



Full wwPDB X-ray Structure Validation Report i

Mar 25, 2024 – 04:41 pm GMT

PDB ID : 8OZ7
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 i 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](#) i) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

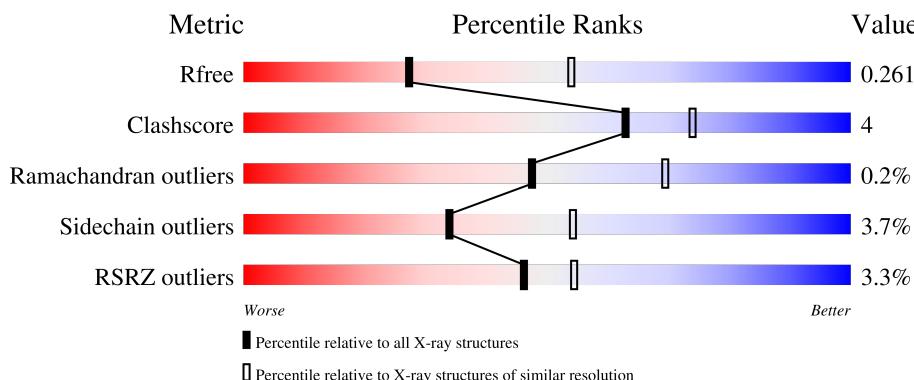
1 Overall quality at a glance

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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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.



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

2 Entry composition [\(i\)](#)

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 (three-letter code: 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		

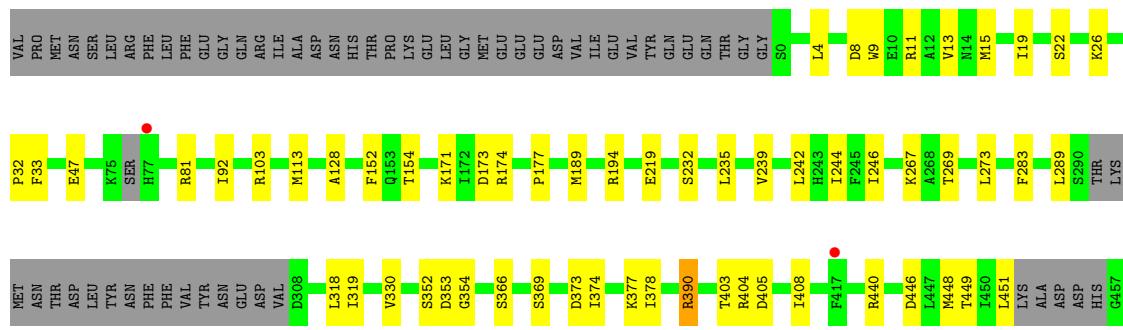
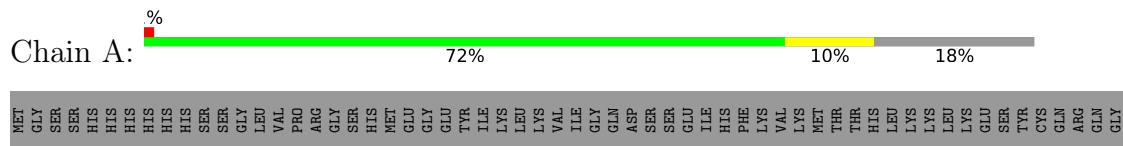
- Molecule 4 is water.

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

3 Residue-property plots

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

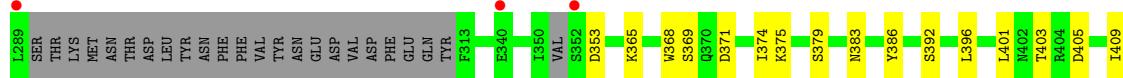
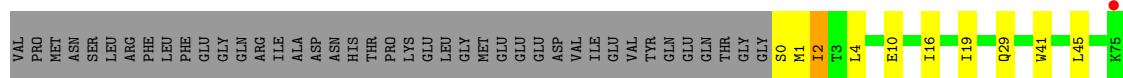
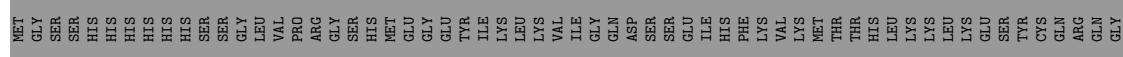
- Molecule 1: AbiA





- Molecule 1: AbiA

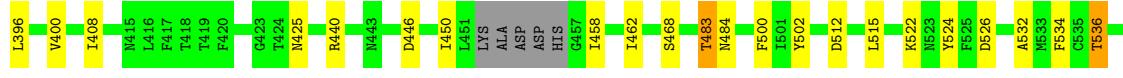
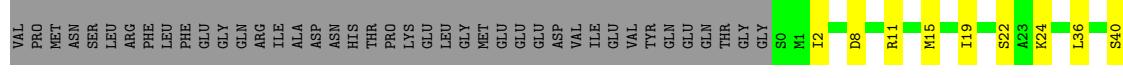
Chain C: 4% • 69% 11% • 20%

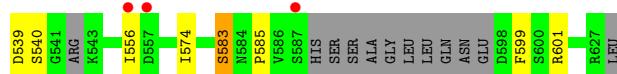


- Molecule 1: AbiA

A horizontal bar chart titled "Chain D" showing its distribution across four categories. The categories are represented by colored segments: red (4%), green (69%), yellow (10%), and grey (20%).

Category	Percentage
Red	4%
Green	69%
Yellow	10%
Grey	20%





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

Chain E:
56% 44%



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

Chain F:
56% 44%



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

Chain G:
56% 44%



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

Chain H:
78% 22%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	84.09 Å 86.10 Å 117.01 Å 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 2.77 Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R , R_{free}	0.220 , 0.264 0.218 , 0.261	Depositor DCC
R_{free} test set	2100 reflections (2.62%)	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 , 42.4	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	0.25	0/4990	0.42	0/6749
1	B	0.24	0/4868	0.42	0/6604
1	C	0.24	0/4788	0.42	0/6489
1	D	0.24	0/4762	0.42	0/6455
2	E	0.51	0/201	0.71	0/308
2	F	0.50	0/117	0.83	0/178
2	G	0.49	0/117	0.85	0/178
2	H	0.50	0/156	0.70	0/238
All	All	0.25	0/19999	0.44	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	34	0
1	B	4757	0	4518	48	0
1	C	4687	0	4446	43	0
1	D	4662	0	4426	43	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	0	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	164	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 4.

All (164) 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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:483:THR:OG1	1:C:484:ASN:N	2.40	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: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: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: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:B:539:ASP:OD2	1:B:549:TYR:OH	2.25	0.49
1:A:405:ASP:HB3	1:A:408:ILE:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:LEU:HG	1:D:40:SER:HB2	1.94	0.49
1:C:239:VAL:HG12	1:C:240:ASP:N	2.27	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: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: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: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: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
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:D:440:ARG:HH21	1:D:446:ASP:CG	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:D:315:LYS:HZ3	1:D:315:LYS:HG3	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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 (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	588/730 (80%)	572 (97%)	15 (3%)	1 (0%)	47 69
1	B	589/730 (81%)	574 (98%)	14 (2%)	1 (0%)	47 69
1	C	576/730 (79%)	552 (96%)	23 (4%)	1 (0%)	47 69
1	D	576/730 (79%)	552 (96%)	23 (4%)	1 (0%)	47 69
All	All	2329/2920 (80%)	2250 (97%)	75 (3%)	4 (0%)	47 69

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 [\(i\)](#)

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	537/680 (79%)	520 (97%)	17 (3%)	39 59
1	B	507/680 (75%)	485 (96%)	22 (4%)	29 48
1	C	495/680 (73%)	480 (97%)	15 (3%)	41 61
1	D	492/680 (72%)	469 (95%)	23 (5%)	26 45
All	All	2031/2720 (75%)	1954 (96%)	77 (4%)	34 53

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	47	GLU
1	A	81	ARG
1	A	154	THR
1	A	171	LYS
1	A	189	MET
1	A	194	ARG
1	A	269	THR
1	A	273	LEU
1	A	352	SER
1	A	390	ARG
1	A	448	MET
1	A	449	THR
1	A	451	LEU
1	A	512	ASP
1	A	608	LEU
1	A	618	LEU
1	B	1	MET

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Mol	Chain	Res	Type
1	B	45	LEU
1	B	64[A]	GLU
1	B	64[B]	GLU
1	B	82	GLN
1	B	111	ASN
1	B	133	SER
1	B	202	SER
1	B	223	SER
1	B	240	ASP
1	B	272	HIS
1	B	284	THR
1	B	330	VAL
1	B	377	LYS
1	B	385	ASN
1	B	476	LYS
1	B	516[A]	GLU
1	B	516[B]	GLU
1	B	533	MET
1	B	547	LYS
1	B	548	LEU
1	B	623	GLN
1	C	2	ILE
1	C	133	SER
1	C	140	GLU
1	C	146	GLU
1	C	152	PHE
1	C	157	SER
1	C	273	LEU
1	C	284	THR
1	C	353	ASP
1	C	386	TYR
1	C	401	LEU
1	C	482	TYR
1	C	522	LYS
1	C	567	SER
1	C	626	ASN
1	D	22	SER
1	D	74	GLN
1	D	95	ILE
1	D	155	ASP
1	D	174	ARG
1	D	218	LYS

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Mol	Chain	Res	Type
1	D	250	ASN
1	D	253	LEU
1	D	315	LYS
1	D	333	ASP
1	D	343	TYR
1	D	356	TYR
1	D	425	ASN
1	D	468	SER
1	D	483	THR
1	D	500[A]	PHE
1	D	500[B]	PHE
1	D	512	ASP
1	D	534	PHE
1	D	536	THR
1	D	539	ASP
1	D	540	SER
1	D	583	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	B	82	GLN
1	B	385	ASN
1	B	578	HIS
1	C	29	GLN
1	C	142	ASN
1	D	414	ASN
1	D	578	HIS

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

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 [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data [\(i\)](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	597/730 (81%)	-0.12	4 (0%)	87	91	39, 59, 95, 137	0
1	B	594/730 (81%)	0.07	22 (3%)	41	49	42, 67, 118, 152	0
1	C	586/730 (80%)	0.12	27 (4%)	32	39	46, 73, 118, 163	0
1	D	587/730 (80%)	0.19	26 (4%)	34	41	44, 73, 124, 160	0
2	E	9/9 (100%)	0.30	0	100	100	58, 70, 149, 152	0
2	F	5/9 (55%)	-0.30	0	100	100	83, 86, 101, 102	0
2	G	5/9 (55%)	-0.20	0	100	100	88, 89, 103, 111	0
2	H	7/9 (77%)	0.35	0	100	100	84, 97, 108, 158	0
All	All	2390/2956 (80%)	0.06	79 (3%)	46	54	39, 68, 117, 163	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	340	GLU	4.0
1	D	451	LEU	4.0
1	B	350	ILE	3.9
1	C	564	PHE	3.6
1	D	352	SER	3.5
1	B	565	LEU	3.5
1	C	568	ASP	3.5
1	B	484	ASN	3.5
1	C	481	PHE	3.5
1	B	351	VAL	3.4
1	D	556	ILE	3.3
1	D	348	PRO	3.2
1	C	75	LYS	3.2
1	D	416	LEU	3.2
1	C	444[A]	HIS	3.2
1	D	349	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	587	SER	3.2
1	B	482	TYR	3.1
1	B	564	PHE	3.1
1	D	418	THR	3.1
1	B	489	TYR	3.0
1	D	417	PHE	3.0
1	B	343	TYR	3.0
1	C	529	VAL	3.0
1	B	348	PRO	3.0
1	C	482	TYR	2.9
1	B	568	ASP	2.9
1	D	557	ASP	2.9
1	B	347	ASN	2.9
1	A	77	HIS	2.8
1	C	288	GLU	2.8
1	C	566	SER	2.8
1	C	528	PHE	2.8
1	D	420	PHE	2.8
1	D	343	TYR	2.8
1	C	559	LEU	2.8
1	D	316	ASN	2.8
1	C	352	SER	2.7
1	B	345	LEU	2.7
1	D	77	HIS	2.7
1	B	288	GLU	2.7
1	C	150	TYR	2.7
1	B	543	LYS	2.7
1	C	549	TYR	2.6
1	B	567	SER	2.5
1	A	628	LEU	2.5
1	D	288	GLU	2.5
1	A	543	LYS	2.5
1	D	289	LEU	2.5
1	C	289	LEU	2.4
1	C	567	SER	2.4
1	D	425	ASN	2.4
1	D	354	GLY	2.4
1	C	287	SER	2.4
1	D	80	TYR	2.4
1	B	531	HIS	2.3
1	C	422	ASN	2.3
1	B	535	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	544	PRO	2.3
1	C	80	TYR	2.3
1	D	370	GLN	2.3
1	C	449	THR	2.3
1	A	417	PHE	2.3
1	D	368	TRP	2.2
1	D	443	ASN	2.2
1	C	340	GLU	2.2
1	B	309	PHE	2.2
1	C	448	MET	2.2
1	C	598	ASP	2.2
1	C	540	SER	2.2
1	B	561	GLN	2.1
1	D	317	THR	2.1
1	C	565	LEU	2.1
1	C	620	THR	2.1
1	B	623	GLN	2.1
1	D	415	ASN	2.1
1	B	566	SER	2.1
1	D	423	GLY	2.1
1	D	369	SER	2.1

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

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

6.3 Carbohydrates [\(i\)](#)

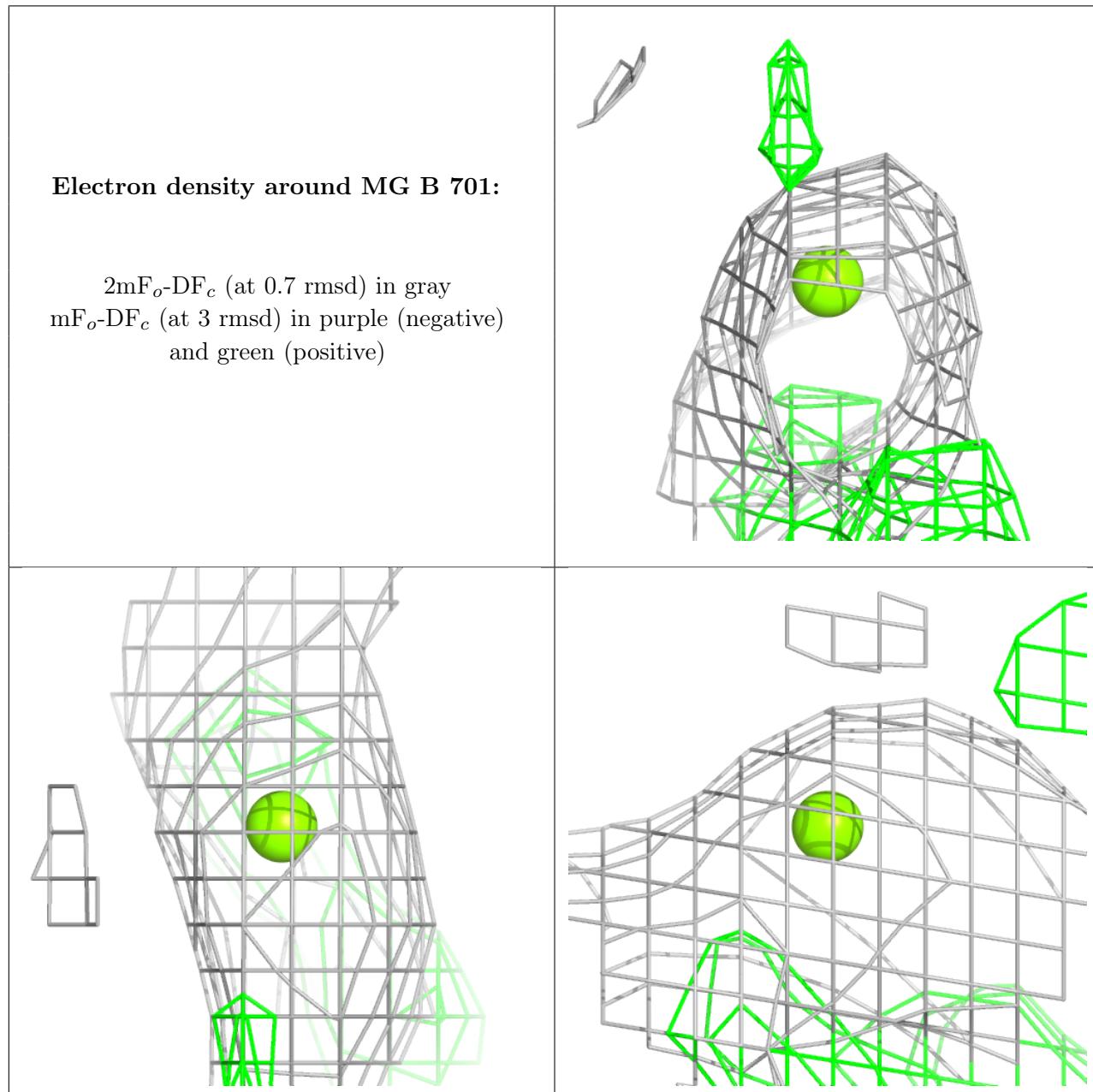
There are no monosaccharides in this entry.

6.4 Ligands [\(i\)](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	B	701	1/1	0.85	0.59	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.



6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.