



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:56 PM GMT

PDB ID : 2BM1
Title : RIBOSOMAL ELONGATION FACTOR G (EF-G) FUSIDIC ACID RESISTANT MUTANT G16V
Authors : Hansson, S.; Singh, R.; Gudkov, A.T.; Liljas, A.; Logan, D.T.
Deposited on : 2005-03-09
Resolution : 2.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

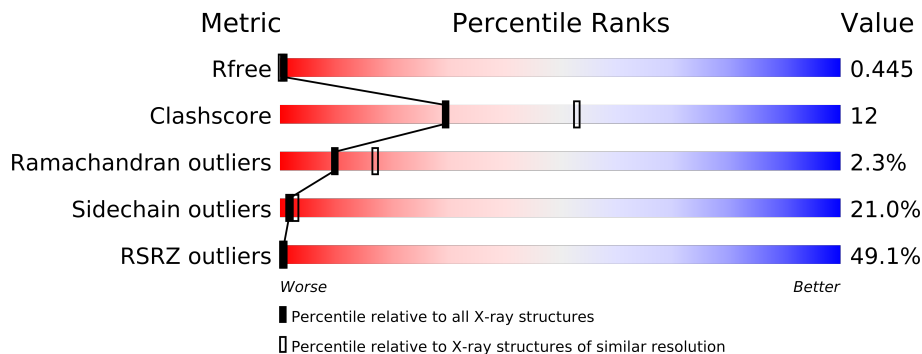
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance


The reported resolution of this entry is 2.60 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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	691	

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 5258 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

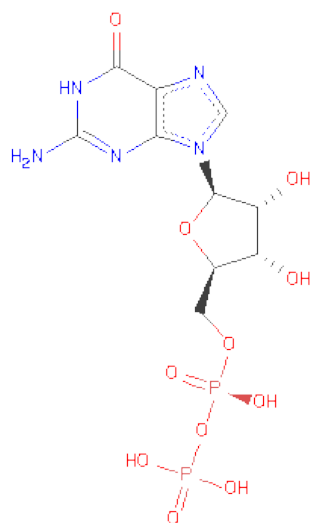
- Molecule 1 is a protein called ELONGATION FACTOR G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	660	5167	3286	882	981	18	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	VAL	GLY	ENGINEERED MUTATION	UNP P13551

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	28	10	5	11	2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	62	Total	O	0	0
			62	62		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.30Å 89.70Å 114.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.00 – 2.60 22.52 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.2 (28.00-2.60) 98.6 (22.52-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.220 , 0.297 0.444 , 0.445	Depositor DCC
R_{free} test set	1247 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	52.9	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 26.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 24503 reflections	Xtriage
F_o, F_c correlation	0.70	EDS
Total number of atoms	5258	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, 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	0.72	0/5264	0.93	23/7131 (0.3%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	562	ASP	CB-CG-OD2	8.08	125.58	118.30
1	A	393	ASP	CB-CG-OD2	7.33	124.90	118.30
1	A	224	ASP	CB-CG-OD2	7.17	124.75	118.30
1	A	252	ASP	CB-CG-OD2	6.87	124.48	118.30
1	A	83	ASP	CB-CG-OD2	6.77	124.39	118.30
1	A	76	ASP	CB-CG-OD2	6.76	124.38	118.30
1	A	410	ASP	CB-CG-OD2	6.66	124.29	118.30
1	A	285	ASP	CB-CG-OD2	6.63	124.27	118.30
1	A	222	ASP	CB-CG-OD2	6.38	124.05	118.30
1	A	89	ASP	CB-CG-OD2	6.33	124.00	118.30
1	A	8	ASP	CB-CG-OD2	6.17	123.85	118.30
1	A	619	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	435	ASP	CB-CG-OD2	5.83	123.54	118.30
1	A	464	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	396	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	A	102	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	13	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	13	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	274	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	319	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	658	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	623	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	357	ARG	NE-CZ-NH2	5.05	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5167	0	5230	127	9
2	A	28	0	12	1	0
3	A	1	0	0	0	1
4	A	62	0	0	10	0
All	All	5258	0	5242	127	9

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (127) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:190:ASN:HD22	1:A:192:LEU:H	1.23	0.82
1:A:190:ASN:ND2	1:A:192:LEU:H	1.76	0.81
1:A:636:PRO:HB3	1:A:641:GLN:HE21	1.45	0.81
1:A:361:ASN:HD22	1:A:361:ASN:H	1.27	0.81
1:A:632:LEU:HD21	1:A:646:PHE:CE2	2.18	0.79
1:A:165:GLN:NE2	1:A:260:LEU:H	1.82	0.77
1:A:132:ARG:CZ	4:A:2011:HOH:O	2.35	0.73
1:A:137:ASN:HD21	1:A:263:ALA:H	1.37	0.73
1:A:4:LYS:HA	1:A:5:VAL:C	2.15	0.67
1:A:580:MET:HG2	4:A:2055:HOH:O	1.95	0.66
1:A:90:PHE:O	1:A:670:VAL:HG12	1.95	0.65
1:A:165:GLN:HE21	1:A:260:LEU:H	1.44	0.64
1:A:18:ALA:HB1	1:A:121:VAL:HG21	1.79	0.62
1:A:415:PRO:HA	1:A:474:ALA:HB1	1.81	0.62
1:A:9:LEU:HD13	1:A:284:LEU:HD13	1.83	0.60
1:A:605:ILE:HG22	1:A:605:ILE:O	2.02	0.60
1:A:343:ASN:HD22	1:A:343:ASN:C	2.05	0.60
1:A:636:PRO:HB3	1:A:641:GLN:NE2	2.16	0.59
1:A:295:GLU:OE2	4:A:2034:HOH:O	2.17	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:116:PRO:O	1:A:117:GLN:HB2	2.04	0.58
1:A:316:ILE:CD1	1:A:326:THR:HB	2.35	0.57
1:A:610:VAL:HG13	1:A:659:LEU:HD11	1.85	0.57
1:A:550:MET:SD	1:A:563:ILE:HD11	2.45	0.57
1:A:546:ILE:HG23	1:A:590:ILE:HG13	1.87	0.57
1:A:113:GLY:HA2	1:A:149:VAL:HG22	1.87	0.56
1:A:391:GLY:O	1:A:392:GLU:CB	2.53	0.56
1:A:517:LEU:HD21	1:A:524:GLU:HG3	1.85	0.56
1:A:409:ILE:HD11	1:A:649:LEU:HD11	1.87	0.56
1:A:316:ILE:HG12	1:A:385:THR:HG22	1.87	0.55
1:A:89:ASP:O	1:A:124:GLN:NE2	2.40	0.55
1:A:326:THR:HG22	4:A:2039:HOH:O	2.05	0.55
1:A:485:GLU:O	1:A:560:VAL:HA	2.07	0.55
1:A:125:ALA:O	1:A:128:TYR:O	2.25	0.55
1:A:388:THR:HG23	1:A:399:LEU:HD22	1.87	0.54
1:A:415:PRO:HB2	1:A:420:ASP:HB3	1.90	0.54
1:A:160:ARG:HG2	1:A:255:ILE:HG22	1.90	0.54
1:A:536:LYS:O	1:A:537:GLU:CB	2.56	0.54
1:A:9:LEU:HD13	1:A:284:LEU:CD1	2.39	0.53
1:A:100:VAL:HG22	1:A:329:ARG:HB2	1.90	0.53
1:A:316:ILE:HD13	1:A:326:THR:HB	1.91	0.52
1:A:549:ALA:HB1	1:A:591:LYS:HD3	1.92	0.52
1:A:181:LEU:HD22	1:A:216:LEU:HD21	1.92	0.52
1:A:94:VAL:HG12	1:A:94:VAL:O	2.10	0.51
1:A:116:PRO:O	1:A:117:GLN:CB	2.59	0.51
1:A:409:ILE:CG1	1:A:649:LEU:HD11	2.42	0.50
1:A:603:GLU:CD	1:A:679:VAL:HG12	2.32	0.50
1:A:351:ARG:HB2	1:A:351:ARG:CZ	2.41	0.50
1:A:632:LEU:HD11	1:A:646:PHE:CE1	2.47	0.49
1:A:96:ARG:HG3	1:A:400:GLU:OE2	2.12	0.49
1:A:7:TYR:OH	1:A:9:LEU:HG	2.12	0.49
1:A:605:ILE:HG21	1:A:675:HIS:CE1	2.48	0.48
1:A:100:VAL:HG22	1:A:329:ARG:CB	2.43	0.48
1:A:549:ALA:HB3	1:A:590:ILE:CG2	2.43	0.48
1:A:351:ARG:HB2	1:A:351:ARG:NH2	2.29	0.48
1:A:148:LEU:O	1:A:152:THR:HG22	2.13	0.48
1:A:361:ASN:HD22	1:A:361:ASN:N	2.02	0.48
1:A:539:ILE:N	1:A:540:PRO:CD	2.76	0.48
1:A:536:LYS:O	1:A:537:GLU:CD	2.52	0.47
1:A:509:HIS:HD1	1:A:570:GLY:HA2	1.78	0.47
1:A:536:LYS:O	1:A:537:GLU:OE1	2.33	0.47
1:A:481:VAL:HG23	1:A:482:ALA:N	2.29	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:301:ILE:HD13	1:A:399:LEU:HD11	1.97	0.46
1:A:190:ASN:C	1:A:190:ASN:HD22	2.18	0.46
1:A:165:GLN:HA	1:A:178:ILE:O	2.14	0.46
1:A:319:ASP:OD1	1:A:363:ARG:NH2	2.44	0.46
1:A:506:GLN:HE21	1:A:581:ALA:HB2	1.80	0.46
1:A:65:ILE:O	1:A:66:THR:C	2.54	0.46
1:A:454:MET:CG	1:A:458:HIS:CD2	2.99	0.46
1:A:20:HIS:ND1	1:A:116:PRO:O	2.49	0.46
1:A:166:LEU:HD22	1:A:180:VAL:HG11	1.98	0.46
1:A:355:LEU:HD22	1:A:369:LEU:CD2	2.46	0.46
1:A:415:PRO:O	1:A:416:LYS:HB2	2.16	0.45
1:A:114:VAL:H	1:A:152:THR:HG21	1.81	0.45
1:A:325:LEU:HD21	1:A:356:LEU:HD12	1.98	0.45
1:A:458:HIS:ND1	1:A:462:ILE:HD11	2.32	0.45
1:A:5:VAL:O	1:A:6:GLU:C	2.55	0.45
1:A:345:THR:C	1:A:346:LYS:O	2.52	0.45
1:A:354:ARG:HB2	1:A:378:VAL:HB	1.98	0.45
1:A:411:VAL:O	1:A:450:ILE:HA	2.17	0.45
1:A:573:HIS:O	1:A:577:SER:HB2	2.17	0.45
1:A:536:LYS:O	1:A:537:GLU:CG	2.65	0.45
1:A:584:ILE:O	1:A:588:MET:HG3	2.17	0.44
1:A:166:LEU:HD22	1:A:180:VAL:CG1	2.47	0.44
1:A:361:ASN:H	1:A:361:ASN:ND2	2.06	0.44
1:A:609:GLU:HB3	1:A:670:VAL:CG2	2.47	0.44
1:A:409:ILE:O	1:A:452:SER:HA	2.18	0.44
1:A:497:PHE:CZ	1:A:499:ARG:HD2	2.53	0.44
1:A:607:ARG:C	4:A:2057:HOH:O	2.56	0.44
1:A:185:ALA:HB3	1:A:199:ILE:HG13	2.00	0.44
1:A:114:VAL:HG23	1:A:152:THR:HG23	2.01	0.43
1:A:336:THR:HG22	1:A:339:SER:HB3	1.99	0.43
1:A:312:LEU:O	1:A:328:ILE:HA	2.18	0.43
1:A:407:PRO:HA	1:A:453:GLY:O	2.19	0.43
1:A:186:TYR:HA	1:A:197:ARG:O	2.18	0.43
1:A:413:ILE:HG23	1:A:413:ILE:O	2.19	0.43
1:A:601:ILE:HG13	1:A:684:GLN:HE21	1.84	0.43
1:A:415:PRO:HG2	1:A:421:GLN:HG2	2.01	0.42
1:A:309:LEU:HD21	1:A:335:LEU:CD1	2.49	0.42
1:A:105:ILE:HD11	1:A:276:VAL:CG2	2.49	0.42
1:A:409:ILE:CG2	1:A:459:LEU:HD13	2.49	0.42
1:A:409:ILE:HG21	1:A:459:LEU:HD13	2.00	0.42
1:A:498:ILE:HA	1:A:506:GLN:O	2.18	0.42
1:A:408:VAL:HG21	1:A:606:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:423:LYS:HA	1:A:426:GLN:HB2	2.02	0.42
1:A:522:GLY:O	1:A:562:ASP:HA	2.19	0.42
1:A:115:GLU:O	1:A:118:SER:HB2	2.19	0.42
1:A:554:PRO:HB3	1:A:595:GLN:HG2	2.01	0.42
1:A:413:ILE:HD13	1:A:424:LEU:HD21	2.01	0.42
1:A:132:ARG:NH1	4:A:2011:HOH:O	2.49	0.41
1:A:671:MET:CG	4:A:2057:HOH:O	2.68	0.41
1:A:644:ARG:HB3	4:A:2058:HOH:O	2.20	0.41
1:A:409:ILE:CD1	1:A:649:LEU:HD11	2.50	0.41
1:A:138:LYS:HG2	2:A:1689:GDP:C6	2.55	0.41
1:A:608:VAL:CG2	1:A:647:VAL:CG1	2.99	0.41
1:A:627:ARG:HB2	1:A:651:GLU:O	2.21	0.41
1:A:357:ARG:NH1	1:A:373:ASP:OD2	2.54	0.41
1:A:74:TRP:CD1	1:A:75:LYS:HG2	2.56	0.41
1:A:123:ARG:HG3	1:A:611:THR:HG21	2.02	0.41
1:A:498:ILE:HG12	1:A:507:TYR:CD2	2.55	0.41
1:A:335:LEU:HD11	1:A:341:VAL:HG11	2.02	0.41
1:A:94:VAL:CG1	1:A:94:VAL:O	2.69	0.41
1:A:506:GLN:NE2	1:A:581:ALA:HB2	2.36	0.41
1:A:499:ARG:NE	4:A:2049:HOH:O	2.54	0.41
1:A:413:ILE:HD11	1:A:424:LEU:HD11	2.03	0.40
1:A:601:ILE:HG12	4:A:2048:HOH:O	2.22	0.40
1:A:303:PRO:HA	1:A:331:TYR:O	2.21	0.40
1:A:470:PHE:HB3	1:A:472:VAL:HG23	2.01	0.40

All (9) 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	Distance(Å)	Clash(Å)
1:A:295:GLU:OE2	3:A:1690:MG:MG[3_555]	1.18	1.02
1:A:226:ASN:ND2	1:A:685:GLU:OE1[1_655]	1.49	0.71
1:A:367:GLU:OE1	1:A:500:GLN:OE1[1_655]	1.59	0.61
1:A:194:THR:O	1:A:521:SER:O[3_545]	2.05	0.15
1:A:367:GLU:CB	1:A:500:GLN:CB[1_655]	2.06	0.14
1:A:306:ASN:ND2	1:A:496:LYS:CE[1_655]	2.15	0.05
1:A:194:THR:CA	1:A:521:SER:O[3_545]	2.16	0.04
1:A:194:THR:OG1	1:A:521:SER:O[3_545]	2.17	0.03
1:A:367:GLU:CD	1:A:500:GLN:OE1[1_655]	2.18	0.02

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	656/691 (95%)	578 (88%)	63 (10%)	15 (2%)	10 17

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	THR
1	A	416	LYS
1	A	537	GLU
1	A	91	THR
1	A	117	GLN
1	A	392	GLU
1	A	403	GLU
1	A	171	GLU
1	A	628	ARG
1	A	346	LYS
1	A	380	LEU
1	A	87	HIS
1	A	320	PRO
1	A	554	PRO
1	A	556	ILE

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	558/583 (96%)	441 (79%)	117 (21%)	1 3

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	6	GLU
1	A	7	TYR
1	A	9	LEU
1	A	10	LYS
1	A	12	LEU
1	A	13	ARG
1	A	16	VAL
1	A	22	ASP
1	A	33	LEU
1	A	66	THR
1	A	88	VAL
1	A	89	ASP
1	A	92	ILE
1	A	95	GLU
1	A	98	MET
1	A	99	ARG
1	A	100	VAL
1	A	110	SER
1	A	111	SER
1	A	120	THR
1	A	124	GLN
1	A	130	VAL
1	A	132	ARG
1	A	142	THR
1	A	146	LEU
1	A	160	ARG
1	A	162	VAL
1	A	166	LEU
1	A	170	ARG
1	A	180	VAL
1	A	181	LEU
1	A	190	ASN
1	A	194	THR
1	A	214	GLU
1	A	229	LEU
1	A	232	LEU
1	A	233	GLU
1	A	239	GLU
1	A	253	LEU
1	A	260	LEU
1	A	264	LEU
1	A	267	LYS

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Mol	Chain	Res	Type
1	A	273	LEU
1	A	277	VAL
1	A	280	LEU
1	A	284	LEU
1	A	286	ILE
1	A	312	LEU
1	A	315	LYS
1	A	322	VAL
1	A	326	THR
1	A	336	THR
1	A	343	ASN
1	A	345	THR
1	A	348	ARG
1	A	349	LYS
1	A	351	ARG
1	A	352	VAL
1	A	361	ASN
1	A	369	LEU
1	A	373	ASP
1	A	377	VAL
1	A	382	GLU
1	A	385	THR
1	A	389	LEU
1	A	399	LEU
1	A	403	GLU
1	A	404	VAL
1	A	411	VAL
1	A	423	LYS
1	A	439	ARG
1	A	443	HIS
1	A	445	GLU
1	A	449	THR
1	A	461	ILE
1	A	464	ASP
1	A	468	ARG
1	A	471	LYS
1	A	476	VAL
1	A	480	GLN
1	A	481	VAL
1	A	499	ARG
1	A	500	GLN
1	A	511	LYS

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Mol	Chain	Res	Type
1	A	517	LEU
1	A	519	ARG
1	A	551	GLN
1	A	552	SER
1	A	558	PHE
1	A	577	SER
1	A	587	SER
1	A	590	ILE
1	A	592	GLU
1	A	596	LYS
1	A	605	ILE
1	A	606	MET
1	A	607	ARG
1	A	608	VAL
1	A	615	GLU
1	A	621	ILE
1	A	623	ASP
1	A	627	ARG
1	A	628	ARG
1	A	641	GLN
1	A	647	VAL
1	A	649	LEU
1	A	653	PHE
1	A	659	LEU
1	A	660	ARG
1	A	662	LYS
1	A	671	MET
1	A	672	PHE
1	A	681	LYS
1	A	682	GLN
1	A	687	LEU
1	A	688	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	124	GLN
1	A	137	ASN
1	A	154	GLN
1	A	165	GLN
1	A	190	ASN

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Mol	Chain	Res	Type
1	A	208	GLN
1	A	343	ASN
1	A	361	ASN
1	A	448	GLN
1	A	480	GLN
1	A	506	GLN
1	A	551	GLN
1	A	630	GLN
1	A	641	GLN
1	A	675	HIS
1	A	677	GLN
1	A	684	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GDP	A	1689	3	30,30,30	1.16	2 (6%)	44,47,47	2.24	10 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GDP	A	1689	3	-	0/16/32/32	0/1/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1689	GDP	O4'-C1'	-2.77	1.37	1.41
2	A	1689	GDP	C2-N3	2.59	1.36	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1689	GDP	C6-C5-N7	-10.37	132.74	134.14
2	A	1689	GDP	O4'-C1'-N9	5.09	113.17	108.44
2	A	1689	GDP	C2-N3-C4	2.84	119.08	115.09
2	A	1689	GDP	O3B-PB-O2B	2.71	118.15	107.61
2	A	1689	GDP	PA-O3A-PB	-2.68	123.83	131.68
2	A	1689	GDP	N3-C4-N9	2.66	130.82	126.91
2	A	1689	GDP	C5-C4-N3	-2.53	122.28	125.94
2	A	1689	GDP	C1'-N9-C4	-2.44	122.42	126.64
2	A	1689	GDP	N7-C8-N9	-2.39	107.59	114.36
2	A	1689	GDP	C8-N9-C4	2.02	108.44	106.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	660/691 (95%)	2.29	324 (49%) 1 0	29, 50, 115, 126	0

All (324) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	429	ALA	12.6
1	A	284	LEU	11.6
1	A	626	ALA	9.7
1	A	263	ALA	8.8
1	A	640	ALA	8.3
1	A	473	ASP	7.3
1	A	232	LEU	7.0
1	A	471	LYS	7.0
1	A	645	ALA	6.9
1	A	402	ILE	6.8
1	A	446	THR	6.6
1	A	470	PHE	6.5
1	A	465	ARG	6.1
1	A	9	LEU	6.1
1	A	447	GLY	5.8
1	A	201	ILE	5.8
1	A	670	VAL	5.7
1	A	669	PHE	5.4
1	A	663	THR	5.4
1	A	92	ILE	5.4
1	A	445	GLU	5.3
1	A	637	ARG	5.3
1	A	656	ALA	5.2
1	A	632	LEU	5.2
1	A	113	GLY	5.1
1	A	171	GLU	5.1
1	A	431	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	73	PHE	5.1
1	A	413	ILE	5.1
1	A	6	GLU	5.0
1	A	408	VAL	4.9
1	A	301	ILE	4.9
1	A	114	VAL	4.9
1	A	440	VAL	4.9
1	A	94	VAL	4.9
1	A	668	SER	4.9
1	A	235	GLU	4.8
1	A	86	GLY	4.8
1	A	189	GLY	4.7
1	A	283	PRO	4.6
1	A	308	PRO	4.6
1	A	296	GLY	4.6
1	A	426	GLN	4.6
1	A	619	ASP	4.6
1	A	441	SER	4.6
1	A	674	ASP	4.4
1	A	129	LYS	4.4
1	A	404	VAL	4.4
1	A	611	THR	4.4
1	A	226	ASN	4.4
1	A	384	ILE	4.3
1	A	609	GLU	4.3
1	A	610	VAL	4.3
1	A	482	ALA	4.3
1	A	608	VAL	4.3
1	A	229	LEU	4.3
1	A	159	ALA	4.3
1	A	194	THR	4.2
1	A	655	TYR	4.2
1	A	652	MET	4.2
1	A	110	SER	4.2
1	A	90	PHE	4.2
1	A	422	GLU	4.1
1	A	430	ARG	4.1
1	A	177	ILE	4.1
1	A	91	THR	4.0
1	A	244	ALA	4.0
1	A	648	PRO	4.0
1	A	217	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	667	GLY	4.0
1	A	453	GLY	3.9
1	A	455	GLY	3.9
1	A	532	GLY	3.9
1	A	39	ILE	3.9
1	A	620	VAL	3.9
1	A	462	ILE	3.9
1	A	5	VAL	3.9
1	A	681	LYS	3.9
1	A	213	HIS	3.8
1	A	349	LYS	3.8
1	A	415	PRO	3.8
1	A	438	PHE	3.8
1	A	322	VAL	3.8
1	A	251	ILE	3.8
1	A	203	GLU	3.8
1	A	362	HIS	3.8
1	A	133	ILE	3.8
1	A	214	GLU	3.7
1	A	646	PHE	3.7
1	A	225	GLU	3.7
1	A	472	VAL	3.7
1	A	660	ARG	3.7
1	A	344	THR	3.7
1	A	374	LEU	3.7
1	A	93	GLU	3.7
1	A	128	TYR	3.6
1	A	644	ARG	3.6
1	A	273	LEU	3.6
1	A	647	VAL	3.6
1	A	421	GLN	3.6
1	A	418	LYS	3.6
1	A	417	THR	3.6
1	A	451	ILE	3.6
1	A	407	PRO	3.5
1	A	666	ARG	3.5
1	A	397	VAL	3.5
1	A	664	GLN	3.5
1	A	238	THR	3.5
1	A	195	ASP	3.5
1	A	216	LEU	3.4
1	A	106	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	298	VAL	3.4
1	A	572	TYR	3.4
1	A	612	THR	3.4
1	A	37	GLY	3.4
1	A	452	SER	3.4
1	A	627	ARG	3.4
1	A	205	TYR	3.4
1	A	258	VAL	3.4
1	A	302	HIS	3.4
1	A	649	LEU	3.3
1	A	463	VAL	3.3
1	A	4	LYS	3.3
1	A	185	ALA	3.3
1	A	416	LYS	3.3
1	A	328	ILE	3.3
1	A	639	ASN	3.3
1	A	181	LEU	3.3
1	A	206	LEU	3.3
1	A	295	GLU	3.3
1	A	82	ILE	3.3
1	A	130	VAL	3.3
1	A	237	PRO	3.3
1	A	586	GLY	3.3
1	A	183	MET	3.3
1	A	124	GLN	3.2
1	A	10	LYS	3.2
1	A	89	ASP	3.2
1	A	676	TYR	3.2
1	A	478	LYS	3.2
1	A	234	GLY	3.2
1	A	252	ASP	3.2
1	A	502	GLY	3.2
1	A	88	VAL	3.2
1	A	554	PRO	3.2
1	A	658	ASP	3.2
1	A	193	GLY	3.2
1	A	76	ASP	3.1
1	A	475	ASN	3.1
1	A	77	HIS	3.1
1	A	433	GLU	3.1
1	A	21	ILE	3.1
1	A	634	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	144	ALA	3.1
1	A	420	ASP	3.1
1	A	459	LEU	3.1
1	A	533	VAL	3.0
1	A	427	ALA	3.0
1	A	178	ILE	3.0
1	A	623	ASP	3.0
1	A	135	PHE	3.0
1	A	439	ARG	3.0
1	A	299	VAL	3.0
1	A	604	PRO	3.0
1	A	277	VAL	3.0
1	A	170	ARG	3.0
1	A	480	GLN	3.0
1	A	150	ILE	3.0
1	A	262	SER	3.0
1	A	461	ILE	3.0
1	A	118	SER	2.9
1	A	636	PRO	2.9
1	A	671	MET	2.9
1	A	672	PHE	2.9
1	A	424	LEU	2.9
1	A	403	GLU	2.9
1	A	12	LEU	2.9
1	A	290	LYS	2.9
1	A	500	GLN	2.9
1	A	190	ASN	2.9
1	A	560	VAL	2.9
1	A	182	ARG	2.9
1	A	607	ARG	2.9
1	A	556	ILE	2.9
1	A	279	TYR	2.9
1	A	643	ILE	2.9
1	A	469	GLU	2.9
1	A	457	LEU	2.8
1	A	330	VAL	2.8
1	A	503	GLY	2.8
1	A	481	VAL	2.8
1	A	542	VAL	2.8
1	A	353	ALA	2.8
1	A	588	MET	2.8
1	A	338	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	187	THR	2.8
1	A	409	ILE	2.8
1	A	67	ALA	2.8
1	A	317	MET	2.8
1	A	590	ILE	2.8
1	A	679	VAL	2.8
1	A	335	LEU	2.8
1	A	432	ALA	2.8
1	A	140	ASP	2.8
1	A	450	ILE	2.8
1	A	179	ASP	2.8
1	A	606	MET	2.8
1	A	630	GLN	2.7
1	A	386	GLY	2.7
1	A	224	ASP	2.7
1	A	485	GLU	2.7
1	A	223	PHE	2.7
1	A	616	TYR	2.7
1	A	210	ARG	2.7
1	A	153	MET	2.7
1	A	222	ASP	2.7
1	A	261	GLY	2.7
1	A	329	ARG	2.7
1	A	196	ILE	2.7
1	A	621	ILE	2.7
1	A	321	TYR	2.6
1	A	414	GLU	2.6
1	A	306	ASN	2.6
1	A	504	ARG	2.6
1	A	212	TYR	2.6
1	A	33	LEU	2.6
1	A	638	GLY	2.6
1	A	348	ARG	2.6
1	A	108	PHE	2.6
1	A	390	VAL	2.6
1	A	411	VAL	2.6
1	A	231	TYR	2.6
1	A	199	ILE	2.6
1	A	192	LEU	2.6
1	A	122	TRP	2.6
1	A	585	ALA	2.6
1	A	412	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	595	GLN	2.5
1	A	127	LYS	2.5
1	A	483	TYR	2.5
1	A	437	THR	2.5
1	A	687	LEU	2.5
1	A	454	MET	2.5
1	A	265	LYS	2.5
1	A	294	PRO	2.5
1	A	188	TYR	2.5
1	A	466	LEU	2.5
1	A	521	SER	2.5
1	A	396	ARG	2.5
1	A	264	LEU	2.5
1	A	651	GLU	2.4
1	A	11	ARG	2.4
1	A	496	LYS	2.4
1	A	378	VAL	2.4
1	A	456	GLU	2.4
1	A	393	ASP	2.4
1	A	406	GLU	2.4
1	A	180	VAL	2.4
1	A	546	ILE	2.4
1	A	221	ALA	2.4
1	A	398	ILE	2.4
1	A	74	TRP	2.4
1	A	449	THR	2.4
1	A	297	GLU	2.4
1	A	673	PHE	2.4
1	A	423	LYS	2.4
1	A	571	SER	2.4
1	A	139	MET	2.3
1	A	425	SER	2.3
1	A	530	VAL	2.3
1	A	434	GLU	2.3
1	A	276	VAL	2.3
1	A	146	LEU	2.3
1	A	428	LEU	2.3
1	A	29	THR	2.3
1	A	220	ALA	2.3
1	A	112	GLN	2.3
1	A	7	TYR	2.3
1	A	618	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	354	ARG	2.3
1	A	662	LYS	2.3
1	A	207	ASP	2.2
1	A	17	ILE	2.2
1	A	287	PRO	2.2
1	A	624	LEU	2.2
1	A	163	VAL	2.2
1	A	151	ARG	2.2
1	A	347	GLY	2.2
1	A	491	VAL	2.2
1	A	257	PRO	2.2
1	A	158	GLY	2.2
1	A	200	PRO	2.2
1	A	592	GLU	2.2
1	A	266	ASN	2.2
1	A	526	VAL	2.2
1	A	85	PRO	2.2
1	A	507	TYR	2.2
1	A	107	VAL	2.2
1	A	219	VAL	2.2
1	A	677	GLN	2.2
1	A	602	LEU	2.2
1	A	545	GLY	2.1
1	A	377	VAL	2.1
1	A	259	PHE	2.1
1	A	685	GLU	2.1
1	A	527	ASN	2.1
1	A	240	GLU	2.1
1	A	389	LEU	2.1
1	A	476	VAL	2.1
1	A	356	LEU	2.1
1	A	458	HIS	2.1
1	A	65	ILE	2.1
1	A	342	TYR	2.1
1	A	553	GLY	2.1
1	A	141	LYS	2.1
1	A	98	MET	2.1
1	A	8	ASP	2.0
1	A	392	GLU	2.0
1	A	169	GLY	2.0
1	A	326	THR	2.0
1	A	410	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	574	GLU	2.0
1	A	250	THR	2.0
1	A	143	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	GDP	A	1689	28/28	0.27	-0.65	25,36,40,41	0
3	MG	A	1690	1/1	0.11	-2.51	40,40,40,40	0

6.5 Other polymers

There are no such residues in this entry.