



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2026 – 05:28 PM UTC

PDB ID : 2BM1 / pdb_00002bm1
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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

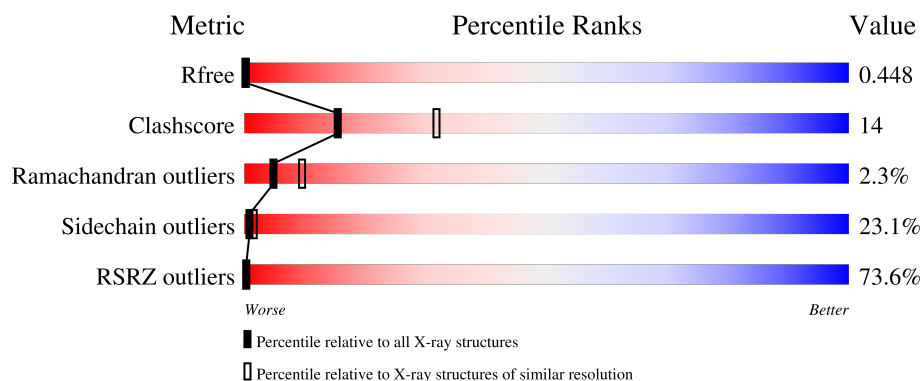
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 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	691	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5258 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.

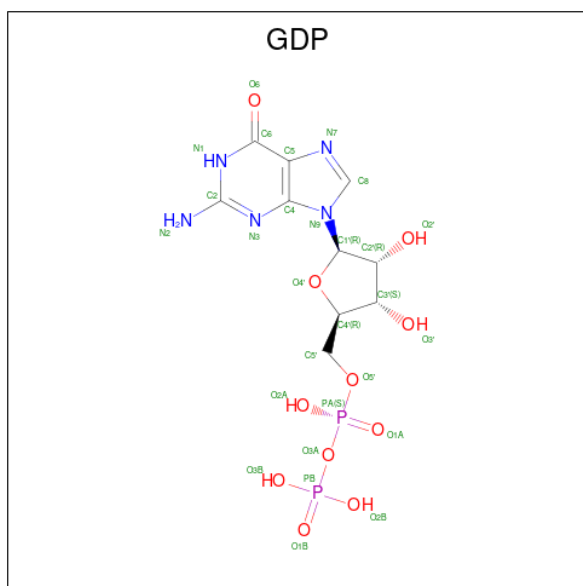
- Molecule 1 is a protein called ELONGATION FACTOR G.

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 (CCD ID: 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 (CCD ID: MG) (formula: Mg).

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

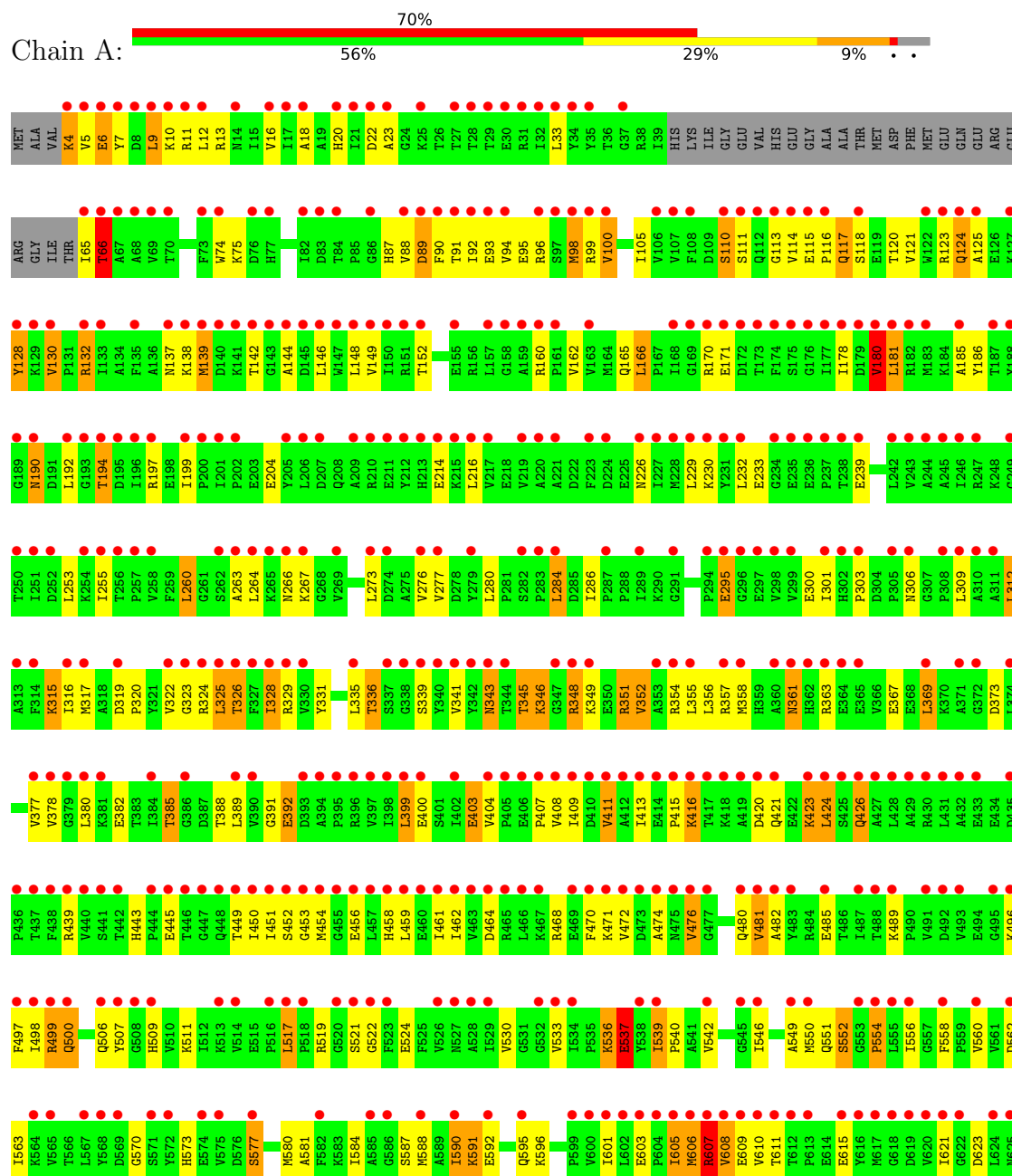
- Molecule 4 is water.

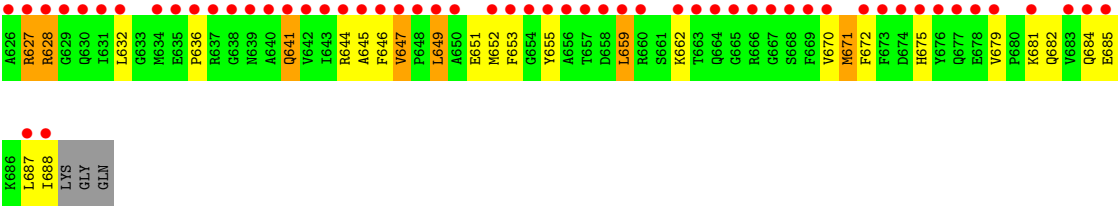
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	62	Total	O	0	0
			62	62		

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: ELONGATION FACTOR G





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 28.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.2 (28.00-2.60) 98.4 (28.00-2.60)	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 , 0.448	Depositor DCC
R_{free} test set	1248 reflections (5.09%)	wwPDB-VP
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 , 32.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

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, GDP

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	0.96	7/5264 (0.1%)	1.05	10/7131 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	352	VAL	CA-CB	7.90	1.62	1.53
1	A	98	MET	SD-CE	7.11	1.97	1.79
1	A	139	MET	SD-CE	-6.64	1.62	1.79
1	A	476	VAL	CA-CB	6.05	1.61	1.54
1	A	530	VAL	CA-CB	5.72	1.60	1.53
1	A	180	VAL	CA-CB	5.41	1.61	1.54
1	A	23	ALA	CA-CB	-5.10	1.44	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	536	LYS	N-CA-C	-6.86	101.29	110.55
1	A	128	TYR	N-CA-C	-6.55	101.26	110.50
1	A	348	ARG	N-CA-C	6.53	118.45	108.52
1	A	607	ARG	N-CA-C	5.60	117.77	108.20
1	A	552	SER	N-CA-C	5.47	117.75	108.02
1	A	130	VAL	N-CA-C	5.42	113.91	107.73
1	A	645	ALA	N-CA-C	5.24	117.04	109.07
1	A	681	LYS	N-CA-C	5.24	117.42	111.02
1	A	424	LEU	N-CA-C	-5.13	106.97	113.43
1	A	266	ASN	N-CA-C	5.08	118.41	111.39

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	5167	0	5230	141	9
2	A	28	0	12	1	0
3	A	1	0	0	0	1
4	A	62	0	0	11	0
All	All	5258	0	5242	141	9

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 14.

All (141) 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: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	0.71
1:A:408:VAL:HG21	1:A:606:MET:HE1	1.75	0.69
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:343:ASN:C	1:A:343:ASN:HD22	2.05	0.65
1:A:110:SER:OG	1:A:139:MET:HE3	1.96	0.64
1:A:165:GLN:HE21	1:A:260:LEU:H	1.44	0.64
1:A:315:LYS:NZ	1:A:317:MET:HE3	2.13	0.63
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:536:LYS:NZ	4:A:2051:HOH:O	2.34	0.60
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: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	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:PRO:O	1:A:117:GLN:HB2	2.04	0.58
1:A:315:LYS:HZ3	1:A:317:MET:HE3	1.68	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:546:ILE:HG23	1:A:590:ILE:HG13	1.87	0.57
1:A:550:MET:SD	1:A:563:ILE:HD11	2.45	0.57
1:A:113:GLY:HA2	1:A:149:VAL:HG22	1.87	0.56
1:A:139:MET:HE2	1:A:144:ALA:HB1	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:603:GLU:CD	1:A:679:VAL:HG12	2.32	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:536:LYS:O	1:A:537:GLU:CD	2.52	0.52
1:A:316:ILE:HD13	1:A:326:THR:HB	1.91	0.52
1:A:181:LEU:HD22	1:A:216:LEU:HD21	1.92	0.52
1:A:549:ALA:HB1	1:A:591:LYS:HD3	1.92	0.52
1:A:358:MET:HE1	1:A:363:ARG:HE	1.75	0.51
1:A:65:ILE:O	1:A:66:THR:C	2.54	0.51
1:A:190:ASN:HD22	1:A:190:ASN:C	2.18	0.51
1:A:606:MET:HE3	1:A:649:LEU:HB3	1.93	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:94:VAL:O	1:A:94:VAL:HG12	2.10	0.50
1:A:351:ARG:CZ	1:A:351:ARG:HB2	2.41	0.50
1:A:345:THR:C	1:A:346:LYS:O	2.52	0.50
1:A:5:VAL:O	1:A:6:GLU:C	2.55	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:VAL:HG22	1:A:329:ARG:CB	2.43	0.48
1:A:148:LEU:O	1:A:152:THR:HG22	2.13	0.48
1:A:351:ARG:HB2	1:A:351:ARG:NH2	2.29	0.48
1:A:549:ALA:HB3	1:A:590:ILE:CG2	2.43	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:607:ARG:C	4:A:2057:HOH:O	2.56	0.47
1:A:358:MET:HE1	1:A:363:ARG:NE	2.29	0.47
1:A:509:HIS:HD1	1:A:570:GLY:HA2	1.78	0.47
1:A:652:MET:HE3	1:A:655:TYR:CD2	2.49	0.47
1:A:536:LYS:O	1:A:537:GLU:OE1	2.33	0.47
1:A:606:MET:HE3	1:A:649:LEU:CB	2.45	0.47
1:A:481:VAL:HG23	1:A:482:ALA:N	2.29	0.47
1:A:301:ILE:HD13	1:A:399:LEU:HD11	1.97	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: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: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:415:PRO:O	1:A:416:LYS:HB2	2.16	0.45
1:A:458:HIS:ND1	1:A:462:ILE:HD11	2.32	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:409:ILE:O	1:A:452:SER:HA	2.18	0.44
1:A:609:GLU:HB3	1:A:670:VAL:CG2	2.47	0.44
1:A:497:PHE:CZ	1:A:499:ARG:HD2	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:ILE:O	1:A:413:ILE:HG23	2.19	0.43
1:A:601:ILE:HG13	1:A:684:GLN:HE21	1.84	0.43
1:A:105:ILE:HD11	1:A:276:VAL:CG2	2.49	0.42
1:A:309:LEU:HD21	1:A:335:LEU:CD1	2.49	0.42
1:A:415:PRO:HG2	1:A:421:GLN:HG2	2.01	0.42
1:A:409:ILE:CG2	1:A:459:LEU:HD13	2.49	0.42
1:A:115:GLU:O	1:A:118:SER:HB2	2.19	0.42
1:A:409:ILE:HG21	1:A:459:LEU:HD13	2.00	0.42
1:A:423:LYS:HA	1:A:426:GLN:HB2	2.02	0.42
1:A:498:ILE:HA	1:A:506:GLN:O	2.18	0.42
1:A:522:GLY:O	1:A:562:ASP:HA	2.19	0.42
1:A:554:PRO:HB3	1:A:595:GLN:HG2	2.01	0.42
1:A:139:MET:HE2	1:A:139:MET:HA	2.02	0.42
1:A:413:ILE:HD13	1:A:424:LEU:HD21	2.01	0.42
1:A:323:GLY:O	1:A:324:ARG:C	2.63	0.41
1:A:132:ARG:NH1	4:A:2011:HOH:O	2.49	0.41
1:A:644:ARG:HB3	4:A:2058:HOH:O	2.20	0.41
1:A:671:MET:CG	4:A:2057:HOH:O	2.68	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:357:ARG:NH1	1:A:373:ASP:OD2	2.54	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: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:O	1:A:94:VAL:CG1	2.69	0.41
1:A:499:ARG:NE	4:A:2049:HOH:O	2.54	0.41
1:A:506:GLN:NE2	1:A:581:ALA:HB2	2.36	0.41
1:A:115:GLU:O	1:A:116:PRO:C	2.64	0.40
1:A:584:ILE:HG22	1:A:588:MET:HE2	2.02	0.40
1:A:303:PRO:HA	1:A:331:TYR:O	2.21	0.40
1:A:413:ILE:HD11	1:A:424:LEU:HD11	2.03	0.40
1:A:470:PHE:HB3	1:A:472:VAL:HG23	2.01	0.40
1:A:601:ILE:HG12	4:A:2048:HOH:O	2.22	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	Interatomic distance (Å)	Clash overlap (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%)	5 9

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%)	429 (77%)	129 (23%)	1 1

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	6	GLU
1	A	9	LEU
1	A	10	LYS
1	A	11	ARG
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	93	GLU
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	162	VAL
1	A	166	LEU
1	A	170	ARG

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Mol	Chain	Res	Type
1	A	180	VAL
1	A	181	LEU
1	A	190	ASN
1	A	194	THR
1	A	204	GLU
1	A	214	GLU
1	A	229	LEU
1	A	230	LYS
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
1	A	273	LEU
1	A	277	VAL
1	A	280	LEU
1	A	284	LEU
1	A	286	ILE
1	A	295	GLU
1	A	300	GLU
1	A	312	LEU
1	A	315	LYS
1	A	322	VAL
1	A	325	LEU
1	A	326	THR
1	A	328	ILE
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	377	VAL
1	A	382	GLU
1	A	385	THR
1	A	389	LEU
1	A	399	LEU

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Mol	Chain	Res	Type
1	A	403	GLU
1	A	404	VAL
1	A	411	VAL
1	A	423	LYS
1	A	426	GLN
1	A	439	ARG
1	A	443	HIS
1	A	445	GLU
1	A	449	THR
1	A	451	ILE
1	A	456	GLU
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	489	LYS
1	A	499	ARG
1	A	500	GLN
1	A	511	LYS
1	A	517	LEU
1	A	519	ARG
1	A	533	VAL
1	A	537	GLU
1	A	539	ILE
1	A	542	VAL
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	591	LYS
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

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Mol	Chain	Res	Type
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	662	LYS
1	A	671	MET
1	A	672	PHE
1	A	682	GLN
1	A	687	LEU
1	A	688	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	124	GLN
1	A	137	ASN
1	A	165	GLN
1	A	190	ASN
1	A	208	GLN
1	A	302	HIS
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	641	GLN
1	A	675	HIS
1	A	684	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	29,30,30	1.09	2 (6%)	45,47,47	1.56	9 (20%)

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	-	2/16/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1689	GDP	PA-O3A	2.88	1.62	1.59
2	A	1689	GDP	O4'-C1'	-2.13	1.37	1.42

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1689	GDP	C2-N3-C4	3.94	119.08	112.30
2	A	1689	GDP	C5-C4-N3	-3.84	122.28	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1689	GDP	N9-C8-N7	-3.13	107.59	113.40
2	A	1689	GDP	O3B-PB-O2B	2.76	118.15	107.80
2	A	1689	GDP	C8-N7-C5	2.73	109.12	104.26
2	A	1689	GDP	N9-C4-N3	2.43	130.82	125.95
2	A	1689	GDP	O6-C6-C5	-2.30	120.47	126.53
2	A	1689	GDP	O2A-PA-O3A	2.26	113.37	107.27
2	A	1689	GDP	O4'-C1'-N9	2.13	113.17	108.36

There are no chirality outliers.

All (2) torsion outliers are listed below:

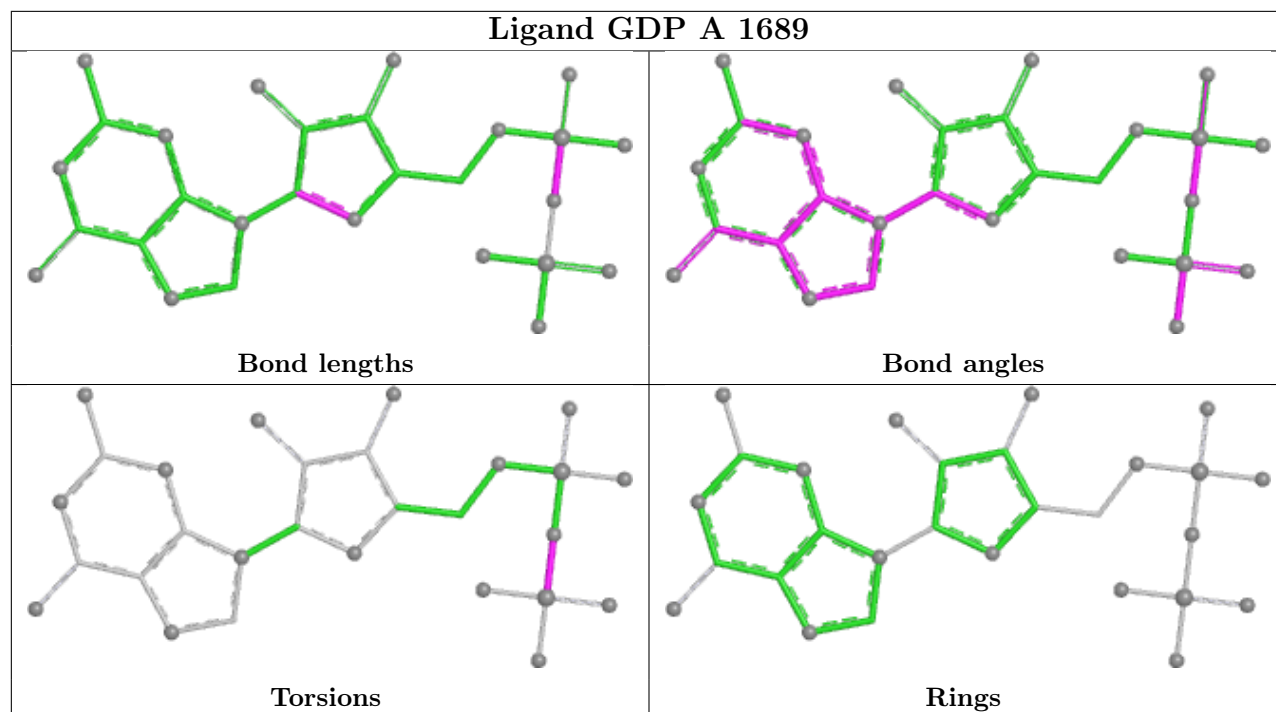
Mol	Chain	Res	Type	Atoms
2	A	1689	GDP	PA-O3A-PB-O2B
2	A	1689	GDP	PA-O3A-PB-O3B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1689	GDP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 ⓘ

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%)	2.86	486 (73%) 0 0	29, 50, 115, 126	0

All (486) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	263	ALA	11.4
1	A	645	ALA	8.9
1	A	620	VAL	8.5
1	A	110	SER	6.9
1	A	284	LEU	6.8
1	A	656	ALA	6.7
1	A	429	ALA	6.5
1	A	408	VAL	6.5
1	A	205	TYR	6.4
1	A	301	ILE	6.4
1	A	232	LEU	6.3
1	A	668	SER	6.2
1	A	413	ILE	6.1
1	A	440	VAL	6.1
1	A	185	ALA	6.1
1	A	177	ILE	6.1
1	A	130	VAL	5.9
1	A	234	GLY	5.9
1	A	201	ILE	5.7
1	A	463	VAL	5.6
1	A	114	VAL	5.6
1	A	94	VAL	5.6
1	A	640	ALA	5.4
1	A	216	LEU	5.4
1	A	431	LEU	5.4
1	A	92	ILE	5.4
1	A	447	GLY	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	106	VAL	5.2
1	A	283	PRO	5.1
1	A	666	ARG	5.1
1	A	188	TYR	5.1
1	A	374	LEU	5.1
1	A	462	ILE	5.1
1	A	213	HIS	5.0
1	A	624	LEU	5.0
1	A	453	GLY	5.0
1	A	146	LEU	4.8
1	A	73	PHE	4.8
1	A	688	ILE	4.8
1	A	432	ALA	4.8
1	A	397	VAL	4.8
1	A	457	LEU	4.8
1	A	416	LYS	4.7
1	A	195	ASP	4.7
1	A	626	ALA	4.7
1	A	402	ILE	4.7
1	A	441	SER	4.7
1	A	251	ILE	4.7
1	A	473	ASP	4.7
1	A	262	SER	4.6
1	A	229	LEU	4.6
1	A	124	GLN	4.6
1	A	616	TYR	4.5
1	A	113	GLY	4.5
1	A	636	PRO	4.5
1	A	437	THR	4.5
1	A	470	PHE	4.5
1	A	5	VAL	4.5
1	A	344	THR	4.5
1	A	670	VAL	4.4
1	A	199	ILE	4.4
1	A	679	VAL	4.4
1	A	455	GLY	4.3
1	A	28	THR	4.3
1	A	194	THR	4.3
1	A	414	GLU	4.3
1	A	474	ALA	4.3
1	A	685	GLU	4.3
1	A	217	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	322	VAL	4.3
1	A	481	VAL	4.3
1	A	100	VAL	4.3
1	A	465	ARG	4.2
1	A	37	GLY	4.2
1	A	446	THR	4.2
1	A	9	LEU	4.2
1	A	652	MET	4.2
1	A	90	PHE	4.2
1	A	86	GLY	4.2
1	A	226	ASN	4.2
1	A	235	GLU	4.2
1	A	133	ILE	4.1
1	A	279	TYR	4.1
1	A	21	ILE	4.1
1	A	599	PRO	4.1
1	A	669	PHE	4.1
1	A	378	VAL	4.1
1	A	142	THR	4.1
1	A	407	PRO	4.1
1	A	676	TYR	4.0
1	A	169	GLY	4.0
1	A	190	ASN	4.0
1	A	163	VAL	4.0
1	A	472	VAL	4.0
1	A	415	PRO	4.0
1	A	6	GLU	4.0
1	A	459	LEU	4.0
1	A	438	PHE	4.0
1	A	604	PRO	4.0
1	A	159	ALA	4.0
1	A	411	VAL	4.0
1	A	514	VAL	4.0
1	A	187	THR	4.0
1	A	449	THR	4.0
1	A	612	THR	4.0
1	A	585	ALA	4.0
1	A	82	ILE	4.0
1	A	108	PHE	4.0
1	A	141	LYS	4.0
1	A	179	ASP	4.0
1	A	390	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	417	THR	3.9
1	A	425	SER	3.9
1	A	308	PRO	3.9
1	A	424	LEU	3.9
1	A	667	GLY	3.9
1	A	687	LEU	3.9
1	A	610	VAL	3.9
1	A	674	ASP	3.9
1	A	456	GLU	3.9
1	A	427	ALA	3.9
1	A	404	VAL	3.9
1	A	464	ASP	3.9
1	A	639	ASN	3.9
1	A	648	PRO	3.9
1	A	171	GLU	3.9
1	A	328	ILE	3.9
1	A	517	LEU	3.9
1	A	631	ILE	3.9
1	A	135	PHE	3.9
1	A	66	THR	3.8
1	A	644	ARG	3.8
1	A	450	ILE	3.8
1	A	533	VAL	3.8
1	A	435	ASP	3.8
1	A	545	GLY	3.8
1	A	647	VAL	3.8
1	A	178	ILE	3.8
1	A	219	VAL	3.8
1	A	257	PRO	3.8
1	A	554	PRO	3.8
1	A	362	HIS	3.8
1	A	405	PRO	3.8
1	A	98	MET	3.7
1	A	196	ILE	3.7
1	A	590	ILE	3.7
1	A	532	GLY	3.7
1	A	258	VAL	3.7
1	A	608	VAL	3.7
1	A	487	ILE	3.7
1	A	237	PRO	3.7
1	A	316	ILE	3.7
1	A	243	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	476	VAL	3.7
1	A	546	ILE	3.7
1	A	74	TRP	3.7
1	A	471	LYS	3.7
1	A	176	GLY	3.7
1	A	649	LEU	3.6
1	A	150	ILE	3.6
1	A	227	ILE	3.6
1	A	231	TYR	3.6
1	A	189	GLY	3.6
1	A	673	PHE	3.6
1	A	361	ASN	3.6
1	A	420	ASP	3.6
1	A	629	GLY	3.6
1	A	560	VAL	3.6
1	A	650	ALA	3.6
1	A	97	SER	3.6
1	A	12	LEU	3.6
1	A	654	GLY	3.6
1	A	406	GLU	3.6
1	A	244	ALA	3.5
1	A	592	GLU	3.5
1	A	451	ILE	3.5
1	A	419	ALA	3.5
1	A	349	LYS	3.5
1	A	421	GLN	3.5
1	A	399	LEU	3.5
1	A	183	MET	3.5
1	A	657	THR	3.5
1	A	475	ASN	3.5
1	A	303	PRO	3.5
1	A	264	LEU	3.5
1	A	646	PHE	3.5
1	A	542	VAL	3.5
1	A	678	GLU	3.5
1	A	430	ARG	3.5
1	A	467	LYS	3.4
1	A	618	GLY	3.4
1	A	197	ARG	3.4
1	A	384	ILE	3.4
1	A	452	SER	3.4
1	A	655	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	296	GLY	3.4
1	A	297	GLU	3.4
1	A	628	ARG	3.4
1	A	386	GLY	3.4
1	A	445	GLU	3.4
1	A	637	ARG	3.4
1	A	224	ASP	3.4
1	A	276	VAL	3.4
1	A	314	PHE	3.4
1	A	289	ILE	3.3
1	A	175	SER	3.3
1	A	663	THR	3.3
1	A	433	GLU	3.3
1	A	125	ALA	3.3
1	A	298	VAL	3.3
1	A	265	LYS	3.3
1	A	192	LEU	3.3
1	A	428	LEU	3.3
1	A	246	ILE	3.3
1	A	500	GLN	3.3
1	A	10	LYS	3.3
1	A	129	LYS	3.3
1	A	139	MET	3.3
1	A	212	TYR	3.3
1	A	291	GLY	3.3
1	A	418	LYS	3.3
1	A	360	ALA	3.3
1	A	32	ILE	3.3
1	A	491	VAL	3.3
1	A	527	ASN	3.3
1	A	627	ARG	3.2
1	A	220	ALA	3.2
1	A	206	LEU	3.2
1	A	273	LEU	3.2
1	A	27	THR	3.2
1	A	7	TYR	3.2
1	A	168	ILE	3.2
1	A	436	PRO	3.2
1	A	67	ALA	3.2
1	A	118	SER	3.2
1	A	144	ALA	3.2
1	A	221	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	492	ASP	3.2
1	A	634	MET	3.2
1	A	65	ILE	3.2
1	A	683	VAL	3.2
1	A	574	GLU	3.1
1	A	193	GLY	3.1
1	A	223	PHE	3.1
1	A	565	VAL	3.1
1	A	238	THR	3.1
1	A	409	ILE	3.1
1	A	632	LEU	3.1
1	A	508	GLY	3.1
1	A	461	ILE	3.1
1	A	643	ILE	3.1
1	A	182	ARG	3.1
1	A	672	PHE	3.1
1	A	567	LEU	3.1
1	A	239	GLU	3.1
1	A	460	GLU	3.1
1	A	442	THR	3.1
1	A	381	LYS	3.1
1	A	140	ASP	3.0
1	A	228	MET	3.0
1	A	35	TYR	3.0
1	A	200	PRO	3.0
1	A	8	ASP	3.0
1	A	480	GLN	3.0
1	A	677	GLN	3.0
1	A	158	GLY	3.0
1	A	555	LEU	3.0
1	A	202	PRO	3.0
1	A	96	ARG	3.0
1	A	23	ALA	3.0
1	A	116	PRO	3.0
1	A	4	LYS	3.0
1	A	305	PRO	2.9
1	A	630	GLN	2.9
1	A	439	ARG	2.9
1	A	330	VAL	2.9
1	A	466	LEU	2.9
1	A	155	GLU	2.9
1	A	458	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	681	LYS	2.9
1	A	294	PRO	2.9
1	A	77	HIS	2.9
1	A	395	PRO	2.9
1	A	448	GLN	2.9
1	A	319	ASP	2.9
1	A	393	ASP	2.9
1	A	29	THR	2.9
1	A	335	LEU	2.9
1	A	161	PRO	2.9
1	A	572	TYR	2.9
1	A	638	GLY	2.9
1	A	310	ALA	2.9
1	A	325	LEU	2.9
1	A	482	ALA	2.9
1	A	93	GLU	2.8
1	A	295	GLU	2.8
1	A	127	LYS	2.8
1	A	209	ALA	2.8
1	A	277	VAL	2.8
1	A	653	PHE	2.8
1	A	122	TRP	2.8
1	A	489	LYS	2.8
1	A	379	GLY	2.8
1	A	33	LEU	2.8
1	A	18	ALA	2.8
1	A	483	TYR	2.8
1	A	88	VAL	2.8
1	A	107	VAL	2.8
1	A	211	GLU	2.8
1	A	160	ARG	2.8
1	A	112	GLN	2.8
1	A	496	LYS	2.8
1	A	622	GLY	2.8
1	A	625	ASN	2.8
1	A	181	LEU	2.8
1	A	410	ASP	2.8
1	A	214	GLU	2.8
1	A	412	ALA	2.8
1	A	642	VAL	2.8
1	A	665	GLY	2.7
1	A	377	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	611	THR	2.7
1	A	518	PRO	2.7
1	A	282	SER	2.7
1	A	323	GLY	2.7
1	A	588	MET	2.7
1	A	609	GLU	2.7
1	A	353	ALA	2.7
1	A	488	THR	2.7
1	A	538	TYR	2.7
1	A	595	GLN	2.7
1	A	621	ILE	2.7
1	A	151	ARG	2.7
1	A	306	ASN	2.7
1	A	660	ARG	2.7
1	A	250	THR	2.7
1	A	606	MET	2.7
1	A	215	LYS	2.7
1	A	498	ILE	2.6
1	A	20	HIS	2.6
1	A	230	LYS	2.6
1	A	267	LYS	2.6
1	A	513	LYS	2.6
1	A	582	PHE	2.6
1	A	684	GLN	2.6
1	A	329	ARG	2.6
1	A	249	GLY	2.6
1	A	313	ALA	2.6
1	A	613	PRO	2.6
1	A	507	TYR	2.6
1	A	444	PRO	2.6
1	A	577	SER	2.6
1	A	76	ASP	2.6
1	A	398	ILE	2.6
1	A	389	LEU	2.6
1	A	602	LEU	2.6
1	A	302	HIS	2.6
1	A	400	GLU	2.6
1	A	469	GLU	2.6
1	A	523	PHE	2.6
1	A	84	THR	2.5
1	A	256	THR	2.5
1	A	506	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	619	ASP	2.5
1	A	17	ILE	2.5
1	A	11	ARG	2.5
1	A	34	TYR	2.5
1	A	115	GLU	2.5
1	A	615	GLU	2.5
1	A	14	ASN	2.5
1	A	266	ASN	2.5
1	A	274	ASP	2.5
1	A	605	ILE	2.5
1	A	148	LEU	2.5
1	A	499	ARG	2.5
1	A	342	TYR	2.5
1	A	16	VAL	2.5
1	A	558	PHE	2.5
1	A	675	HIS	2.5
1	A	338	GLY	2.5
1	A	495	GLY	2.5
1	A	311	ALA	2.5
1	A	91	THR	2.5
1	A	254	LYS	2.5
1	A	147	TRP	2.5
1	A	157	LEU	2.5
1	A	207	ASP	2.5
1	A	454	MET	2.5
1	A	529	ILE	2.4
1	A	556	ILE	2.4
1	A	521	SER	2.4
1	A	600	VAL	2.4
1	A	528	ALA	2.4
1	A	564	LYS	2.4
1	A	299	VAL	2.4
1	A	327	PHE	2.4
1	A	354	ARG	2.4
1	A	369	LEU	2.4
1	A	83	ASP	2.4
1	A	562	ASP	2.4
1	A	658	ASP	2.4
1	A	31	ARG	2.4
1	A	601	ILE	2.4
1	A	571	SER	2.4
1	A	252	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	25	LYS	2.4
1	A	423	LYS	2.4
1	A	132	ARG	2.4
1	A	242	LEU	2.3
1	A	380	LEU	2.3
1	A	568	TYR	2.3
1	A	534	ILE	2.3
1	A	173	THR	2.3
1	A	617	MET	2.3
1	A	357	ARG	2.3
1	A	641	GLN	2.3
1	A	394	ALA	2.3
1	A	255	ILE	2.3
1	A	662	LYS	2.3
1	A	170	ARG	2.3
1	A	520	GLY	2.3
1	A	575	VAL	2.3
1	A	70	THR	2.3
1	A	128	TYR	2.3
1	A	317	MET	2.3
1	A	89	ASP	2.3
1	A	287	PRO	2.3
1	A	396	ARG	2.3
1	A	309	LEU	2.3
1	A	245	ALA	2.3
1	A	138	LYS	2.3
1	A	326	THR	2.3
1	A	337	SER	2.3
1	A	553	GLY	2.3
1	A	586	GLY	2.3
1	A	180	VAL	2.3
1	A	355	LEU	2.3
1	A	526	VAL	2.3
1	A	659	LEU	2.3
1	A	174	PHE	2.3
1	A	365	GLU	2.2
1	A	123	ARG	2.2
1	A	22	ASP	2.2
1	A	477	GLY	2.2
1	A	324	ARG	2.2
1	A	145	ASP	2.2
1	A	372	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	339	SER	2.2
1	A	539	ILE	2.2
1	A	348	ARG	2.2
1	A	137	ASN	2.2
1	A	550	MET	2.2
1	A	69	VAL	2.2
1	A	549	ALA	2.1
1	A	603	GLU	2.1
1	A	516	PRO	2.1
1	A	172	ASP	2.1
1	A	68	ALA	2.1
1	A	30	GLU	2.1
1	A	236	GLU	2.1
1	A	340	TYR	2.1
1	A	143	GLY	2.1
1	A	635	GLU	2.1
1	A	99	ARG	2.1
1	A	210	ARG	2.1
1	A	152	THR	2.1
1	A	343	ASN	2.1
1	A	509	HIS	2.1
1	A	269	VAL	2.1
1	A	497	PHE	2.1
1	A	569	ASP	2.1
1	A	247	ARG	2.1
1	A	363	ARG	2.1
1	A	341	VAL	2.1
1	A	111	SER	2.0
1	A	358	MET	2.0
1	A	426	GLN	2.0
1	A	149	VAL	2.0
1	A	364	GLU	2.0
1	A	485	GLU	2.0
1	A	371	ALA	2.0
1	A	664	GLN	2.0
1	A	347	GLY	2.0
1	A	522	GLY	2.0
1	A	493	VAL	2.0
1	A	607	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

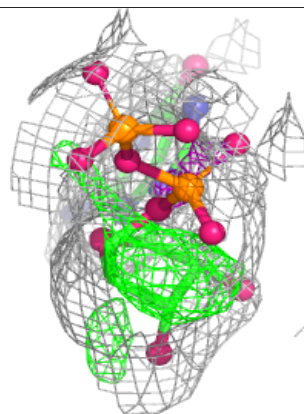
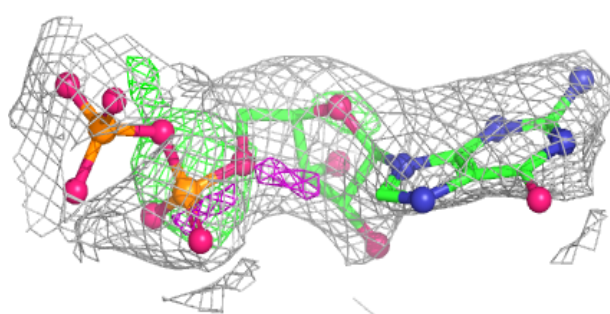
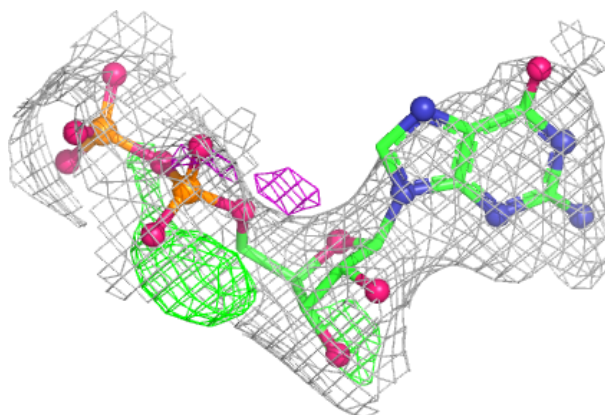
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GDP	A	1689	28/28	0.72	0.19	25,36,40,41	0
3	MG	A	1690	1/1	0.96	0.05	40,40,40,40	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 GDP A 1689:

$2mF_o-DF_c$ (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.