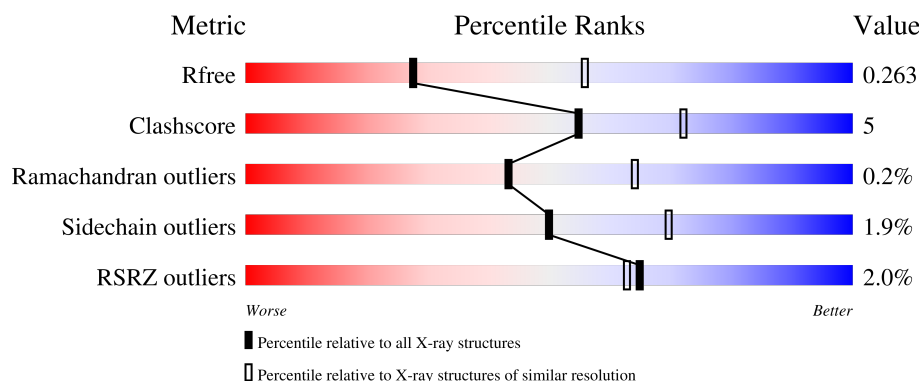
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	730	% 71% 11% 18%
1	B	730	% 69% 12% 19%
1	C	730	2% 69% 11% 20%
1	D	730	2% 71% 9% 20%
2	E	9	% 56% 44%

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Mol	Chain	Length	Quality of chain
2	F	9	56% 44%
2	G	9	44% 11% 44%
2	H	9	78% 22%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19626 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 AbiA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	0	1	0
			4883	3166	777	927	13			
1	B	594	Total	C	N	O	S	0	3	0
			4757	3085	751	909	12			
1	C	586	Total	C	N	O	S	0	2	0
			4687	3034	754	886	13			
1	D	587	Total	C	N	O	S	0	1	0
			4662	3021	746	883	12			

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*AP*AP*AP*AP*AP*AP*T)-3').

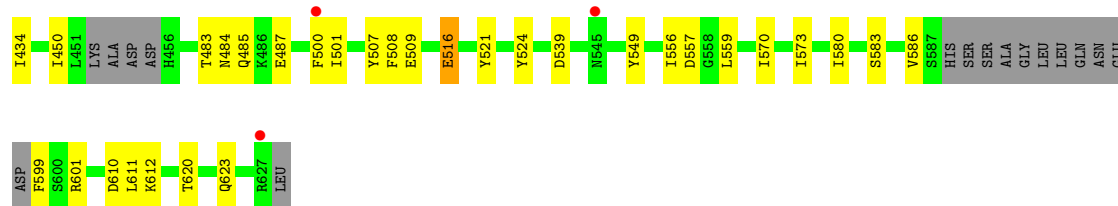
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	9	Total	C	N	O	P	0	0	0
			177	85	41	43	8			
2	F	5	Total	C	N	O	P	0	0	0
			104	50	22	27	5			
2	G	5	Total	C	N	O	P	0	0	0
			104	50	22	27	5			
2	H	7	Total	C	N	O	P	0	0	0
			138	65	31	35	7			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

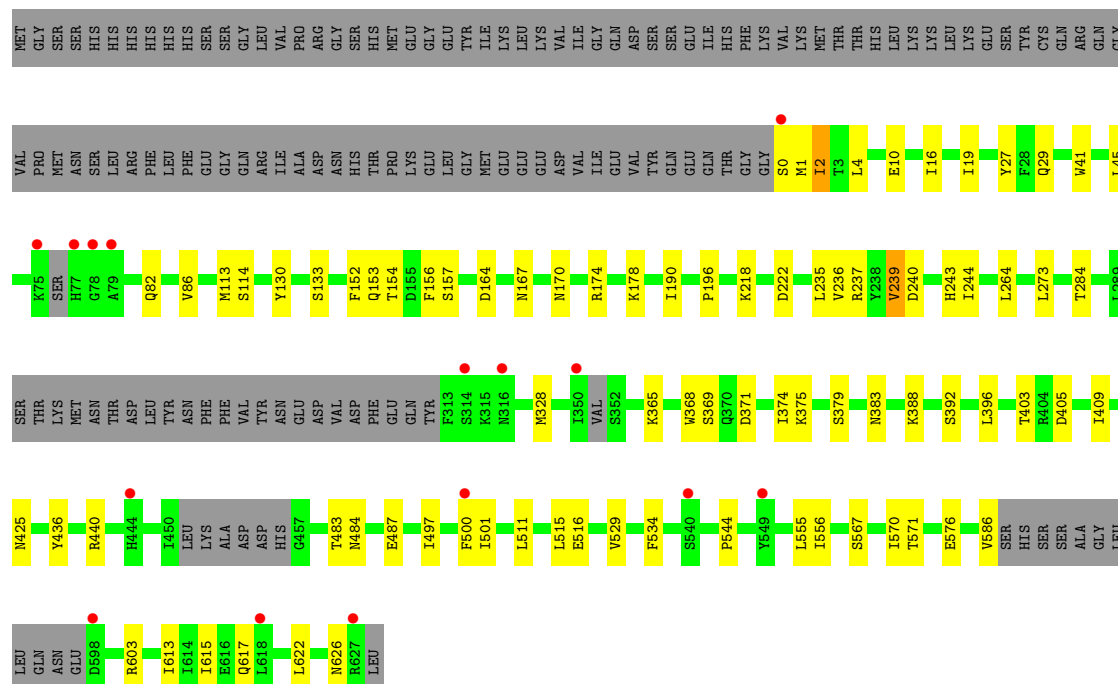
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

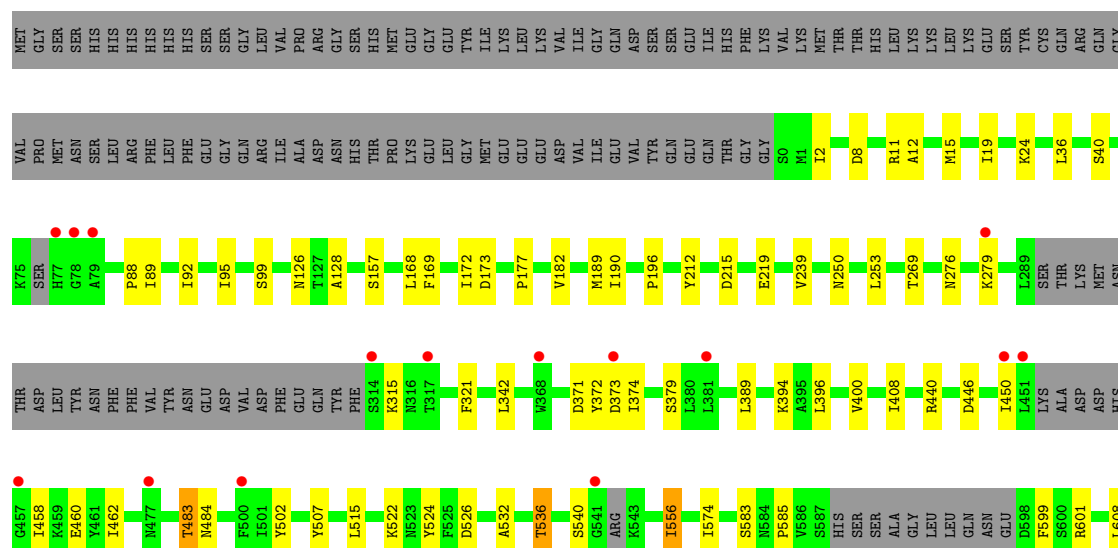
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total 44	O 44	0	0
4	B	22	Total 22	O 22	0	0
4	C	26	Total 26	O 26	0	0
4	D	20	Total 20	O 20	0	0
4	G	1	Total 1	O 1	0	0



● Molecule 1: AbiA

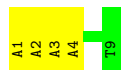


● Molecule 1: AbiA

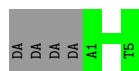




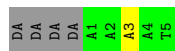
- Molecule 2: DNA (5'-D(*AP*AP*AP*AP*AP*AP*AP*AP*T)-3')



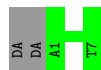
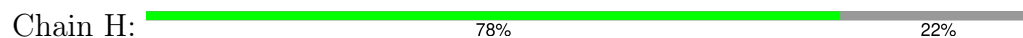
- Molecule 2: DNA (5'-D(*AP*AP*AP*AP*AP*AP*AP*AP*T)-3')



- Molecule 2: DNA (5'-D(*AP*AP*AP*AP*AP*AP*AP*AP*T)-3')



- Molecule 2: DNA (5'-D(*AP*AP*AP*AP*AP*AP*AP*AP*T)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	84.09Å 86.10Å 117.01Å 99.32° 90.18° 90.27°	Depositor
Resolution (Å)	38.49 – 2.75 38.49 – 2.75	Depositor EDS
% Data completeness (in resolution range)	95.1 (38.49-2.75) 95.1 (38.49-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.220 , 0.264 0.220 , 0.263	Depositor DCC
R_{free} test set	2101 reflections (2.49%)	wwPDB-VP
Wilson B-factor (Å ²)	61.7	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19626	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.11	0/4990	0.24	0/6749
1	B	0.09	0/4868	0.23	0/6604
1	C	0.09	0/4788	0.23	0/6489
1	D	0.09	0/4762	0.22	0/6455
2	E	0.20	0/201	0.35	0/308
2	F	0.17	0/117	0.33	0/178
2	G	0.17	0/117	0.32	0/178
2	H	0.17	0/156	0.31	0/238
All	All	0.10	0/19999	0.24	0/27199

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4883	0	4748	38	0
1	B	4757	0	4518	54	0
1	C	4687	0	4446	48	0
1	D	4662	0	4426	46	0
2	E	177	0	97	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	104	0	57	0	0
2	G	104	0	57	1	0
2	H	138	0	74	0	0
3	B	1	0	0	0	0
4	A	44	0	0	0	0
4	B	22	0	0	0	0
4	C	26	0	0	1	0
4	D	20	0	0	0	0
4	G	1	0	0	0	0
All	All	19626	0	18423	181	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 5.

All (181) 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:D:12:ALA:HA	1:D:15:MET:HE2	1.76	0.68
1:B:559:LEU:HB3	1:B:570:ILE:HD13	1.76	0.67
1:B:11:ARG:O	1:B:15:MET:HG3	1.95	0.66
1:B:2:ILE:HG22	1:B:4:LEU:H	1.59	0.66
1:B:389:LEU:HD22	1:B:396:LEU:HB3	1.78	0.65
1:B:113:MET:HB2	1:B:235:LEU:HB2	1.80	0.64
1:D:189:MET:HE3	1:D:507:TYR:HA	1.79	0.63
1:B:195:MET:HE3	1:B:208:ASN:HD21	1.65	0.62
1:C:529:VAL:HG21	1:C:555:LEU:HD11	1.82	0.61
1:C:556:ILE:HD13	1:C:571:THR:HA	1.81	0.61
1:B:556:ILE:HG22	1:B:570:ILE:HG22	1.83	0.61
1:C:16:ILE:HG22	1:C:41:TRP:HH2	1.66	0.60
1:C:153:GLN:OE1	1:C:243:HIS:NE2	2.35	0.59
1:A:219:GLU:HB3	1:A:267:LYS:HD2	1.84	0.59
1:C:29:GLN:HE22	1:C:86:VAL:H	1.50	0.59
1:B:387:ARG:NH2	1:B:426:ASP:OD2	2.36	0.59
1:C:10:GLU:HB2	1:C:45:LEU:HD23	1.85	0.59
1:D:11:ARG:O	1:D:15:MET:HG3	2.03	0.59
1:C:2:ILE:HG23	1:C:4:LEU:H	1.67	0.58
1:B:573:ILE:HD12	1:B:610:ASP:HB3	1.85	0.58
1:D:321:PHE:HE1	1:D:342:LEU:HD12	1.67	0.58
1:C:497:ILE:O	1:C:501:ILE:HG12	2.03	0.58
1:D:173:ASP:N	1:D:173:ASP:OD1	2.34	0.58
1:D:483:THR:OG1	1:D:484:ASN:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:LYS:NZ	1:C:405:ASP:OD2	2.38	0.57
1:B:15:MET:HG2	1:B:126:ASN:HB3	1.84	0.57
1:A:533:MET:HG3	1:A:549:TYR:CZ	2.40	0.57
1:C:576:GLU:OE1	1:C:603:ARG:NH2	2.35	0.57
1:A:22:SER:O	1:A:26:LYS:NZ	2.38	0.56
1:D:389:LEU:HD22	1:D:396:LEU:HB3	1.85	0.56
1:A:177:PRO:HG3	1:B:601:ARG:HG3	1.87	0.56
1:D:169:PHE:HA	1:D:172:ILE:HD12	1.86	0.55
1:B:140:GLU:OE2	1:B:234:LYS:NZ	2.39	0.55
1:A:585:PRO:HB3	1:B:1:MET:HE1	1.89	0.55
1:B:235:LEU:HD23	1:B:242:LEU:HD11	1.89	0.55
1:C:1:MET:HA	1:C:178:LYS:HD2	1.88	0.55
1:A:353:ASP:OD1	1:A:354:GLY:N	2.40	0.54
1:B:509:GLU:OE2	1:B:612:LYS:NZ	2.39	0.54
1:C:409:ILE:HG21	1:C:440:ARG:HH11	1.73	0.54
1:D:2:ILE:HD11	1:D:182:VAL:HG11	1.90	0.54
1:B:371:ASP:OD1	1:B:372:TYR:N	2.41	0.53
1:D:583:SER:O	1:D:583:SER:OG	2.24	0.53
1:D:583:SER:HB3	1:D:599:PHE:HE2	1.74	0.53
1:B:372:TYR:O	1:B:376:ASN:ND2	2.38	0.53
1:B:108:LYS:HB3	1:B:218:LYS:HG3	1.89	0.52
1:A:366:SER:OG	1:A:404:ARG:NH1	2.43	0.52
1:A:11:ARG:O	1:A:15:MET:HG3	2.09	0.52
1:A:113:MET:HE1	1:A:237:ARG:HE	1.75	0.52
1:D:157:SER:OG	1:D:276:ASN:OD1	2.20	0.51
1:A:235:LEU:HD22	1:A:242:LEU:HD11	1.92	0.51
1:C:170:ASN:O	1:D:601:ARG:NH2	2.43	0.51
1:D:19:ILE:HD11	1:D:128:ALA:HB3	1.92	0.51
1:C:0:SER:OG	1:C:1:MET:N	2.43	0.51
1:D:15:MET:HG2	1:D:126:ASN:HB3	1.93	0.51
1:D:19:ILE:O	1:D:24:LYS:NZ	2.41	0.51
1:D:522:LYS:NZ	1:D:526:ASP:OD1	2.43	0.51
1:D:532:ALA:O	1:D:536:THR:OG1	2.24	0.51
1:D:168:LEU:HD13	1:D:212:TYR:HB2	1.93	0.50
1:C:113:MET:HE3	1:C:235:LEU:HB3	1.93	0.50
1:C:483:THR:OG1	1:C:484:ASN:N	2.40	0.50
1:C:516:GLU:HG3	1:C:586:VAL:HG11	1.92	0.50
1:B:189:MET:HB2	1:B:507:TYR:HD1	1.77	0.50
1:B:483:THR:HG23	1:B:485:GLN:H	1.76	0.50
1:C:154:THR:HG21	1:C:264:LEU:HD13	1.93	0.50
1:B:539:ASP:OD2	1:B:549:TYR:OH	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:PHE:HB3	1:A:244:ILE:HB	1.94	0.50
1:A:369:SER:HB3	1:A:403:THR:HG22	1.93	0.50
1:D:371:ASP:HB3	1:D:374:ILE:HB	1.94	0.50
1:C:371:ASP:HB3	1:C:374:ILE:HB	1.94	0.49
1:C:613:ILE:O	1:C:617:GLN:HG2	2.12	0.49
1:A:405:ASP:HB3	1:A:408:ILE:HB	1.95	0.49
1:D:36:LEU:HG	1:D:40:SER:HB2	1.94	0.49
1:D:556:ILE:HD11	1:D:574:ILE:HB	1.95	0.49
1:B:501:ILE:HG22	1:B:524:TYR:HB2	1.95	0.49
1:A:33:PHE:HE2	1:A:92:ILE:HD11	1.77	0.49
1:A:330:VAL:O	1:A:390:ARG:NH2	2.46	0.49
1:C:190:ILE:HB	1:C:196:PRO:HG3	1.94	0.48
1:D:440:ARG:HH21	1:D:446:ASP:CG	2.20	0.48
1:C:239:VAL:HG12	1:C:240:ASP:N	2.27	0.48
1:B:116:TYR:OH	1:B:140:GLU:OE1	2.25	0.48
1:B:325:LEU:HB2	1:B:341:VAL:HG11	1.96	0.48
1:B:224:LEU:HA	1:B:227:ILE:HD12	1.95	0.48
1:B:195:MET:HE3	1:B:208:ASN:ND2	2.28	0.48
1:A:232:SER:HB2	1:C:174:ARG:HH21	1.78	0.47
1:A:319:ILE:HG23	1:A:377:LYS:HE3	1.95	0.47
1:A:66:LEU:HB3	1:A:189:MET:HE1	1.96	0.47
1:B:430:GLU:O	1:B:434:ILE:HG12	2.14	0.47
1:C:425:ASN:OD1	1:C:425:ASN:N	2.48	0.47
1:C:392:SER:HB2	1:C:396:LEU:HG	1.96	0.47
1:A:404:ARG:HH21	2:E:3:DA:H62	1.63	0.47
1:C:218:LYS:NZ	4:C:703:HOH:O	2.37	0.47
1:D:190:ILE:HB	1:D:196:PRO:HG3	1.97	0.47
1:B:413:LEU:HD11	1:B:450:ILE:HD11	1.97	0.47
1:C:156:PHE:HB2	1:C:240:ASP:HB2	1.97	0.47
1:B:41:TRP:O	1:B:45:LEU:HD12	2.14	0.47
1:B:113:MET:HE3	1:B:237:ARG:HB3	1.97	0.46
1:C:436:TYR:CE1	1:C:440:ARG:HD3	2.50	0.46
1:A:479:VAL:O	1:A:480:ILE:HD13	2.15	0.46
1:D:515:LEU:HD13	1:D:585:PRO:HD2	1.98	0.46
1:B:137:TYR:CZ	1:B:141:LEU:HD11	2.51	0.46
1:A:9:TRP:O	1:A:13:VAL:HG23	2.16	0.45
1:C:369:SER:HB3	1:C:403:THR:HG22	1.97	0.45
2:E:1:DA:H4'	2:E:2:DA:OP1	2.16	0.45
1:A:8:ASP:OD2	1:A:103:ARG:NH2	2.32	0.45
1:A:113:MET:HG3	1:A:235:LEU:HB3	1.98	0.45
1:C:379:SER:O	1:C:383:ASN:ND2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:PHE:CD1	1:B:516[B]:GLU:HG3	2.51	0.45
1:B:321:PHE:HB2	1:B:345:LEU:HD21	1.97	0.45
1:B:342:LEU:HD23	1:B:342:LEU:HA	1.80	0.45
1:B:227:ILE:HB	1:B:230:ILE:HD12	1.99	0.45
1:D:502:TYR:HB2	1:D:524:TYR:CD1	2.52	0.45
1:A:373:ASP:O	1:A:377:LYS:HG3	2.17	0.44
1:B:580:ILE:HG12	1:B:599:PHE:HE2	1.81	0.44
1:B:516[A]:GLU:HG3	1:B:586:VAL:HG11	1.99	0.44
1:C:615:ILE:HD13	1:C:615:ILE:HA	1.87	0.44
1:A:174:ARG:HA	1:A:174:ARG:HD2	1.83	0.44
1:D:253:LEU:HD23	1:D:253:LEU:HA	1.84	0.44
1:A:32:PRO:HD3	1:A:466:GLN:OE1	2.18	0.44
1:C:515:LEU:HD23	1:C:515:LEU:HA	1.87	0.44
1:A:374:ILE:O	1:A:378:ILE:HG13	2.18	0.44
1:A:515:LEU:HD13	1:A:585:PRO:HD2	2.00	0.44
1:D:371:ASP:OD2	1:D:372:TYR:N	2.51	0.44
1:A:19:ILE:HD11	1:A:128:ALA:HB3	2.00	0.44
1:B:68:PHE:HE2	1:B:189:MET:HG2	1.81	0.44
1:C:500[A]:PHE:CE2	1:D:585:PRO:HB3	2.52	0.44
1:D:446:ASP:O	1:D:450:ILE:HG22	2.18	0.44
1:B:2:ILE:HD12	1:B:500[B]:PHE:HZ	1.83	0.43
1:D:462:ILE:HD12	1:D:462:ILE:H	1.83	0.43
1:A:68:PHE:HE2	1:A:189:MET:HE2	1.82	0.43
1:B:22:SER:O	1:B:26:LYS:HE2	2.18	0.43
1:C:114:SER:HB2	1:C:236:VAL:HG22	1.99	0.43
2:E:3:DA:H4'	2:E:4:DA:OP2	2.18	0.43
1:C:19:ILE:H	1:C:19:ILE:HD12	1.83	0.43
1:C:218:LYS:NZ	1:C:222:ASP:OD2	2.41	0.43
1:C:82:GLN:HG2	1:D:269:THR:HG22	1.99	0.43
1:A:440:ARG:HD3	1:A:446:ASP:OD2	2.18	0.43
1:A:489:TYR:HE2	1:A:492:ILE:HG13	1.83	0.43
1:B:521:TYR:HE2	1:B:611:LEU:HB3	1.84	0.43
1:B:76:SER:OG	1:B:77:HIS:ND1	2.49	0.43
1:B:113:MET:HE2	1:B:115:VAL:HB	2.01	0.43
1:D:88:PRO:O	1:D:92:ILE:HG13	2.19	0.43
1:B:190:ILE:HB	1:B:196:PRO:HG3	2.01	0.43
1:B:109:ARG:HH12	1:B:210:VAL:HA	1.83	0.43
1:B:240:ASP:OD1	1:B:240:ASP:N	2.49	0.43
1:D:556:ILE:HD13	1:D:556:ILE:HA	1.74	0.43
1:A:173:ASP:N	1:A:173:ASP:OD1	2.52	0.42
1:A:318:LEU:HD23	1:A:374:ILE:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:460:GLU:CD	1:D:460:GLU:H	2.27	0.42
1:C:27:TYR:OH	2:G:3:DA:OP2	2.31	0.42
1:C:328:MET:O	1:C:388:LYS:NZ	2.41	0.42
1:C:152:PHE:HB3	1:C:244:ILE:HB	2.02	0.42
1:C:534:PHE:CD1	1:C:544:PRO:HD3	2.55	0.42
1:D:371:ASP:OD2	1:D:373:ASP:N	2.50	0.42
1:A:246:ILE:HD13	1:A:283:PHE:CE1	2.55	0.42
1:A:556:ILE:HG23	1:A:570:ILE:HG22	2.02	0.42
1:B:330:VAL:HG22	1:B:390:ARG:HH12	1.84	0.42
1:B:484:ASN:N	1:B:484:ASN:OD1	2.52	0.42
1:D:279:LYS:HE2	1:D:279:LYS:HB3	1.83	0.42
1:D:396:LEU:O	1:D:400:VAL:HG23	2.19	0.42
1:D:8:ASP:HB3	1:D:99:SER:HB3	2.01	0.41
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.89	0.41
1:C:130:TYR:CD1	1:C:130:TYR:C	2.99	0.41
1:D:215:ASP:O	1:D:219:GLU:HG3	2.20	0.41
1:C:567:SER:HA	1:C:570:ILE:HG12	2.02	0.41
1:D:379:SER:HB2	1:D:408:ILE:HD11	2.01	0.41
1:D:394:LYS:HD2	1:D:394:LYS:HA	1.80	0.41
1:D:458:ILE:HG12	1:D:462:ILE:HD11	2.03	0.41
1:D:315:LYS:HZ3	1:D:315:LYS:HG3	1.79	0.41
1:A:502:TYR:HB2	1:A:524:TYR:CD1	2.56	0.41
1:B:378:ILE:HG21	1:B:403:THR:HG21	2.03	0.41
1:C:113:MET:HE2	1:C:237:ARG:HB2	2.02	0.41
1:C:365:LYS:HB3	1:C:368:TRP:CG	2.56	0.41
1:B:152:PHE:HB2	1:B:283:PHE:CE1	2.56	0.40
1:B:321:PHE:CE1	1:B:341:VAL:HG12	2.56	0.40
1:B:556:ILE:HD12	1:B:557:ASP:N	2.36	0.40
1:C:483:THR:HG22	1:C:487:GLU:O	2.21	0.40
1:C:515:LEU:HG	1:D:177:PRO:HB2	2.03	0.40
1:D:89:ILE:HD13	1:D:89:ILE:HA	1.88	0.40
1:B:508:PHE:CE2	1:B:516[A]:GLU:HG2	2.56	0.40
1:C:164:ASP:HB3	1:C:167:ASN:HB3	2.04	0.40
1:B:483:THR:HG22	1:B:487:GLU:H	1.86	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	588/730 (80%)	572 (97%)	15 (3%)	1 (0%)	43	64
1	B	589/730 (81%)	574 (98%)	14 (2%)	1 (0%)	43	64
1	C	576/730 (79%)	552 (96%)	23 (4%)	1 (0%)	43	64
1	D	576/730 (79%)	552 (96%)	23 (4%)	1 (0%)	43	64
All	All	2329/2920 (80%)	2250 (97%)	75 (3%)	4 (0%)	43	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	239	VAL
1	D	239	VAL
1	A	239	VAL
1	B	239	VAL

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	537/680 (79%)	523 (97%)	14 (3%)	40	63
1	B	507/680 (75%)	496 (98%)	11 (2%)	45	67
1	C	495/680 (73%)	487 (98%)	8 (2%)	55	73
1	D	492/680 (72%)	485 (99%)	7 (1%)	59	75
All	All	2031/2720 (75%)	1991 (98%)	40 (2%)	50	69

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	115	VAL
1	A	154	THR
1	A	171	LYS
1	A	260	VAL
1	A	269	THR
1	A	273	LEU
1	A	275	ILE
1	A	284	THR
1	A	352	SER
1	A	449	THR
1	A	451	LEU
1	A	512	ASP
1	A	618	LEU
1	B	133	SER
1	B	202	SER
1	B	240	ASP
1	B	284	THR
1	B	330	VAL
1	B	397	ILE
1	B	516[A]	GLU
1	B	516[B]	GLU
1	B	583	SER
1	B	620	THR
1	B	623	GLN
1	C	2	ILE
1	C	133	SER
1	C	157	SER
1	C	273	LEU
1	C	284	THR
1	C	511	LEU
1	C	622	LEU
1	C	626	ASN
1	D	95	ILE
1	D	250	ASN
1	D	483	THR
1	D	536	THR
1	D	540	SER
1	D	556	ILE
1	D	608	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	132	GLN
1	A	153	GLN
1	A	316	ASN
1	A	444	HIS
1	A	623	GLN
1	A	624	ASN
1	B	82	GLN
1	B	243	HIS
1	B	262	ASN
1	B	385	ASN
1	B	531	HIS
1	B	578	HIS
1	B	623	GLN
1	C	29	GLN
1	C	100	GLN
1	C	132	GLN
1	C	142	ASN
1	C	422	ASN
1	D	14	ASN
1	D	63	GLN
1	D	326	ASN
1	D	414	ASN
1	D	578	HIS

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

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	597/730 (81%)	-0.05	7 (1%) 76 76	34, 59, 95, 137	1 (0%)
1	B	594/730 (81%)	0.14	10 (1%) 69 67	36, 67, 118, 152	3 (0%)
1	C	586/730 (80%)	0.28	15 (2%) 57 55	40, 73, 118, 163	2 (0%)
1	D	587/730 (80%)	0.28	15 (2%) 57 55	37, 73, 124, 160	1 (0%)
2	E	9/9 (100%)	0.21	0 100 100	58, 70, 149, 152	0
2	F	5/9 (55%)	-0.06	0 100 100	83, 86, 101, 102	0
2	G	5/9 (55%)	0.32	0 100 100	88, 89, 103, 111	0
2	H	7/9 (77%)	0.71	0 100 100	84, 97, 108, 158	0
All	All	2390/2956 (80%)	0.16	47 (1%) 65 63	34, 68, 117, 163	7 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	77	HIS	4.3
1	C	75	LYS	4.0
1	B	0	SER	3.6
1	C	500[A]	PHE	3.5
1	A	597	GLU	3.5
1	D	381	LEU	3.3
1	D	317	THR	3.3
1	D	77	HIS	3.2
1	A	311	GLN	3.2
1	C	627	ARG	3.0
1	D	500[A]	PHE	2.9
1	C	79	ALA	2.9
1	A	628	LEU	2.8
1	A	500[A]	PHE	2.8
1	D	314	SER	2.7
1	C	540	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	78	GLY	2.6
1	C	598	ASP	2.6
1	D	450	ILE	2.6
1	C	444[A]	HIS	2.6
1	B	308	ASP	2.5
1	D	368	TRP	2.5
1	B	316	ASN	2.4
1	A	308	ASP	2.4
1	B	500[A]	PHE	2.4
1	C	618	LEU	2.4
1	A	309	PHE	2.3
1	B	627	ARG	2.3
1	C	314	SER	2.2
1	D	373	ASP	2.2
1	B	545	ASN	2.2
1	D	477	ASN	2.2
1	B	279	LYS	2.2
1	D	451	LEU	2.2
1	C	316	ASN	2.1
1	D	279	LYS	2.1
1	C	78	GLY	2.1
1	B	75	LYS	2.1
1	B	78	GLY	2.1
1	D	79	ALA	2.1
1	C	549	TYR	2.1
1	B	118	SER	2.1
1	C	350	ILE	2.1
1	A	369	SER	2.0
1	D	457	GLY	2.0
1	C	0	SER	2.0
1	D	541	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

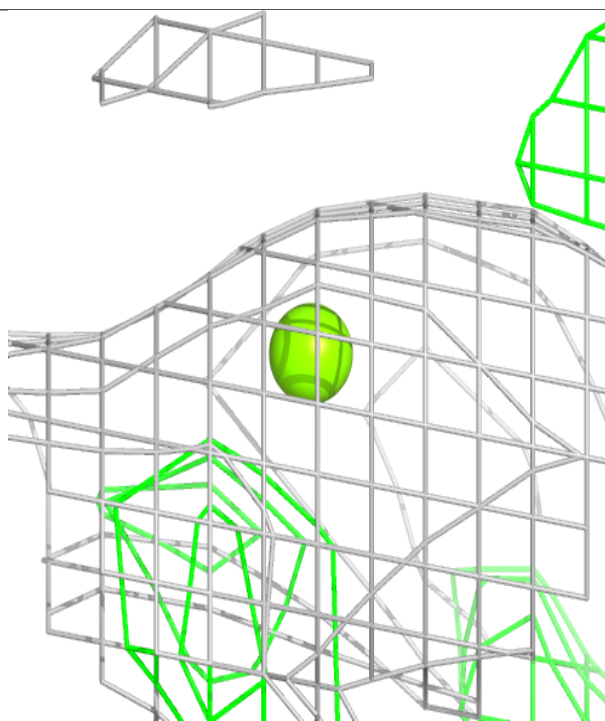
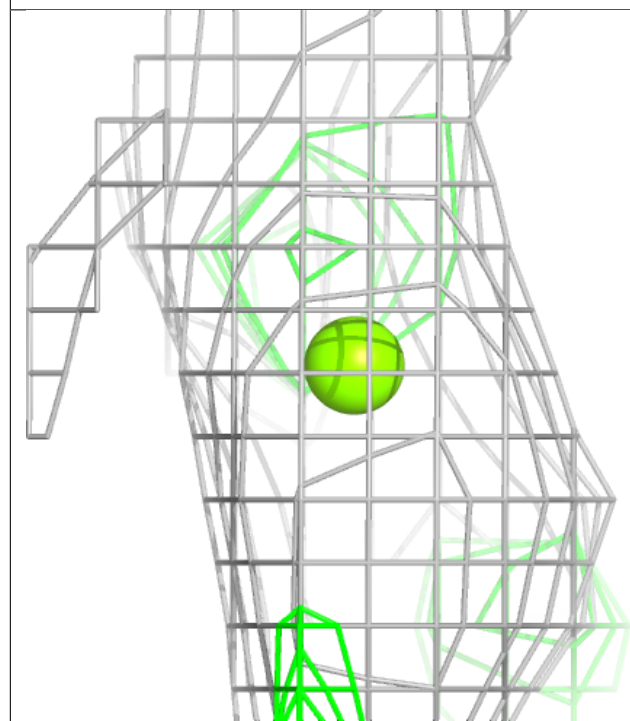
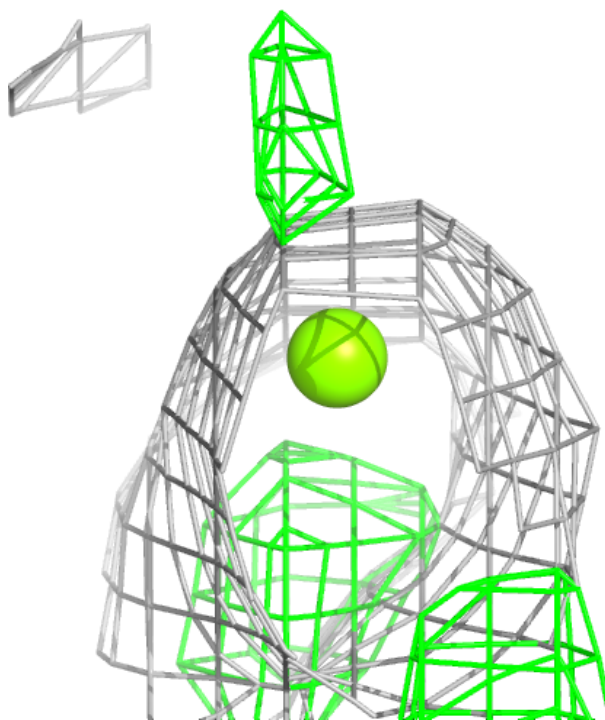
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	B	701	1/1	0.92	0.30	84,84,84,84	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around MG B 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.