



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 11, 2023 – 12:34 PM EST

PDB ID : 8F72
Title : Phage P32 gp64- RNA polymerase
Authors : Bae, B.; Nair, S.K.
Deposited on : 2022-11-17
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 : 4.02b-467
Xtrriage (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

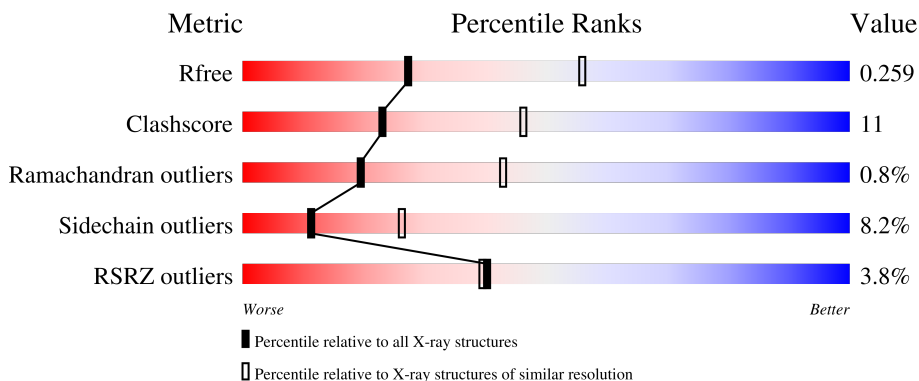
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

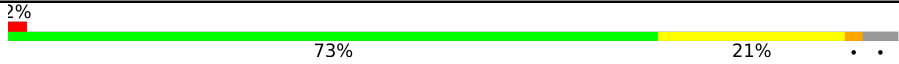
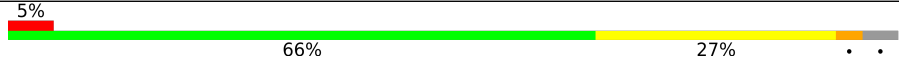
The reported resolution of this entry is 2.70 Å.

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))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 $\leq 5\%$. 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	617	
1	B	617	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9478 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 TPR_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	593	4656	2991	814	841	10	0	0	0
1	B	595	4674	3002	818	843	11	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

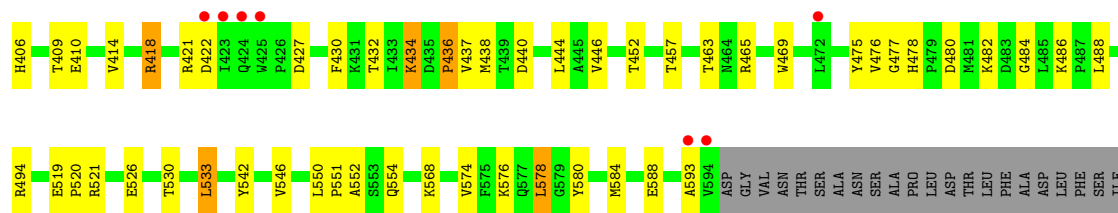
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP A7XX94
B	0	HIS	-	expression tag	UNP A7XX94

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	76	Total	O	0	0
			76	76		
3	B	70	Total	O	0	0
			70	70		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	210.33Å 106.32Å 112.36Å 90.00° 102.26° 90.00°	Depositor
Resolution (Å)	25.00 – 2.70 38.66 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (25.00-2.70) 99.8 (38.66-2.70)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.69Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.205 , 0.257 0.207 , 0.259	Depositor DCC
R_{free} test set	3322 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	65.8	Xtrriage
Anisotropy	0.516	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9478	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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	0.33	0/4791	0.72	0/6525
1	B	0.34	0/4810	0.72	1/6550 (0.0%)
All	All	0.34	0/9601	0.72	1/13075 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	246	THR	CA-CB-OG1	-5.26	97.96	109.00

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	4656	0	4607	80	0
1	B	4674	0	4626	132	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	76	0	0	3	0
3	B	70	0	0	8	0
All	All	9478	0	9233	212	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 11.

All (212) 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:475:TYR:O	1:B:482:LYS:HE2	1.44	1.15
1:B:127:PRO:O	1:B:153:THR:HG22	1.57	1.02
1:A:538:ARG:HD3	3:A:1062:HOH:O	1.59	1.01
1:B:139:ARG:HB3	1:B:142:GLU:HB2	1.43	0.99
1:B:352:LEU:HD12	1:B:406:HIS:HB3	1.53	0.88
1:A:127:PRO:O	1:A:153:THR:HG22	1.74	0.87
1:A:57:LEU:CD1	1:A:64:VAL:HG13	2.06	0.86
1:B:3:THR:HG21	3:B:1038:HOH:O	1.75	0.85
1:B:127:PRO:O	1:B:153:THR:CG2	2.28	0.82
1:B:208:HIS:NE2	3:B:1001:HOH:O	2.13	0.80
1:A:144:PHE:O	1:A:169:GLY:HA3	1.82	0.79
1:B:288:ARG:HG3	1:B:325:ALA:HB2	1.63	0.79
1:B:6:GLY:HA3	1:B:65:MET:CE	2.13	0.78
1:B:24:LEU:HD21	1:B:41:ALA:HB3	1.68	0.73
1:A:57:LEU:HD11	1:A:64:VAL:HG13	1.70	0.73
1:A:212:ASP:HB2	1:A:242:LYS:HD3	1.72	0.70
1:B:50:LEU:HD23	1:B:51:GLY:H	1.56	0.70
1:B:278:TRP:CH2	1:B:334:VAL:HG12	2.28	0.68
1:B:1:MET:O	1:B:3:THR:HG23	1.94	0.68
1:B:388:ARG:NH1	1:B:440:ASP:OD2	2.28	0.67
1:B:521:ARG:CB	1:B:554:GLN:HE21	2.06	0.67
1:B:388:ARG:HG2	1:B:437:VAL:HG21	1.76	0.66
1:B:494:ARG:HH11	1:B:494:ARG:HG3	1.61	0.66
1:B:116:ILE:O	1:B:161:LEU:HB2	1.96	0.66
1:A:118:PRO:HB3	1:A:157:VAL:O	1.96	0.65
1:B:116:ILE:HG22	1:B:157:VAL:HG21	1.78	0.64
1:B:145:ARG:NH1	1:B:164:PHE:O	2.32	0.63
1:B:521:ARG:NE	1:B:526:GLU:OE2	2.25	0.62
1:B:317:GLU:HG3	1:B:327:TYR:HE2	1.64	0.62
1:B:321:ALA:N	1:B:322:PRO:HD2	2.15	0.62
1:A:237:GLN:CB	1:A:462:ILE:HD12	2.29	0.62
1:B:385:ASN:HD21	1:B:432:THR:HG22	1.64	0.62
1:B:437:VAL:HG22	1:B:440:ASP:OD1	1.99	0.62
1:B:128:ASN:HA	1:B:153:THR:O	2.00	0.62
1:B:390:LEU:HD22	1:B:394:TRP:CZ2	2.35	0.61
1:B:593:ALA:HB2	3:B:1040:HOH:O	1.99	0.61
1:A:236:ALA:HA	1:A:239:LEU:HD12	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:PRO:HG2	1:A:99:SER:OG	2.02	0.60
1:B:293:PRO:HD2	1:B:409:THR:OG1	2.01	0.60
1:A:4:ARG:HH22	1:A:63:VAL:HG21	1.67	0.60
1:B:521:ARG:HA	1:B:554:GLN:NE2	2.17	0.60
1:B:288:ARG:CG	1:B:325:ALA:HB2	2.32	0.59
1:A:321:ALA:N	1:A:322:PRO:HD2	2.18	0.59
1:B:139:ARG:HB2	1:B:144:PHE:CE1	2.37	0.59
1:B:6:GLY:HA3	1:B:65:MET:HE1	1.84	0.59
1:B:193:THR:O	1:B:197:LEU:HD12	2.03	0.59
1:B:320:ILE:HD12	1:B:325:ALA:HB3	1.84	0.58
1:B:478:HIS:CE1	1:B:480:ASP:HB2	2.38	0.58
1:B:47:GLU:HA	1:B:47:GLU:OE1	2.03	0.58
1:A:164:PHE:HE2	1:A:173:LEU:HD12	1.69	0.57
1:A:139:ARG:HB3	1:A:142:GLU:HB2	1.85	0.57
1:A:204:GLY:O	1:A:207:LYS:HB2	2.04	0.57
1:A:519:GLU:HB3	1:A:520:PRO:HD2	1.87	0.57
1:B:434:LYS:O	1:B:434:LYS:HG3	2.04	0.57
1:A:57:LEU:HD11	1:A:64:VAL:CG1	2.36	0.56
1:A:388:ARG:HG2	1:A:437:VAL:CG2	2.36	0.56
1:B:205:TRP:CE3	1:B:206:TRP:N	2.74	0.56
1:B:317:GLU:HG3	1:B:327:TYR:CE2	2.40	0.55
1:B:410:GLU:O	1:B:414:VAL:HG23	2.06	0.55
1:B:478:HIS:HE1	1:B:480:ASP:HB2	1.71	0.55
1:B:436:PRO:O	1:B:476:VAL:HG22	2.06	0.55
1:A:95:LEU:HD13	1:A:96:PRO:HD2	1.88	0.55
1:B:126:SER:HB2	1:B:185:GLN:OE1	2.07	0.55
1:B:19:GLU:O	1:B:23:GLU:HB2	2.07	0.54
1:A:258:LEU:N	1:A:259:PRO:HD2	2.23	0.54
1:A:234:PRO:HD2	1:A:237:GLN:NE2	2.21	0.54
1:B:437:VAL:O	1:B:440:ASP:HB2	2.07	0.54
1:B:463:THR:HG23	3:B:1036:HOH:O	2.08	0.54
1:A:274:TYR:CG	1:A:310:ALA:HA	2.42	0.54
1:B:119:PRO:HA	1:B:153:THR:HG23	1.90	0.54
1:B:139:ARG:CB	1:B:142:GLU:HB2	2.28	0.54
1:B:271:VAL:HG12	1:B:315:ALA:HB2	1.89	0.54
1:B:6:GLY:HA3	1:B:65:MET:HE3	1.90	0.53
1:A:528:LEU:HD22	1:A:541:VAL:HG13	1.89	0.53
1:B:438:MET:HE2	1:B:482:LYS:HG3	1.89	0.53
1:A:135:MET:HE3	1:A:151:ILE:HG21	1.91	0.53
1:A:532:GLY:HA3	1:A:541:VAL:HG21	1.90	0.52
1:B:494:ARG:HG3	1:B:494:ARG:NH1	2.23	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:LEU:HD12	1:A:551:PRO:HD2	1.92	0.52
1:A:147:TRP:CZ2	1:A:162:LEU:HD21	2.44	0.52
1:B:47:GLU:O	1:B:50:LEU:O	2.27	0.52
1:B:484:GLY:HA3	3:B:1031:HOH:O	2.09	0.52
1:B:326:ASP:O	1:B:330:ASP:HB2	2.10	0.51
1:A:490:SER:HB3	1:A:494:ARG:HH12	1.75	0.51
1:A:117:PHE:HB3	1:A:118:PRO:HD2	1.93	0.51
1:B:58:ILE:HD11	1:B:65:MET:HB2	1.92	0.51
1:B:521:ARG:HA	1:B:554:GLN:HE21	1.76	0.50
1:A:82:SER:OG	1:A:86:ARG:NH1	2.45	0.50
1:B:223:VAL:HG22	1:B:232:LEU:HD11	1.93	0.50
1:B:288:ARG:HG3	1:B:325:ALA:CB	2.37	0.50
1:A:490:SER:HB3	1:A:494:ARG:NH1	2.27	0.50
1:A:211:LEU:HD11	1:A:239:LEU:HD22	1.94	0.49
1:A:388:ARG:HG2	1:A:437:VAL:HG21	1.94	0.49
1:B:159:GLU:O	1:B:161:LEU:HD23	2.13	0.49
1:B:12:ASN:HB2	1:B:66:TRP:CE2	2.48	0.49
1:A:278:TRP:CH2	1:A:334:VAL:HG12	2.47	0.49
1:B:430:PHE:O	1:B:432:THR:HG23	2.13	0.49
1:B:446:VAL:HG12	1:B:446:VAL:O	2.13	0.49
1:B:550:LEU:HD12	1:B:551:PRO:CD	2.43	0.49
1:A:105:GLY:O	1:A:108:VAL:HG22	2.13	0.49
1:B:578:LEU:HB3	1:B:580:TYR:CE2	2.47	0.49
1:A:274:TYR:CD1	1:A:310:ALA:HA	2.48	0.49
1:B:251:ILE:HD11	1:B:329:GLY:HA2	1.95	0.49
1:A:54:PRO:HB2	1:A:66:TRP:CD1	2.49	0.48
1:B:79:TRP:HE3	1:B:368:ARG:HD2	1.79	0.48
1:B:578:LEU:CB	1:B:580:TYR:CE2	2.97	0.48
1:B:289:ARG:HB3	1:B:290:PRO:HA	1.96	0.48
1:B:477:GLY:O	1:B:478:HIS:C	2.52	0.48
1:A:538:ARG:NH2	1:A:560:GLU:OE2	2.47	0.48
1:B:191:GLU:O	1:B:289:ARG:NH2	2.46	0.48
1:A:204:GLY:HA2	1:A:206:TRP:CZ2	2.49	0.48
1:A:388:ARG:O	1:A:391:ASP:HB2	2.14	0.47
1:B:117:PHE:HD2	1:B:120:MET:SD	2.37	0.47
1:B:418:ARG:NH2	1:B:422:ASP:OD2	2.47	0.47
1:A:521:ARG:NH1	1:A:554:GLN:O	2.44	0.47
1:B:102:LEU:HD12	1:B:102:LEU:N	2.30	0.47
1:B:484:GLY:CA	3:B:1031:HOH:O	2.61	0.47
1:B:469:TRP:CZ3	1:B:488:LEU:HD23	2.49	0.47
1:B:274:TYR:CD1	1:B:310:ALA:HA	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LEU:HD21	1:A:41:ALA:CB	2.45	0.46
1:B:418:ARG:HA	1:B:421:ARG:O	2.16	0.46
1:B:117:PHE:O	1:B:153:THR:HA	2.16	0.46
1:B:438:MET:HE2	1:B:482:LYS:CG	2.46	0.46
1:B:521:ARG:CA	1:B:554:GLN:HE21	2.28	0.46
1:A:317:GLU:H	1:A:317:GLU:CD	2.18	0.46
1:B:550:LEU:HD12	1:B:551:PRO:HD2	1.97	0.46
1:A:57:LEU:HD23	1:A:366:LEU:HD12	1.98	0.46
1:A:135:MET:HA	1:A:178:GLU:O	2.15	0.46
1:A:145:ARG:HG2	1:A:147:TRP:CH2	2.51	0.46
1:B:102:LEU:HD23	1:B:164:PHE:CD2	2.50	0.46
1:B:135:MET:HA	1:B:178:GLU:O	2.15	0.46
1:B:252:LEU:O	1:B:327:TYR:HD1	1.99	0.45
1:A:94:GLU:O	1:A:95:LEU:HD22	2.15	0.45
1:A:124:VAL:HG12	1:A:131:ALA:HB2	1.98	0.45
1:B:278:TRP:CH2	1:B:334:VAL:CG1	2.99	0.45
1:B:130:TRP:CD2	1:B:251:ILE:HG21	2.51	0.45
1:A:195:GLN:OE1	1:A:195:GLN:N	2.30	0.45
1:B:400:VAL:HG11	1:B:404:TYR:HD2	1.80	0.45
1:B:486:LYS:HD3	1:B:486:LYS:HA	1.81	0.45
1:B:584:MET:O	1:B:588:GLU:HG2	2.17	0.45
1:A:4:ARG:NH2	1:A:63:VAL:HG11	2.31	0.45
1:B:379:LEU:C	1:B:379:LEU:HD23	2.37	0.45
1:A:478:HIS:HA	1:A:479:PRO:HD2	1.85	0.45
1:B:388:ARG:HG2	1:B:437:VAL:CG2	2.44	0.45
1:B:542:TYR:O	1:B:546:VAL:HG23	2.17	0.45
1:A:538:ARG:CD	3:A:1062:HOH:O	2.38	0.44
1:B:369:TRP:O	1:B:373:VAL:HG23	2.17	0.44
1:B:438:MET:HE1	1:B:482:LYS:HG2	1.98	0.44
1:A:13:LEU:HD11	1:A:63:VAL:HG13	1.99	0.44
1:B:355:LYS:HD3	1:B:356:ASP:N	2.33	0.44
1:A:300:GLU:HB2	1:A:346:PRO:HB3	1.99	0.44
1:B:387:ARG:HA	1:B:390:LEU:HD12	1.99	0.44
1:B:294:THR:OG1	1:B:296:GLN:HB3	2.18	0.44
1:B:352:LEU:CD1	1:B:406:HIS:HB3	2.38	0.44
1:A:437:VAL:O	1:A:440:ASP:N	2.46	0.44
1:A:537:LYS:O	1:A:541:VAL:HG23	2.17	0.44
1:B:533:LEU:HD12	1:B:533:LEU:HA	1.84	0.44
1:B:17:PRO:C	1:B:19:GLU:H	2.21	0.43
1:B:22:ARG:O	1:B:22:ARG:HG2	2.18	0.43
1:B:139:ARG:HB2	1:B:144:PHE:CZ	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:LYS:C	1:A:421:ARG:HG3	2.38	0.43
1:A:475:TYR:O	1:A:482:LYS:NZ	2.37	0.43
1:A:14:LEU:HD12	1:A:15:GLU:H	1.84	0.43
1:A:96:PRO:C	1:A:98:SER:H	2.21	0.43
1:A:439:THR:O	1:A:443:ARG:HG2	2.18	0.43
1:B:297:SER:HB2	3:B:1011:HOH:O	2.18	0.43
1:A:205:TRP:CE3	1:A:206:TRP:N	2.87	0.43
1:B:103:VAL:HG12	1:B:108:VAL:HG11	2.00	0.43
1:B:208:HIS:CE1	3:B:1001:HOH:O	2.66	0.43
1:B:80:ARG:O	1:B:82:SER:N	2.52	0.43
1:B:287:ASN:HA	1:B:297:SER:O	2.19	0.43
1:A:532:GLY:CA	1:A:541:VAL:HG21	2.48	0.42
1:B:12:ASN:HB2	1:B:66:TRP:CZ2	2.54	0.42
1:B:390:LEU:HD22	1:B:394:TRP:HZ2	1.84	0.42
1:B:519:GLU:HB3	1:B:520:PRO:CD	2.48	0.42
1:B:48:GLU:C	1:B:50:LEU:H	2.22	0.42
1:B:438:MET:CE	1:B:482:LYS:HG2	2.49	0.42
1:B:11:TRP:CD1	1:B:71:GLY:CA	3.03	0.42
1:B:253:LEU:HB2	1:B:314:ILE:HG12	2.00	0.42
1:B:294:THR:HG23	1:B:409:THR:OG1	2.20	0.42
1:A:58:ILE:HD12	1:A:58:ILE:C	2.40	0.42
1:A:294:THR:OG1	1:A:296:GLN:HB3	2.20	0.42
1:A:589:GLU:O	1:A:593:ALA:HB2	2.20	0.42
1:A:237:GLN:HB3	1:A:462:ILE:HD12	2.00	0.41
1:B:354:ARG:NH2	1:B:357:LEU:HB3	2.36	0.41
1:B:102:LEU:HD23	1:B:164:PHE:HD2	1.85	0.41
1:B:240:LYS:HE3	1:B:452:THR:OG1	2.20	0.41
1:B:253:LEU:O	1:B:314:ILE:HA	2.20	0.41
1:A:113:ILE:HD11	1:A:253:LEU:HA	2.03	0.41
1:A:89:SER:OG	1:A:92:ARG:HD3	2.20	0.41
1:A:109:PHE:CD1	1:A:116:ILE:HD12	2.56	0.41
1:A:491:LYS:O	1:A:492:VAL:C	2.59	0.41
1:B:58:ILE:C	1:B:58:ILE:HD12	2.41	0.41
1:B:219:LYS:HG3	1:B:238:TYR:OH	2.20	0.41
1:B:457:THR:HG21	1:B:465:ARG:HH22	1.85	0.41
1:B:258:LEU:N	1:B:259:PRO:CD	2.84	0.41
1:A:5:ILE:HD11	1:A:182:ILE:HG22	2.03	0.41
1:A:145:ARG:HG2	1:A:147:TRP:CZ2	2.56	0.41
1:A:433:ILE:HG22	1:A:435:ASP:H	1.86	0.41
1:B:28:ALA:HA	1:B:34:SER:OG	2.20	0.41
1:B:76:LEU:HB3	1:B:169:GLY:HA2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:GLU:HG3	1:B:568:LYS:NZ	2.36	0.41
1:A:380:GLY:O	1:A:384:VAL:HG23	2.21	0.41
1:A:57:LEU:CD1	1:A:64:VAL:CG1	2.87	0.40
1:B:199:TYR:CG	1:B:293:PRO:HA	2.56	0.40
1:A:456:ASN:OD1	1:A:457:THR:N	2.55	0.40
1:B:70:THR:HB	1:B:71:GLY:H	1.64	0.40
1:B:552:ALA:C	1:B:554:GLN:H	2.24	0.40
1:A:112:GLY:HA3	1:A:327:TYR:C	2.41	0.40
1:A:119:PRO:HA	1:A:153:THR:HG23	2.03	0.40
1:A:264:HIS:HA	3:A:1036:HOH:O	2.20	0.40
1:B:308:PRO:HD2	1:B:314:ILE:HD12	2.04	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	591/617 (96%)	540 (91%)	47 (8%)	4 (1%)	22 46
1	B	593/617 (96%)	534 (90%)	54 (9%)	5 (1%)	19 43
All	All	1184/1234 (96%)	1074 (91%)	101 (8%)	9 (1%)	19 43

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	399	GLU
1	B	2	GLY
1	B	206	TRP
1	B	160	PRO
1	A	16	PHE
1	B	71	GLY
1	A	30	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	436	PRO
1	A	140	GLY

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	483/503 (96%)	451 (93%)	32 (7%)	16	38
1	B	485/503 (96%)	438 (90%)	47 (10%)	8	19
All	All	968/1006 (96%)	889 (92%)	79 (8%)	11	26

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	21	VAL
1	A	24	LEU
1	A	27	SER
1	A	64	VAL
1	A	70	THR
1	A	76	LEU
1	A	80	ARG
1	A	92	ARG
1	A	95	LEU
1	A	99	SER
1	A	108	VAL
1	A	126	SER
1	A	128	ASN
1	A	136	PHE
1	A	137	SER
1	A	150	VAL
1	A	153	THR
1	A	170	VAL
1	A	173	LEU
1	A	176	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	189	THR
1	A	237	GLN
1	A	246	THR
1	A	267	GLU
1	A	326	ASP
1	A	383	GLU
1	A	389	LEU
1	A	401	SER
1	A	444	LEU
1	A	462	ILE
1	A	476	VAL
1	B	14	LEU
1	B	19	GLU
1	B	20	ARG
1	B	24	LEU
1	B	37	ASN
1	B	45	LEU
1	B	47	GLU
1	B	48	GLU
1	B	50	LEU
1	B	70	THR
1	B	76	LEU
1	B	92	ARG
1	B	93	THR
1	B	95	LEU
1	B	124	VAL
1	B	135	MET
1	B	137	SER
1	B	145	ARG
1	B	151	ILE
1	B	153	THR
1	B	162	LEU
1	B	170	VAL
1	B	172	GLU
1	B	175	ASP
1	B	176	VAL
1	B	182	ILE
1	B	189	THR
1	B	202	ILE
1	B	211	LEU
1	B	246	THR
1	B	275	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	306	LEU
1	B	330	ASP
1	B	350	GLU
1	B	353	HIS
1	B	355	LYS
1	B	356	ASP
1	B	403	ASP
1	B	418	ARG
1	B	427	ASP
1	B	434	LYS
1	B	444	LEU
1	B	530	THR
1	B	533	LEU
1	B	574	VAL
1	B	576	LYS
1	B	578	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	ASN
1	A	237	GLN
1	A	534	GLN
1	B	141	ASN
1	B	385	ASN
1	B	402	GLN
1	B	554	GLN

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

Of 2 ligands modelled in this entry, 2 are 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	593/617 (96%)	0.01	15 (2%) 57 59	43, 71, 133, 182	0
1	B	595/617 (96%)	0.15	30 (5%) 28 27	41, 76, 129, 173	0
All	All	1188/1234 (96%)	0.08	45 (3%) 40 39	41, 73, 130, 182	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	353	HIS	6.0
1	B	39	PHE	5.5
1	B	352	LEU	5.3
1	A	55	HIS	5.1
1	A	39	PHE	4.9
1	A	352	LEU	4.5
1	B	423	ILE	4.2
1	A	44	HIS	4.2
1	A	354	ARG	3.9
1	B	20	ARG	3.9
1	B	41	ALA	3.8
1	B	55	HIS	3.8
1	B	24	LEU	3.7
1	B	594	VAL	3.6
1	B	1	MET	3.4
1	A	21	VAL	3.2
1	A	20	ARG	3.1
1	B	40	ASP	3.0
1	B	21	VAL	2.9
1	A	355	LYS	2.9
1	B	425	TRP	2.8
1	B	44	HIS	2.8
1	B	366	LEU	2.8
1	B	364	SER	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	534	GLN	2.7
1	A	11	TRP	2.7
1	B	362	TYR	2.7
1	B	424	GLN	2.5
1	A	17	PRO	2.4
1	B	42	LEU	2.4
1	B	422	ASP	2.3
1	A	455	GLY	2.3
1	B	176	VAL	2.3
1	B	593	ALA	2.3
1	A	356	ASP	2.3
1	B	360	LYS	2.2
1	B	38	ILE	2.2
1	B	358	PRO	2.2
1	B	0	HIS	2.2
1	B	367	HIS	2.2
1	B	472	LEU	2.1
1	B	394	TRP	2.1
1	B	404	TYR	2.0
1	B	356	ASP	2.0
1	A	594	VAL	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](#)

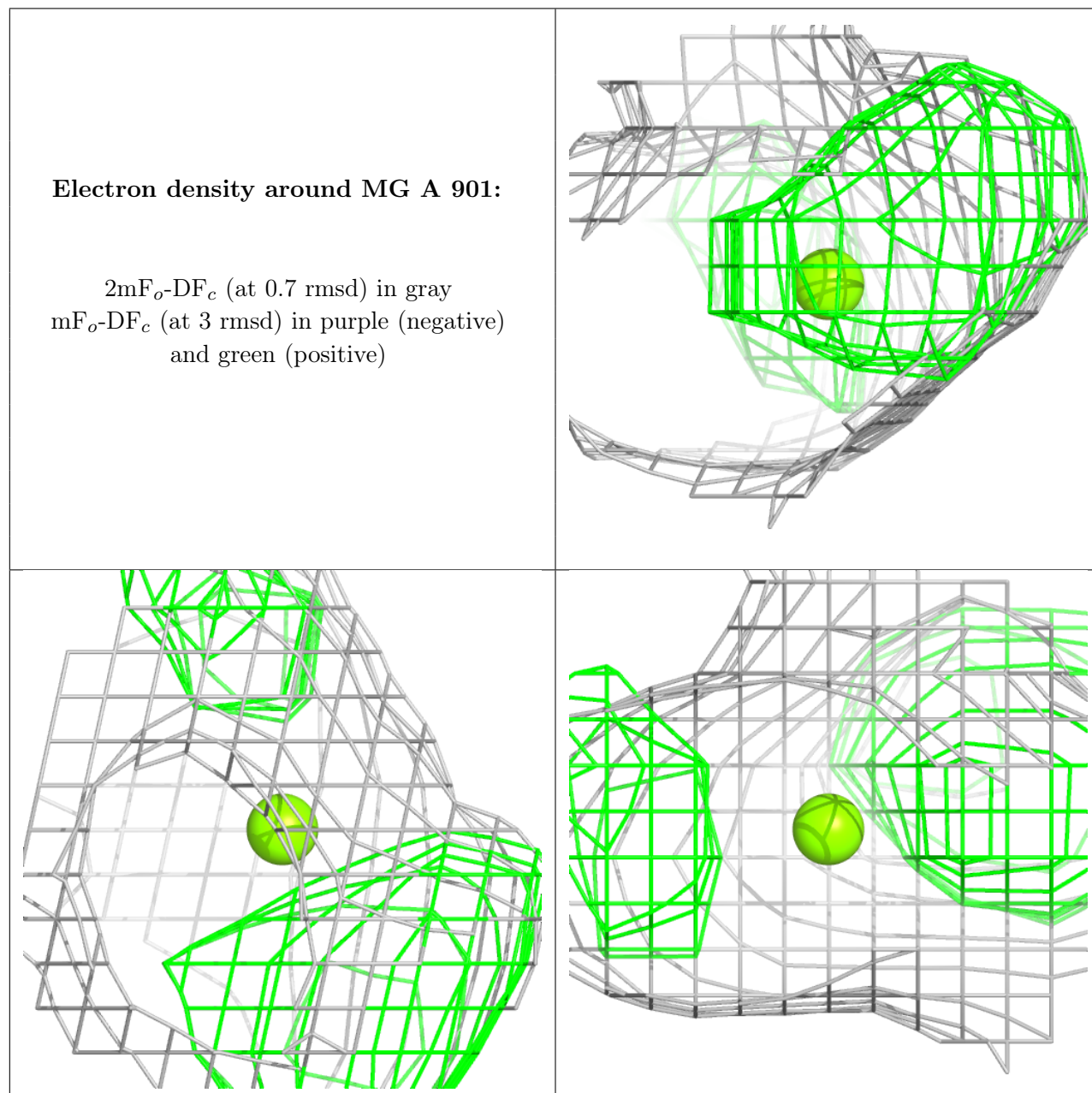
There are no monosaccharides in this entry.

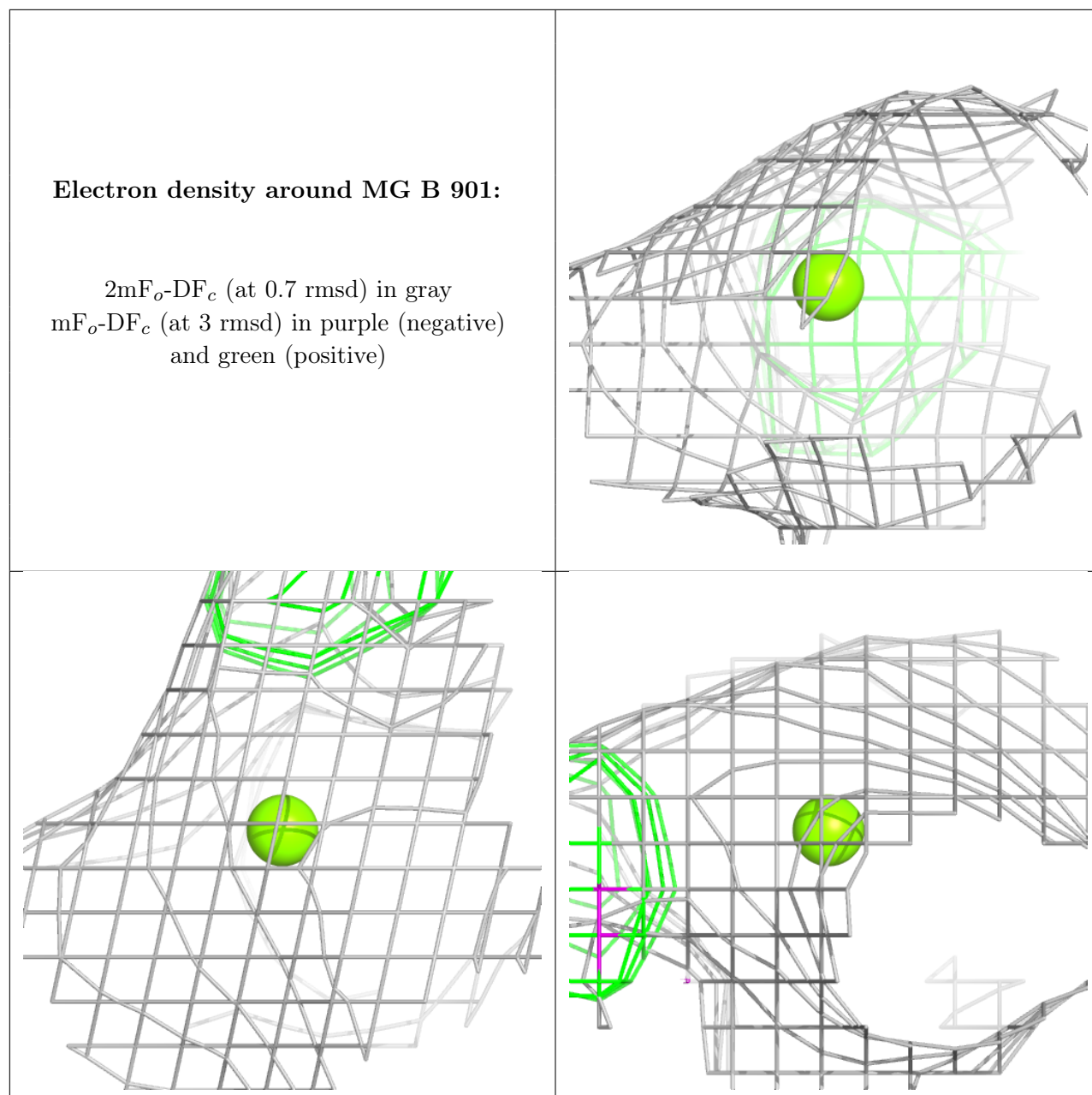
6.4 Ligands [i](#)

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
2	MG	A	901	1/1	0.98	0.40	68,68,68,68	0
2	MG	B	901	1/1	0.98	0.35	71,71,71,71	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.