Full wwPDB X-ray Structure Validation Report (i)

Jan 9, 2024 – 05:00 PM EST

PDB ID	:	8F5M
Title	:	Crystal structure of P74 gp62
Authors	:	Bae, B.; Nair, S.K.
Deposited on	:	2022-11-14
Resolution	:	2.40 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 (1)) were used in the production of this report:

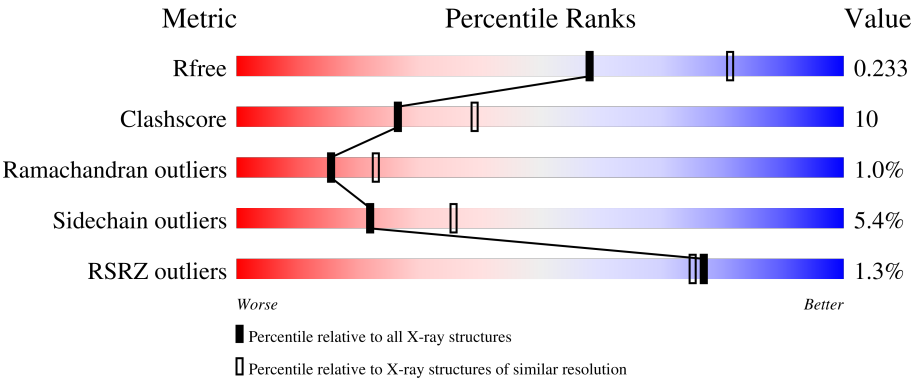
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	81% 13%
1	B	617	2% 75% 17%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10150 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 Envelope glycoprotein gp62.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	592	Total	C	N	O	S	0	0	0
			4662	2995	816	842	9			
1	B	591	Total	C	N	O	S	0	0	0
			4655	2991	815	840	9			

- 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.

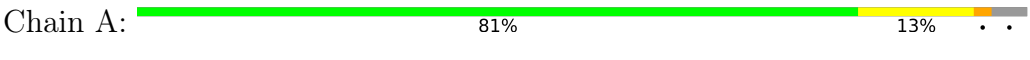
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	454	Total	O	0	0
			454	454		
3	B	377	Total	O	0	0
			377	377		

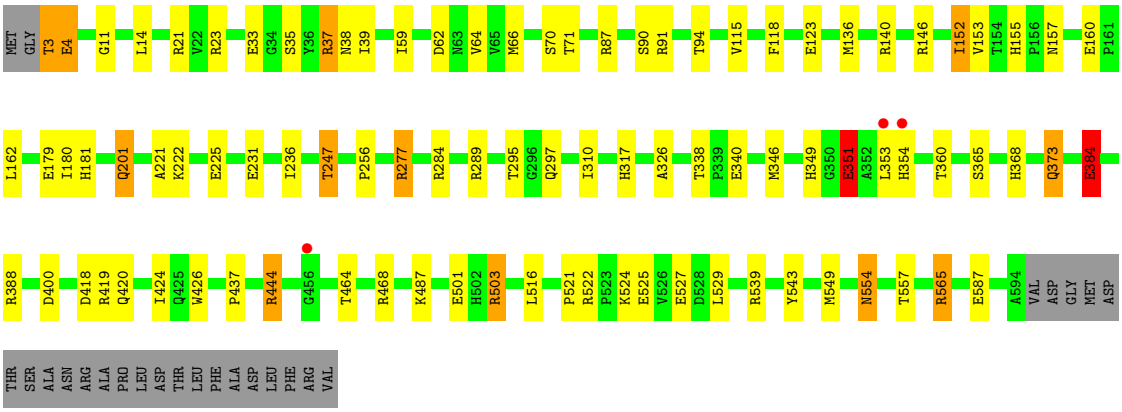
3 Residue-property plots (i)

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: Envelope glycoprotein gp62

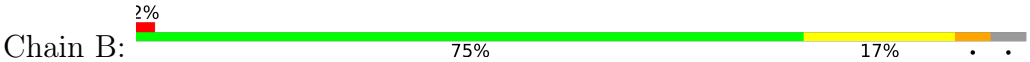
Chain A:

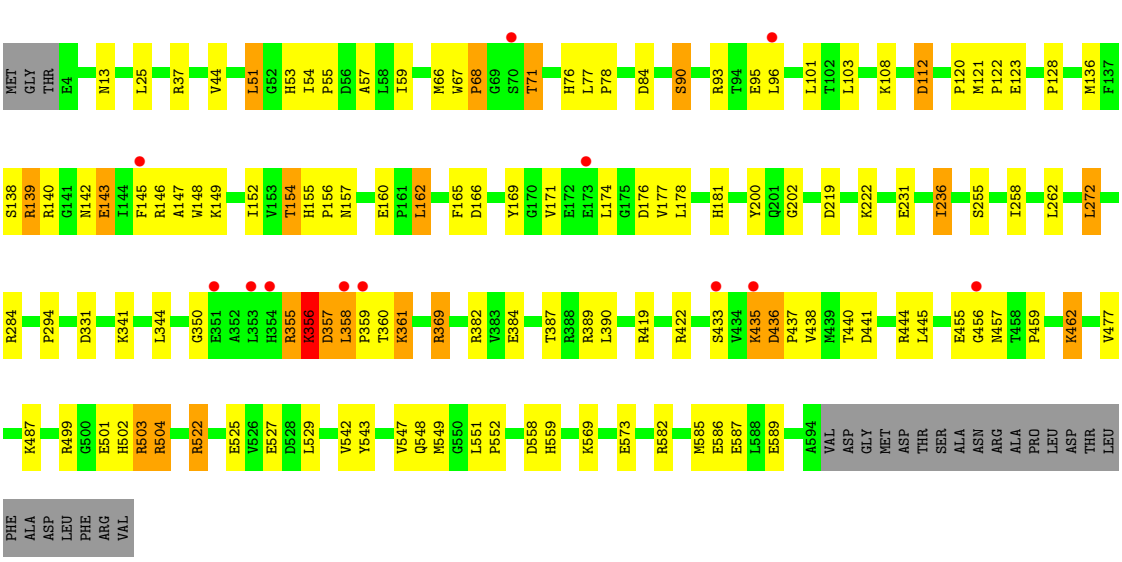




• Molecule 1: Envelope glycoprotein gp62

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	110.94Å 210.10Å 181.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.40 47.34 – 2.38	Depositor EDS
% Data completeness (in resolution range)	94.5 (25.00-2.40) 92.3 (47.34-2.38)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 2.37Å)	Xtriage
Refinement program	REFMAC refmac5	Depositor
R, R_{free}	0.186 , 0.231 0.187 , 0.233	Depositor DCC
R_{free} test set	3955 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	35.5	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10150	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.87 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.7668e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.38	0/4793	0.77	5/6527 (0.1%)
1	B	0.36	0/4786	0.75	4/6517 (0.1%)
All	All	0.37	0/9579	0.76	9/13044 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	201	GLN	CB-CA-C	-8.14	94.13	110.40
1	B	503	ARG	CG-CD-NE	-8.12	94.74	111.80
1	A	384	GLU	CB-CA-C	6.84	124.08	110.40
1	B	503	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	A	503	ARG	CG-CD-NE	-6.58	97.99	111.80
1	B	499	ARG	NE-CZ-NH2	-6.45	117.07	120.30
1	A	554	ASN	CB-CA-C	-6.25	97.91	110.40
1	A	146	ARG	CG-CD-NE	-6.21	98.77	111.80
1	B	499	ARG	NE-CZ-NH1	5.49	123.05	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	350	GLY	Peptide
1	B	436	ASP	Peptide

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	4662	0	4631	84	0
1	B	4655	0	4624	109	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	454	0	0	25	0
3	B	377	0	0	27	1
All	All	10150	0	9255	191	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (191) 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:A:565:ARG:HG2	1:A:565:ARG:HH11	1.14	1.08
1:A:66:MET:HE1	1:A:87:ARG:HA	1.30	1.06
1:A:136:MET:SD	3:A:1180:HOH:O	2.15	1.05
1:B:160:GLU:O	1:B:162:LEU:HD13	1.61	1.00
1:A:179:GLU:OE2	1:A:181:HIS:HE1	1.44	0.98
1:A:155:HIS:HD2	1:A:157:ASN:H	1.12	0.95
1:A:66:MET:HE3	1:A:87:ARG:HG2	1.49	0.94
1:A:66:MET:CE	1:A:87:ARG:HA	2.04	0.88
1:A:37:ARG:HD3	3:A:1019:HOH:O	1.74	0.87
1:A:123:GLU:HG2	3:A:1172:HOH:O	1.74	0.87
1:B:504:ARG:HH11	1:B:504:ARG:HG2	1.44	0.82
1:A:71:THR:HG22	3:A:1002:HOH:O	1.80	0.81
1:B:171:VAL:HG13	3:B:1021:HOH:O	1.81	0.79
1:A:62:ASP:H	1:A:373:GLN:NE2	1.80	0.78
1:B:219:ASP:HB2	3:B:998:HOH:O	1.84	0.78
1:B:384:GLU:CG	3:B:857:HOH:O	2.31	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:GLU:HG3	3:A:1019:HOH:O	1.84	0.77
1:A:179:GLU:OE2	1:A:181:HIS:CE1	2.34	0.77
1:A:565:ARG:HG2	1:A:565:ARG:NH1	1.94	0.76
1:A:565:ARG:HH11	1:A:565:ARG:CG	1.95	0.76
1:B:543:TYR:OH	1:B:559:HIS:HD2	1.68	0.76
1:A:277:ARG:HH11	1:A:277:ARG:HG2	1.51	0.75
1:A:444:ARG:HH21	1:A:444:ARG:HB3	1.51	0.74
1:A:365:SER:OG	1:A:368:HIS:HD2	1.68	0.74
1:A:62:ASP:H	1:A:373:GLN:HE22	1.34	0.73
1:A:155:HIS:CD2	1:A:157:ASN:H	2.03	0.72
1:B:53:HIS:HB2	3:B:1109:HOH:O	1.90	0.72
1:B:95:GLU:HG2	1:B:177:VAL:HG11	1.73	0.71
1:A:11:GLY:O	1:A:71:THR:HG23	1.91	0.70
1:A:247:THR:CG2	3:A:1008:HOH:O	2.39	0.70
1:B:357:ASP:O	1:B:358:LEU:HG	1.92	0.70
1:B:501:GLU:O	3:B:801:HOH:O	2.09	0.70
1:B:95:GLU:HG2	1:B:177:VAL:CG1	2.23	0.69
1:A:160:GLU:O	1:A:162:LEU:HD13	1.93	0.68
1:B:569:LYS:CE	1:B:573:GLU:OE2	2.42	0.68
1:B:487:LYS:HE2	3:B:1096:HOH:O	1.93	0.67
1:B:128:PRO:O	1:B:154:THR:HG22	1.95	0.67
1:A:66:MET:HE3	1:A:87:ARG:CG	2.25	0.67
1:B:155:HIS:CD2	1:B:157:ASN:H	2.14	0.66
1:B:155:HIS:HD2	1:B:157:ASN:H	1.42	0.66
1:B:95:GLU:OE2	1:B:177:VAL:HG11	1.95	0.66
1:B:503:ARG:NH2	1:B:587:GLU:OE1	2.29	0.66
1:B:389:ARG:NH1	1:B:441:ASP:OD1	2.30	0.65
1:B:136:MET:HG3	1:B:148:TRP:HB2	1.80	0.64
1:B:177:VAL:HG12	1:B:178:LEU:N	2.12	0.64
1:B:139:ARG:HB2	1:B:143:GLU:O	1.98	0.64
1:A:136:MET:HE2	1:A:180:ILE:HG12	1.80	0.64
1:B:384:GLU:HG2	3:B:857:HOH:O	1.96	0.63
1:A:464:THR:O	1:A:468:ARG:HG2	1.99	0.62
1:B:13:ASN:O	1:B:66:MET:HA	2.00	0.62
1:A:565:ARG:NH2	3:A:801:HOH:O	2.19	0.62
1:A:373:GLN:HB2	1:A:420:GLN:HG2	1.82	0.61
1:B:459:PRO:HG2	1:B:462:LYS:HG2	1.82	0.61
1:A:90:SER:OG	1:A:181:HIS:HD2	1.84	0.61
1:B:569:LYS:HE3	1:B:573:GLU:OE2	2.00	0.61
1:B:504:ARG:HH11	1:B:504:ARG:CG	2.11	0.60
1:B:78:PRO:HG3	3:B:1115:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:SER:O	1:B:258:ILE:HG12	2.01	0.60
1:A:35:SER:O	1:A:38:ASN:HB2	2.02	0.60
1:A:118:PHE:CE2	1:A:152:ILE:HG13	2.36	0.59
1:A:277:ARG:HH11	1:A:277:ARG:CG	2.16	0.59
1:B:435:LYS:HD3	3:B:1053:HOH:O	2.03	0.58
1:B:502:HIS:H	1:B:504:ARG:HH12	1.52	0.58
1:A:349:HIS:O	1:A:351:GLU:HG2	2.04	0.58
1:B:501:GLU:HG3	3:B:1127:HOH:O	2.04	0.57
1:B:582:ARG:HD2	1:B:586:GLU:OE1	2.05	0.57
1:B:582:ARG:HD3	3:B:1065:HOH:O	2.05	0.57
1:B:95:GLU:CG	1:B:177:VAL:HG11	2.33	0.57
1:A:539:ARG:HB2	3:A:1059:HOH:O	2.05	0.57
1:A:349:HIS:CD2	3:A:910:HOH:O	2.58	0.56
1:B:569:LYS:HE2	1:B:573:GLU:OE2	2.05	0.56
1:B:522:ARG:HD2	1:B:527:GLU:OE2	2.05	0.56
1:B:84:ASP:CG	1:B:369:ARG:HH22	2.09	0.55
1:B:569:LYS:HD3	3:B:842:HOH:O	2.06	0.55
1:B:457:ASN:HB3	3:B:1072:HOH:O	2.06	0.55
1:A:522:ARG:HD2	1:A:527:GLU:OE2	2.08	0.54
1:B:236:ILE:HD12	1:B:236:ILE:N	2.23	0.54
1:B:145:PHE:HB3	3:B:1021:HOH:O	2.07	0.54
1:B:231:GLU:OE2	1:B:503:ARG:HD2	2.08	0.54
1:A:539:ARG:HG2	1:A:543:TYR:CZ	2.43	0.54
1:B:384:GLU:HG3	3:B:857:HOH:O	2.02	0.54
1:B:503:ARG:HH22	1:B:587:GLU:CD	2.11	0.54
1:B:522:ARG:NH2	1:B:558:ASP:OD1	2.41	0.54
1:A:338:THR:HB	1:A:340:GLU:OE1	2.07	0.53
3:A:1239:HOH:O	1:B:549:MET:HE3	2.07	0.53
1:A:136:MET:CE	1:A:180:ILE:CD1	2.86	0.53
1:A:136:MET:CE	1:A:180:ILE:HG12	2.39	0.53
1:B:390:LEU:HG	3:B:811:HOH:O	2.08	0.53
1:A:503:ARG:NH2	1:A:587:GLU:OE1	2.42	0.53
1:B:90:SER:HB3	1:B:93:ARG:HH11	1.73	0.52
1:B:55:PRO:HB2	1:B:67:TRP:CD1	2.44	0.52
1:B:236:ILE:HD12	1:B:236:ILE:H	1.73	0.52
1:B:76:HIS:NE2	1:B:143:GLU:HG3	2.25	0.52
1:B:284:ARG:HG3	3:B:1160:HOH:O	2.10	0.52
1:B:101:LEU:HD21	1:B:178:LEU:HD22	1.92	0.52
1:B:55:PRO:CB	1:B:67:TRP:CD1	2.93	0.51
1:A:91:ARG:NH1	3:A:813:HOH:O	2.43	0.51
1:A:284:ARG:HG3	3:A:1226:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:PRO:HA	3:A:823:HOH:O	2.10	0.51
1:B:360:THR:O	1:B:361:LYS:HB2	2.11	0.51
1:B:90:SER:OG	1:B:181:HIS:ND1	2.45	0.50
1:B:57:ALA:HA	3:B:985:HOH:O	2.11	0.50
1:B:78:PRO:CG	3:B:1115:HOH:O	2.59	0.50
1:B:59:ILE:C	1:B:59:ILE:HD12	2.32	0.49
1:A:419:ARG:HD3	1:A:426:TRP:CZ2	2.48	0.49
1:A:418:ASP:HB3	1:A:424:ILE:CD1	2.42	0.49
1:B:71:THR:HG22	3:B:975:HOH:O	2.12	0.49
1:A:3:THR:O	1:A:4:GLU:HB2	2.13	0.48
1:A:277:ARG:CG	1:A:277:ARG:NH1	2.76	0.48
1:A:136:MET:HE3	1:A:180:ILE:HD13	1.94	0.48
1:B:90:SER:HB3	1:B:93:ARG:NH1	2.29	0.48
1:B:258:ILE:HD12	1:B:262:LEU:HD11	1.96	0.47
1:B:551:LEU:HD12	1:B:552:PRO:HD2	1.95	0.47
1:A:549:MET:HG2	1:B:548:GLN:NE2	2.29	0.47
1:A:565:ARG:NE	3:A:801:HOH:O	2.32	0.47
1:B:437:PRO:HB2	3:B:926:HOH:O	2.14	0.47
1:A:418:ASP:HB3	1:A:424:ILE:HD11	1.97	0.47
1:A:247:THR:HG22	3:A:1008:HOH:O	2.08	0.47
3:A:988:HOH:O	1:B:525:GLU:HG3	2.15	0.47
1:B:382:ARG:HD2	3:B:1020:HOH:O	2.14	0.47
1:B:529:LEU:HB3	1:B:542:VAL:HG13	1.97	0.47
1:A:365:SER:OG	1:A:368:HIS:CD2	2.59	0.47
1:A:289:ARG:HG3	1:A:326:ALA:HB2	1.96	0.47
1:A:384:GLU:HG2	3:A:1178:HOH:O	2.15	0.46
1:B:177:VAL:CG1	1:B:178:LEU:N	2.78	0.46
1:B:165:PHE:HD2	1:B:166:ASP:OD1	1.98	0.46
1:B:355:ARG:O	1:B:356:LYS:CB	2.63	0.46
1:A:38:ASN:HB3	3:A:948:HOH:O	2.15	0.46
1:B:121:MET:O	1:B:123:GLU:N	2.49	0.46
1:B:543:TYR:O	1:B:547:VAL:HG23	2.16	0.46
1:A:503:ARG:HH22	1:A:587:GLU:CD	2.19	0.45
3:A:988:HOH:O	1:B:525:GLU:CG	2.64	0.45
1:B:171:VAL:HG22	3:B:1017:HOH:O	2.16	0.45
1:B:341:LYS:HD2	3:B:829:HOH:O	2.17	0.45
1:A:115:VAL:HG23	1:A:152:ILE:CD1	2.47	0.45
1:B:272:LEU:C	1:B:272:LEU:HD12	2.38	0.45
1:B:355:ARG:O	1:B:356:LYS:HB3	2.17	0.45
1:A:527:GLU:HG2	3:A:925:HOH:O	2.17	0.44
1:B:149:LYS:HD2	3:B:931:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:MET:HG2	3:A:1244:HOH:O	2.17	0.44
1:B:202:GLY:HA2	1:B:344:LEU:O	2.18	0.44
1:A:59:ILE:C	1:A:59:ILE:HD12	2.37	0.44
1:B:146:ARG:HA	1:B:169:TYR:O	2.17	0.44
1:B:501:GLU:O	1:B:502:HIS:HB2	2.18	0.44
1:A:136:MET:CE	1:A:180:ILE:HD13	2.48	0.44
1:B:128:PRO:O	1:B:154:THR:CG2	2.64	0.44
1:B:44:VAL:HG13	1:B:54:ILE:HD11	1.99	0.44
1:B:294:PRO:HB3	1:B:387:THR:HG21	1.99	0.43
1:A:529:LEU:HD23	1:A:529:LEU:HA	1.79	0.43
1:A:118:PHE:HE2	1:A:152:ILE:HG13	1.83	0.43
1:A:351:GLU:HG2	1:A:351:GLU:H	1.54	0.43
1:B:68:PRO:O	1:B:71:THR:HG23	2.19	0.43
1:B:501:GLU:O	1:B:502:HIS:CB	2.66	0.43
1:A:256:PRO:HG2	1:A:317:HIS:ND1	2.34	0.42
1:A:388:ARG:HH11	1:A:388:ARG:HD2	1.73	0.42
1:B:140:ARG:NH2	1:B:176:ASP:HB3	2.34	0.42
1:A:437:PRO:HD2	3:A:851:HOH:O	2.20	0.42
1:B:96:LEU:HD11	1:B:121:MET:CE	2.50	0.42
1:B:419:ARG:HA	1:B:422:ARG:O	2.19	0.42
1:A:14:LEU:CD1	1:A:64:VAL:HG13	2.50	0.42
1:B:136:MET:O	1:B:147:ALA:HA	2.20	0.42
1:A:549:MET:HG2	1:B:548:GLN:HE21	1.84	0.42
1:B:95:GLU:CD	1:B:177:VAL:HG11	2.39	0.42
1:B:108:LYS:HD2	1:B:112:ASP:HB2	2.02	0.42
1:B:585:MET:O	1:B:589:GLU:HG2	2.19	0.42
1:A:153:VAL:HG13	1:A:310:ILE:HD12	2.01	0.42
1:A:360:THR:HG23	1:A:424:ILE:HG12	2.01	0.42
1:B:440:THR:O	1:B:444:ARG:HG3	2.19	0.42
1:A:522:ARG:NH1	1:A:527:GLU:OE2	2.46	0.41
1:B:435:LYS:HG3	3:B:945:HOH:O	2.20	0.41
1:A:349:HIS:C	1:A:351:GLU:H	2.22	0.41
1:B:96:LEU:HD11	1:B:121:MET:HE1	2.02	0.41
1:A:516:LEU:HB3	1:A:557:THR:HB	2.02	0.41
1:B:155:HIS:HA	1:B:156:PRO:HD3	1.96	0.41
1:B:358:LEU:CB	1:B:359:PRO:HD3	2.51	0.41
1:B:543:TYR:OH	1:B:559:HIS:CD2	2.59	0.41
1:A:231:GLU:OE2	1:A:503:ARG:HD2	2.20	0.41
1:A:487:LYS:HD3	1:A:487:LYS:HA	1.92	0.41
1:A:501:GLU:HA	3:A:803:HOH:O	2.20	0.41
1:B:59:ILE:HD12	1:B:59:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:MET:C	1:B:123:GLU:H	2.25	0.41
1:B:589:GLU:HB2	3:B:882:HOH:O	2.20	0.41
1:A:38:ASN:CB	3:A:948:HOH:O	2.69	0.41
1:A:66:MET:CE	1:A:87:ARG:HG2	2.36	0.41
1:A:384:GLU:CG	3:A:1178:HOH:O	2.68	0.41
1:B:103:LEU:HD21	1:B:174:LEU:HD11	2.03	0.40
1:A:295:THR:OG1	1:A:297:GLN:NE2	2.51	0.40
1:B:120:PRO:HA	1:B:154:THR:HG23	2.03	0.40
1:A:221:ALA:O	1:A:225:GLU:HG2	2.20	0.40
1:B:200:TYR:CD1	1:B:294:PRO:HA	2.56	0.40
1:B:438:VAL:HA	1:B:477:VAL:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1087:HOH:O	3:B:1087:HOH:O[3_655]	2.04	0.16

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	590/617 (96%)	565 (96%)	21 (4%)	4 (1%)	22	32
1	B	589/617 (96%)	557 (95%)	24 (4%)	8 (1%)	11	15
All	All	1179/1234 (96%)	1122 (95%)	45 (4%)	12 (1%)	15	23

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	351	GLU
1	B	356	LYS

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Mol	Chain	Res	Type
1	B	358	LEU
1	B	361	LYS
1	B	456	GLY
1	A	353	LEU
1	B	112	ASP
1	B	51	LEU
1	A	4	GLU
1	A	554	ASN
1	B	68	PRO
1	B	122	PRO

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	484/504 (96%)	461 (95%)	23 (5%)	25 41
1	B	483/504 (96%)	454 (94%)	29 (6%)	19 31
All	All	967/1008 (96%)	915 (95%)	52 (5%)	22 36

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	21	ARG
1	A	23	ARG
1	A	37	ARG
1	A	39	ILE
1	A	70	SER
1	A	94	THR
1	A	140	ARG
1	A	152	ILE
1	A	201	GLN
1	A	222	LYS
1	A	236	ILE
1	A	247	THR

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Mol	Chain	Res	Type
1	A	277	ARG
1	A	351	GLU
1	A	354	HIS
1	A	373	GLN
1	A	384	GLU
1	A	400	ASP
1	A	444	ARG
1	A	524	LYS
1	A	525	GLU
1	A	565	ARG
1	B	25	LEU
1	B	37	ARG
1	B	51	LEU
1	B	71	THR
1	B	77	LEU
1	B	90	SER
1	B	138	SER
1	B	139	ARG
1	B	142	ASN
1	B	143	GLU
1	B	152	ILE
1	B	154	THR
1	B	162	LEU
1	B	222	LYS
1	B	236	ILE
1	B	272	LEU
1	B	331	ASP
1	B	355	ARG
1	B	356	LYS
1	B	357	ASP
1	B	369	ARG
1	B	433	SER
1	B	435	LYS
1	B	436	ASP
1	B	445	LEU
1	B	455	GLU
1	B	462	LYS
1	B	504	ARG
1	B	522	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	HIS
1	A	181	HIS
1	A	288	ASN
1	A	368	HIS
1	A	373	GLN
1	B	155	HIS
1	B	375	HIS
1	B	457	ASN
1	B	548	GLN
1	B	559	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 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 (i)

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, 95^{th} 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	592/617 (95%)	-0.53	3 (0%)	91	89	17, 34, 65, 138	0
1	B	591/617 (95%)	-0.36	12 (2%)	65	63	20, 40, 84, 142	0
All	All	1183/1234 (95%)	-0.45	15 (1%)	77	75	17, 37, 75, 142	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	354	HIS	4.8
1	B	358	LEU	3.7
1	A	354	HIS	3.7
1	B	351	GLU	3.1
1	B	435	LYS	3.1
1	B	145	PHE	3.0
1	B	353	LEU	2.9
1	B	96	LEU	2.6
1	B	70	SER	2.5
1	B	456	GLY	2.3
1	B	173	GLU	2.3
1	A	353	LEU	2.2
1	B	359	PRO	2.2
1	B	433	SER	2.1
1	A	456	GLY	2.0

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

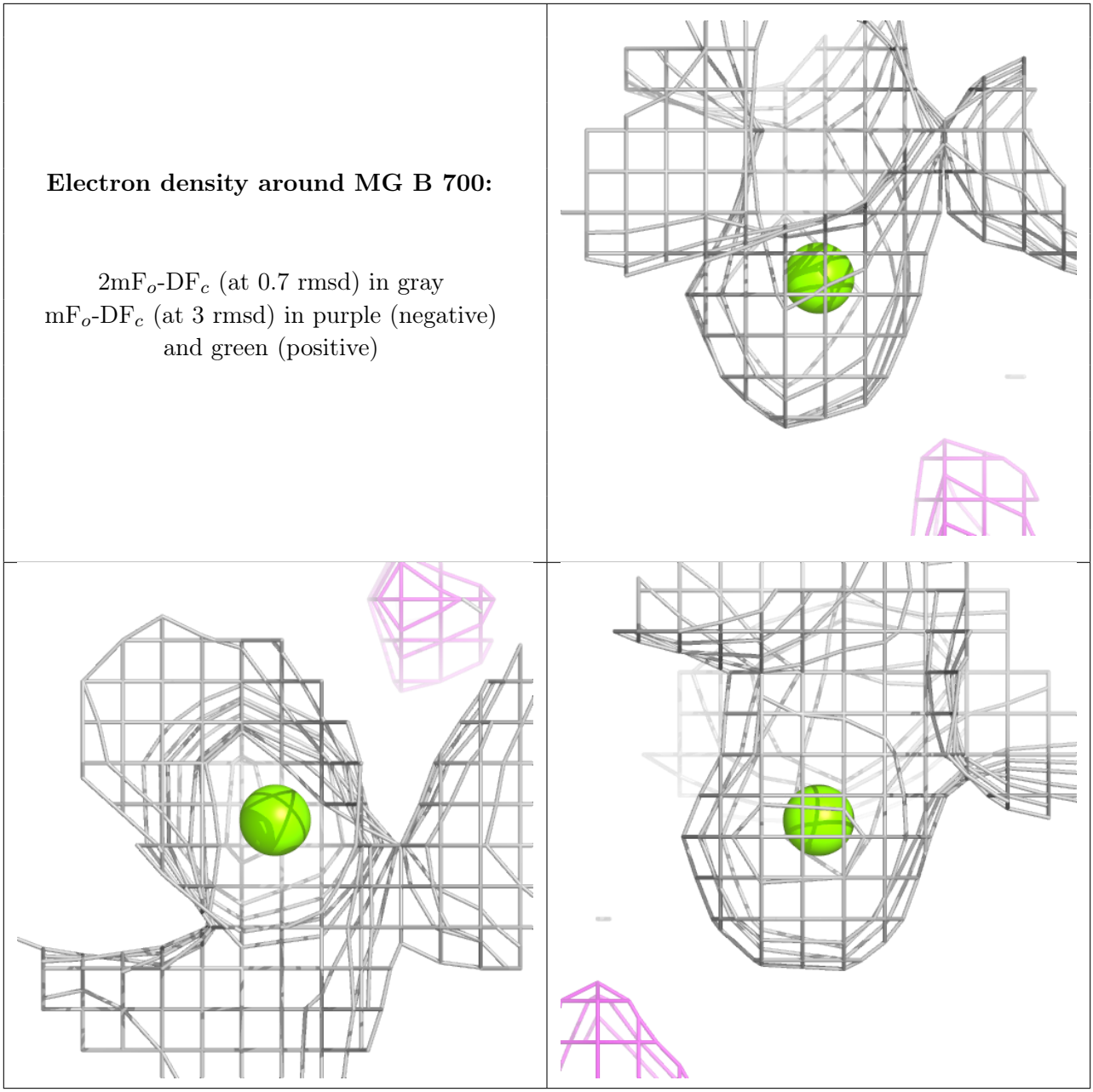
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	B	700	1/1	0.95	0.10	47,47,47,47	0
2	MG	A	700	1/1	0.99	0.11	49,49,49,49	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.

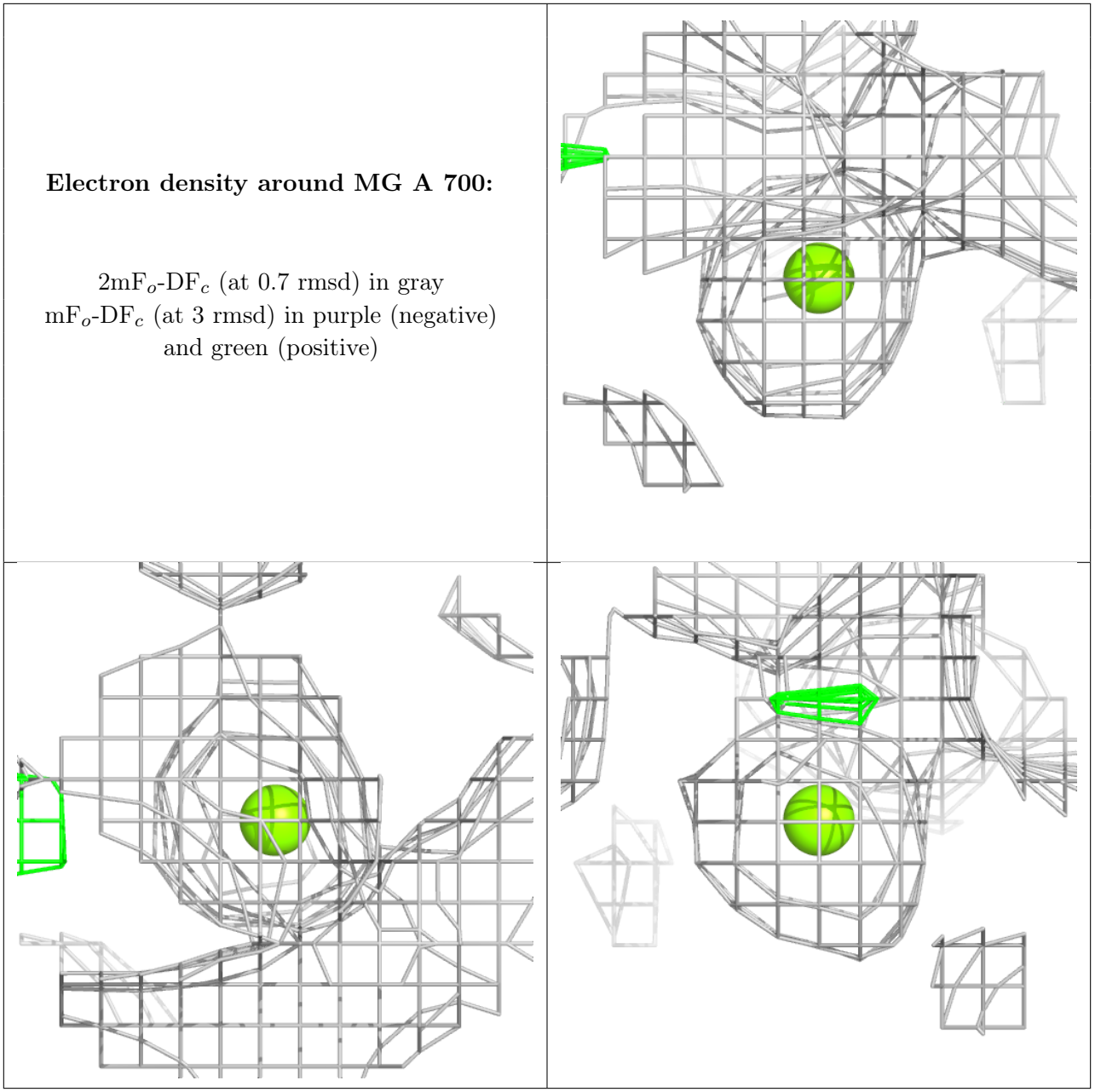
Electron density around MG B 700:

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



Electron density around MG A 700:

$2mF_o$-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 (i)

There are no such residues in this entry.