



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:39 PM UTC

PDB ID : 2B92 / pdb_00002b92
Title : Crystal-structure of the N-terminal Large GTPase Domain of human Guanylate Binding protein 1 (hGBP1) in complex with GDP/AlF3
Authors : Ghosh, A.; Praefcke, G.J.K.; Renault, L.; Wittinghofer, A.; Herrmann, C.
Deposited on : 2005-10-10
Resolution : 3.20 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

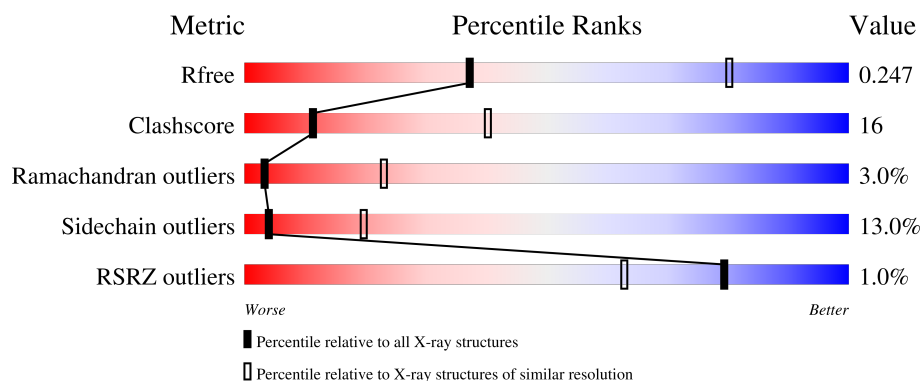
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	328	% 53% 25% 9% • 12%
1	B	328	% 48% 29% 8% • 12%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4666 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 Interferon-induced guanylate-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2284	1466	385	421	12			
1	B	290	Total	C	N	O	S	0	0	0
			2301	1478	387	424	12			

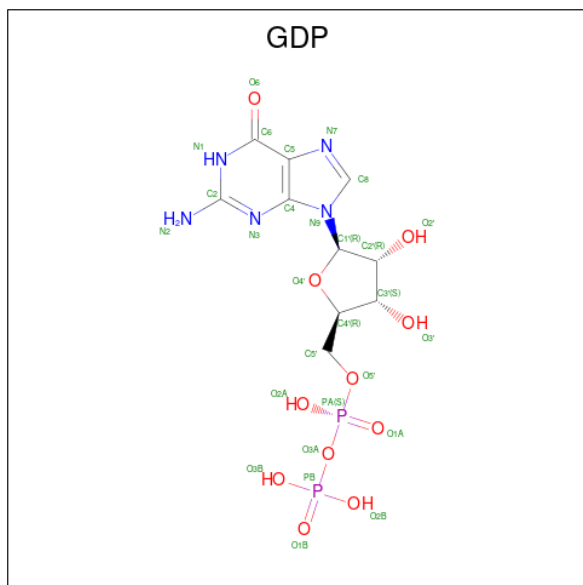
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	cloning artifact	UNP P32455
A	-9	HIS	-	expression tag	UNP P32455
A	-8	HIS	-	expression tag	UNP P32455
A	-7	HIS	-	expression tag	UNP P32455
A	-6	HIS	-	expression tag	UNP P32455
A	-5	HIS	-	expression tag	UNP P32455
A	-4	HIS	-	expression tag	UNP P32455
A	-3	MET	-	cloning artifact	UNP P32455
A	-2	ARG	-	cloning artifact	UNP P32455
A	-1	GLY	-	cloning artifact	UNP P32455
A	0	SER	-	cloning artifact	UNP P32455
B	-10	MET	-	cloning artifact	UNP P32455
B	-9	HIS	-	expression tag	UNP P32455
B	-8	HIS	-	expression tag	UNP P32455
B	-7	HIS	-	expression tag	UNP P32455
B	-6	HIS	-	expression tag	UNP P32455
B	-5	HIS	-	expression tag	UNP P32455
B	-4	HIS	-	expression tag	UNP P32455
B	-3	MET	-	cloning artifact	UNP P32455
B	-2	ARG	-	cloning artifact	UNP P32455
B	-1	GLY	-	cloning artifact	UNP P32455
B	0	SER	-	cloning artifact	UNP P32455

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

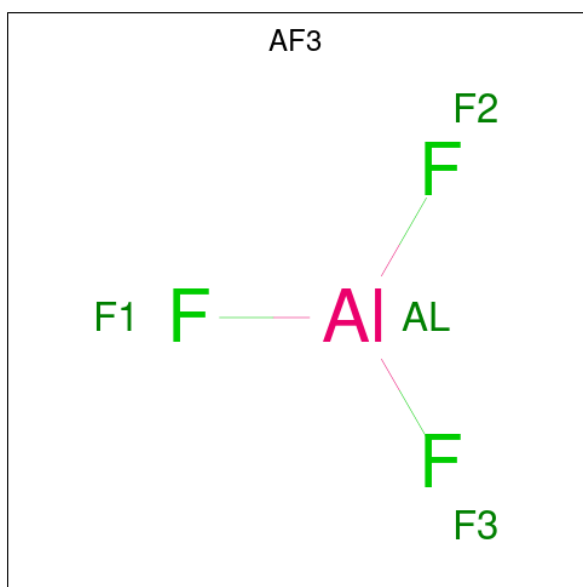
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 4 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Al	F	0	0
			4	1	3		
4	B	1	Total	Al	F	0	0
			4	1	3		

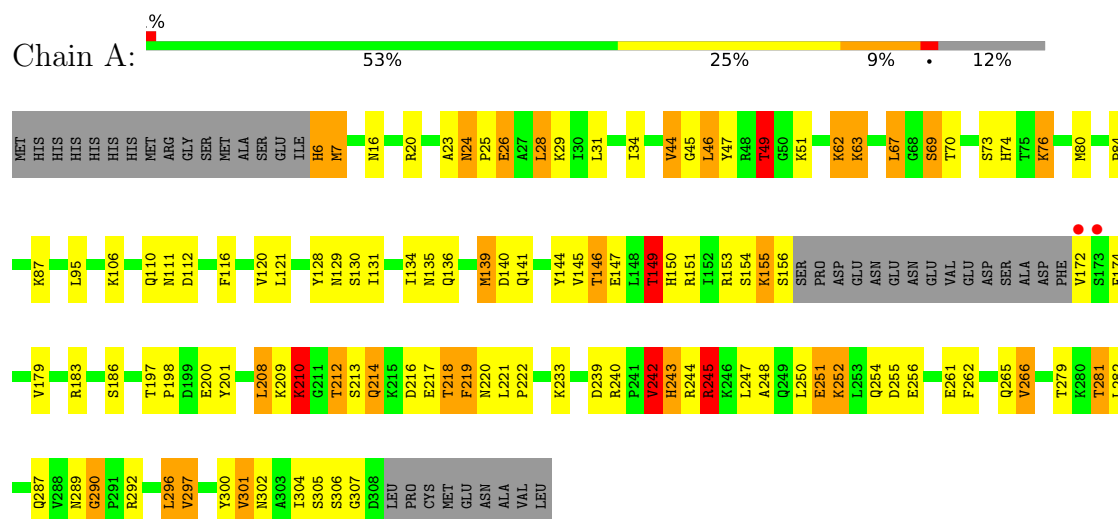
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total	O	0	0
			9	9		
5	B	6	Total	O	0	0
			6	6		

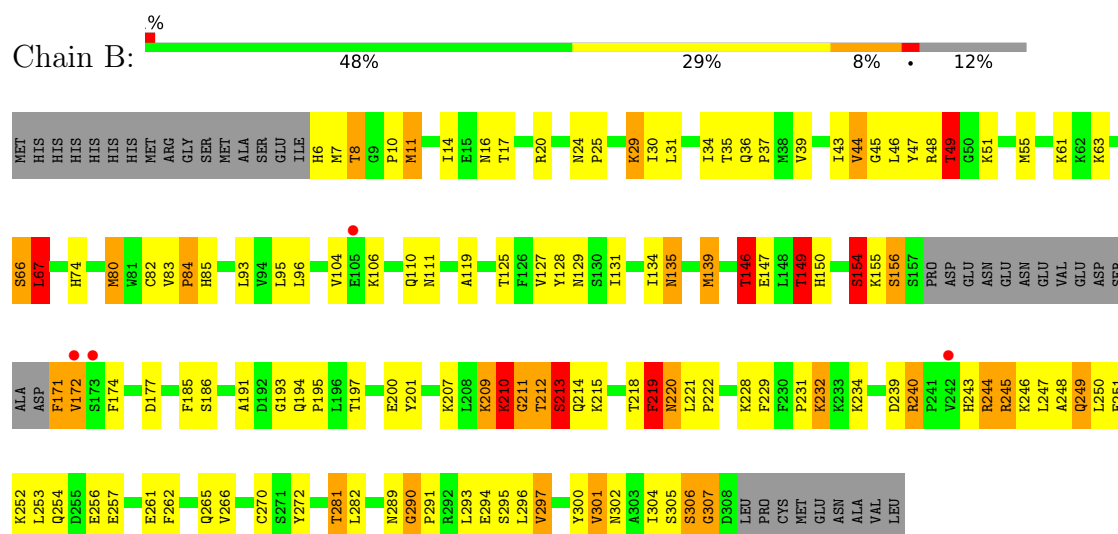
3 Residue-property plots

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: Interferon-induced guanylate-binding protein 1



• Molecule 1: Interferon-induced guanylate-binding protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	148.82Å 103.92Å 55.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 30.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-3.20) 99.1 (30.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.18 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.204 , 0.250 0.198 , 0.247	Depositor DCC
R_{free} test set	989 reflections (6.68%)	wwPDB-VP
Wilson B-factor (Å ²)	79.0	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4666	wwPDB-VP
Average B, all atoms (Å ²)	60.0	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 65.95 % 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 6.5306e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, AF3, 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	1.69	41/2334 (1.8%)	0.66	0/3156
1	B	1.74	48/2352 (2.0%)	0.71	4/3180 (0.1%)
All	All	1.72	89/4686 (1.9%)	0.69	4/6336 (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	A	0	3
1	B	0	5
All	All	0	8

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	85	HIS	N-CA	-12.56	1.26	1.46
1	A	243	HIS	CA-C	12.41	1.68	1.52
1	B	84	PRO	N-CA	-11.52	1.32	1.47
1	B	84	PRO	CA-C	-11.39	1.39	1.52
1	B	306	SER	N-CA	9.88	1.58	1.46
1	B	49	THR	N-CA	-9.71	1.35	1.46
1	A	297	VAL	N-CA	-9.38	1.35	1.46
1	B	213	SER	N-CA	9.02	1.57	1.46
1	B	131	ILE	CA-CB	-8.62	1.44	1.54
1	A	266	VAL	CA-C	-8.53	1.42	1.52
1	A	245	ARG	CA-C	8.50	1.63	1.52
1	A	251	GLU	N-CA	8.50	1.57	1.46
1	A	242	VAL	N-CA	8.41	1.56	1.46
1	B	135	ASN	N-CA	-8.22	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	296	LEU	CA-C	-7.66	1.43	1.52
1	B	127	VAL	CA-CB	-7.54	1.45	1.54
1	A	255	ASP	N-CA	-7.47	1.36	1.46
1	B	80	MET	CA-C	-7.46	1.43	1.52
1	A	131	ILE	CA-CB	-7.46	1.44	1.53
1	A	256	GLU	CA-C	-7.41	1.42	1.52
1	B	210	LYS	C-O	7.28	1.33	1.24
1	A	46	LEU	CA-C	-7.17	1.43	1.53
1	A	135	ASN	N-CA	-7.17	1.37	1.46
1	B	305	SER	CA-C	7.08	1.62	1.52
1	B	8	THR	CA-CB	6.99	1.64	1.53
1	B	125	THR	CA-C	-6.99	1.44	1.52
1	B	146	THR	N-CA	-6.98	1.38	1.46
1	A	256	GLU	N-CA	6.87	1.54	1.46
1	A	49	THR	N-CA	-6.86	1.37	1.46
1	B	110	GLN	CA-CB	6.85	1.64	1.53
1	B	211	GLY	N-CA	6.75	1.55	1.45
1	B	174	PHE	N-CA	6.74	1.53	1.46
1	B	243	HIS	N-CA	6.71	1.54	1.46
1	A	255	ASP	CA-C	6.54	1.61	1.52
1	B	219	PHE	N-CA	6.53	1.54	1.46
1	B	48	ARG	CA-C	-6.35	1.46	1.53
1	A	243	HIS	CA-CB	6.32	1.63	1.53
1	A	149	THR	N-CA	-6.32	1.38	1.46
1	A	301	VAL	CA-CB	-6.32	1.47	1.54
1	A	251	GLU	CA-CB	6.28	1.64	1.53
1	B	253	LEU	N-CA	6.25	1.53	1.46
1	B	74	HIS	CA-CB	-6.18	1.44	1.53
1	B	270	CYS	N-CA	-6.13	1.39	1.46
1	B	243	HIS	CA-C	6.08	1.60	1.52
1	B	119	ALA	CA-CB	-6.02	1.44	1.53
1	B	8	THR	N-CA	-6.01	1.38	1.46
1	A	179	VAL	CA-C	-6.00	1.45	1.52
1	A	304	ILE	N-CA	-5.96	1.38	1.46
1	A	208	LEU	N-CA	5.94	1.53	1.45
1	A	252	LYS	CA-C	5.93	1.60	1.52
1	A	120	VAL	N-CA	-5.84	1.39	1.46
1	A	135	ASN	CB-CG	-5.82	1.37	1.52
1	B	149	THR	N-CA	-5.80	1.39	1.46
1	A	214	GLN	CG-CD	5.74	1.66	1.52
1	A	130	SER	CA-C	-5.73	1.45	1.52
1	B	84	PRO	N-CD	5.70	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	240	ARG	CA-C	-5.68	1.45	1.52
1	B	212	THR	CA-C	5.67	1.60	1.52
1	B	297	VAL	N-CA	-5.65	1.40	1.46
1	A	302	ASN	N-CA	5.59	1.53	1.46
1	B	135	ASN	CB-CG	-5.57	1.38	1.52
1	B	185	PHE	CA-C	5.53	1.60	1.52
1	A	140	ASP	CA-C	-5.47	1.45	1.52
1	B	307	GLY	N-CA	5.44	1.53	1.45
1	B	302	ASN	N-CA	5.40	1.53	1.46
1	B	49	THR	CA-C	5.39	1.59	1.52
1	A	76	LYS	N-CA	5.36	1.52	1.45
1	B	10	PRO	CA-C	-5.36	1.44	1.52
1	B	249	GLN	CA-C	-5.35	1.46	1.52
1	B	67	LEU	C-O	5.34	1.30	1.23
1	B	301	VAL	N-CA	-5.30	1.40	1.46
1	B	210	LYS	C-N	5.30	1.41	1.33
1	A	24	ASN	N-CA	-5.29	1.39	1.46
1	B	135	ASN	CA-C	5.25	1.58	1.52
1	A	245	ARG	N-CA	-5.23	1.40	1.46
1	A	26	GLU	CB-CG	5.22	1.68	1.52
1	B	39	VAL	CA-CB	-5.19	1.47	1.54
1	A	112	ASP	CA-C	-5.17	1.46	1.52
1	B	186	SER	N-CA	5.17	1.52	1.46
1	B	35	THR	CA-CB	-5.17	1.46	1.54
1	A	141	GLN	N-CA	-5.13	1.40	1.46
1	B	11	MET	SD-CE	5.10	1.92	1.79
1	A	28	LEU	N-CA	-5.09	1.40	1.46
1	A	128	TYR	CA-CB	5.09	1.60	1.53
1	A	292	ARG	CA-C	5.07	1.59	1.52
1	B	43	ILE	N-CA	-5.03	1.40	1.46
1	B	257	GLU	CA-C	5.03	1.59	1.52
1	A	136	GLN	CA-C	5.02	1.59	1.52
1	A	139	MET	N-CA	5.01	1.52	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	219	PHE	O-C-N	-6.65	113.75	122.59
1	B	154	SER	O-C-N	-6.40	115.23	122.08
1	B	210	LYS	CA-C-N	-6.32	109.02	121.41
1	B	210	LYS	C-N-CA	-6.32	109.02	121.41

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	212	THR	Peptide
1	A	243	HIS	Peptide
1	A	245	ARG	Peptide
1	B	154	SER	Mainchain
1	B	156	SER	Peptide
1	B	219	PHE	Mainchain
1	B	248	ALA	Peptide
1	B	66	SER	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	2284	0	2308	70	0
1	B	2301	0	2323	83	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	28	0	12	1	0
3	B	28	0	12	1	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	A	9	0	0	1	0
5	B	6	0	0	1	0
All	All	4666	0	4655	151	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 16.

All (151) 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:219:PHE:O	1:A:222:PRO:HD2	1.39	1.19
1:B:171:PHE:O	1:B:172:VAL:HG12	1.42	1.16
1:A:49:THR:HG23	1:A:129:ASN:ND2	1.63	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:ARG:HH11	1:B:244:ARG:HG3	1.11	1.11
1:B:49:THR:HG23	1:B:129:ASN:ND2	1.76	1.01
1:B:154:SER:C	1:B:156:SER:H	1.69	1.00
1:B:244:ARG:HH11	1:B:244:ARG:CG	1.76	0.98
1:A:242:VAL:HG23	1:A:244:ARG:O	1.65	0.95
1:B:49:THR:CG2	1:B:129:ASN:HD22	1.79	0.95
1:A:49:THR:CG2	1:A:129:ASN:ND2	2.29	0.94
1:A:242:VAL:HG22	1:A:247:LEU:HD13	1.45	0.94
1:A:16:ASN:HD21	1:A:111:ASN:HD21	1.12	0.94
1:B:171:PHE:O	1:B:172:VAL:CG1	2.17	0.93
1:A:49:THR:CG2	1:A:129:ASN:HD22	1.82	0.92
1:A:62:LYS:NZ	1:A:254:GLN:HA	1.85	0.92
1:B:244:ARG:HG3	1:B:244:ARG:NH1	1.74	0.91
1:B:16:ASN:HD21	1:B:111:ASN:HD21	1.15	0.90
1:B:154:SER:C	1:B:156:SER:N	2.34	0.82
1:B:197:THR:OG1	1:B:200:GLU:HG3	1.80	0.81
1:B:49:THR:CG2	1:B:129:ASN:ND2	2.38	0.81
1:A:174:PHE:HB2	1:A:281:THR:HG22	1.64	0.79
1:A:49:THR:HG21	1:A:129:ASN:HD22	1.48	0.77
1:B:213:SER:OG	1:B:214:GLN:N	2.16	0.76
1:A:49:THR:HG23	1:A:129:ASN:HD21	1.48	0.76
1:A:62:LYS:HZ3	1:A:254:GLN:HA	1.48	0.75
1:B:154:SER:O	1:B:156:SER:N	2.19	0.75
1:A:73:SER:OG	1:A:76:LYS:HE2	1.90	0.72
1:B:82:CYS:O	1:B:83:VAL:CG1	2.37	0.72
1:A:219:PHE:O	1:A:221:LEU:N	2.24	0.70
1:A:281:THR:HG23	1:A:282:LEU:O	1.92	0.70
1:B:82:CYS:O	1:B:83:VAL:HG13	1.92	0.70
1:B:49:THR:HG23	1:B:129:ASN:HD21	1.53	0.69
1:A:155:LYS:O	1:A:156:SER:CB	2.41	0.69
1:B:245:ARG:C	1:B:247:LEU:H	2.01	0.68
1:B:171:PHE:C	1:B:172:VAL:HG12	2.18	0.68
1:A:31:LEU:HA	1:A:34:ILE:HD12	1.74	0.68
1:B:82:CYS:C	1:B:83:VAL:HG13	2.19	0.68
1:B:49:THR:HG21	1:B:129:ASN:HD22	1.55	0.68
1:A:151:ARG:O	1:A:154:SER:HB2	1.94	0.67
1:A:155:LYS:O	1:A:156:SER:HB3	1.93	0.67
1:A:6:HIS:HB2	1:A:84:PRO:HD3	1.77	0.67
1:A:218:THR:O	1:A:219:PHE:O	2.13	0.66
1:B:49:THR:HG22	1:B:51:LYS:HG3	1.77	0.66
1:A:197:THR:OG1	1:A:200:GLU:HG3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:ASP:O	1:B:240:ARG:C	2.38	0.66
1:B:261:GLU:O	1:B:265:GLN:HG3	1.97	0.65
1:A:49:THR:HG22	1:A:51:LYS:HG3	1.77	0.64
1:B:296:LEU:HD22	1:B:300:TYR:CE1	2.32	0.64
1:A:213:SER:H	1:A:216:ASP:HB2	1.64	0.63
1:A:62:LYS:O	1:A:63:LYS:HB3	1.99	0.62
1:A:219:PHE:O	1:A:222:PRO:CD	2.33	0.62
1:B:297:VAL:O	1:B:301:VAL:HG23	2.00	0.62
1:B:262:PHE:O	1:B:266:VAL:HG23	2.02	0.60
1:B:16:ASN:ND2	1:B:111:ASN:HD21	1.93	0.60
1:B:234:LYS:HD3	1:B:272:TYR:CE1	2.37	0.60
1:B:44:VAL:HG23	1:B:45:GLY:N	2.15	0.59
1:A:146:THR:HG22	1:A:147:GLU:N	2.17	0.59
1:B:134:ILE:HD12	1:B:201:TYR:CE2	2.38	0.59
1:B:219:PHE:O	1:B:221:LEU:N	2.31	0.59
1:A:221:LEU:N	1:A:222:PRO:HD2	2.18	0.58
1:B:16:ASN:HD21	1:B:111:ASN:ND2	1.96	0.58
1:B:106:LYS:NZ	1:B:111:ASN:HD22	2.01	0.58
1:A:149:THR:HG22	1:A:150:HIS:N	2.19	0.57
1:A:149:THR:CG2	1:A:153:ARG:NH2	2.68	0.57
1:B:219:PHE:O	1:B:220:ASN:HB2	2.05	0.57
1:A:24:ASN:OD1	1:A:24:ASN:C	2.47	0.57
1:B:244:ARG:CG	1:B:244:ARG:NH1	2.46	0.56
1:B:221:LEU:N	1:B:222:PRO:HD2	2.21	0.55
1:B:171:PHE:N	1:B:171:PHE:CD2	2.74	0.55
1:A:172:VAL:O	1:A:172:VAL:HG12	2.08	0.54
1:A:262:PHE:O	1:A:266:VAL:HG23	2.08	0.53
1:B:149:THR:HG22	1:B:150:HIS:N	2.22	0.53
1:B:239:ASP:O	1:B:240:ARG:O	2.27	0.53
1:B:82:CYS:C	1:B:83:VAL:CG1	2.80	0.53
1:B:24:ASN:OD1	1:B:24:ASN:C	2.51	0.52
1:B:49:THR:HG23	1:B:49:THR:O	2.09	0.52
1:A:209:LYS:O	1:A:210:LYS:C	2.53	0.51
1:B:31:LEU:HA	1:B:34:ILE:HD12	1.91	0.51
1:A:296:LEU:HD22	1:A:300:TYR:CE1	2.45	0.51
1:A:239:ASP:OD2	1:B:245:ARG:CZ	2.59	0.51
1:A:242:VAL:CG2	1:A:247:LEU:HD13	2.31	0.51
1:B:245:ARG:C	1:B:247:LEU:N	2.68	0.51
1:B:209:LYS:O	1:B:211:GLY:N	2.44	0.51
1:A:297:VAL:O	1:A:301:VAL:HG23	2.12	0.50
1:A:250:LEU:C	1:A:252:LYS:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:LEU:N	1:B:222:PRO:CD	2.75	0.49
1:A:44:VAL:HG23	1:A:45:GLY:N	2.26	0.49
1:A:49:THR:HG23	1:A:49:THR:O	2.11	0.49
1:B:128:TYR:CD2	1:B:128:TYR:C	2.89	0.49
1:B:46:LEU:O	1:B:49:THR:HB	2.13	0.49
1:A:289:ASN:O	1:A:290:GLY:C	2.56	0.49
1:B:36:GLN:HB3	1:B:37:PRO:HD2	1.95	0.48
1:B:289:ASN:O	1:B:290:GLY:C	2.56	0.48
1:B:172:VAL:O	1:B:172:VAL:HG13	2.13	0.48
1:A:67:LEU:O	3:A:593:GDP:O2A	2.31	0.48
1:B:244:ARG:HH11	1:B:244:ARG:CB	2.24	0.48
1:A:46:LEU:O	1:A:49:THR:HB	2.13	0.48
1:B:34:ILE:O	1:B:290:GLY:HA3	2.13	0.48
1:B:281:THR:CG2	1:B:282:LEU:O	2.62	0.48
1:A:116:PHE:CG	1:A:145:VAL:HG21	2.49	0.47
1:B:289:ASN:OD1	1:B:291:PRO:HD2	2.14	0.47
1:B:82:CYS:O	1:B:83:VAL:HG12	2.14	0.47
1:B:218:THR:C	1:B:219:PHE:O	2.57	0.47
1:A:245:ARG:HB2	1:A:247:LEU:HB2	1.97	0.47
1:A:261:GLU:O	1:A:265:GLN:HG3	2.14	0.47
1:B:146:THR:O	1:B:149:THR:HB	2.14	0.47
1:B:210:LYS:HB2	1:B:210:LYS:HE2	1.71	0.47
1:A:134:ILE:HG22	1:B:104:VAL:HG11	1.96	0.46
1:B:67:LEU:HG	1:B:251:GLU:CG	2.45	0.46
1:B:134:ILE:HD12	1:B:201:TYR:CZ	2.51	0.46
1:B:29:LYS:HB2	1:B:29:LYS:HE2	1.51	0.46
1:B:139:MET:HE2	1:B:139:MET:HB3	1.78	0.46
1:B:95:LEU:O	1:B:96:LEU:HD23	2.17	0.45
1:B:229:PHE:CD2	1:B:229:PHE:C	2.95	0.45
1:A:149:THR:O	1:A:150:HIS:C	2.60	0.45
1:A:144:TYR:CD2	1:A:144:TYR:C	2.94	0.45
1:B:83:VAL:O	1:B:93:LEU:N	2.47	0.44
1:B:250:LEU:C	1:B:252:LYS:H	2.25	0.44
1:A:80:MET:HA	1:A:95:LEU:O	2.17	0.44
1:A:242:VAL:HG23	1:A:242:VAL:O	2.16	0.44
1:B:80:MET:HA	1:B:95:LEU:O	2.18	0.44
1:A:149:THR:HG21	1:A:153:ARG:NH2	2.33	0.44
1:B:11:MET:SD	1:B:30:ILE:HD12	2.57	0.44
1:A:121:LEU:HD22	1:A:300:TYR:CZ	2.53	0.43
1:A:67:LEU:C	1:A:74:HIS:HD2	2.27	0.43
1:A:87:LYS:HE2	1:A:87:LYS:HB3	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:HIS:HB3	1:A:7:MET:H	1.53	0.43
1:A:69:SER:OG	1:A:248:ALA:HB1	2.19	0.43
1:A:116:PHE:CD2	1:A:145:VAL:HG11	2.53	0.43
1:B:281:THR:HG23	1:B:282:LEU:O	2.18	0.43
1:A:31:LEU:O	1:A:290:GLY:HA3	2.19	0.43
1:A:242:VAL:CG2	1:A:242:VAL:O	2.66	0.43
1:B:220:ASN:C	1:B:222:PRO:HD2	2.44	0.43
1:B:191:ALA:C	1:B:193:GLY:H	2.27	0.42
1:A:106:LYS:NZ	1:A:111:ASN:HD22	2.17	0.42
1:A:279:THR:HG21	1:A:287:GLN:HG2	2.01	0.42
1:B:24:ASN:HA	1:B:25:PRO:HD2	1.77	0.42
1:A:24:ASN:HA	1:A:25:PRO:HD3	1.88	0.42
1:B:191:ALA:C	1:B:193:GLY:N	2.76	0.42
1:B:177:ASP:OD1	1:B:232:LYS:HB2	2.20	0.42
1:B:250:LEU:C	1:B:252:LYS:N	2.76	0.42
1:A:183:ARG:HA	1:A:183:ARG:HD2	1.86	0.42
1:A:23:ALA:HB1	1:A:28:LEU:HD11	2.02	0.41
1:A:20:ARG:HA	1:A:20:ARG:HD3	1.92	0.41
1:A:198:PRO:O	1:A:201:TYR:HB3	2.19	0.41
1:B:67:LEU:O	3:B:593:GDP:O2A	2.39	0.41
1:B:293:LEU:O	1:B:294:GLU:C	2.65	0.40
1:A:67:LEU:HG	1:A:251:GLU:HG2	2.03	0.40
1:B:6:HIS:N	5:B:596:HOH:O	2.53	0.40
1:B:146:THR:HG22	1:B:147:GLU:N	2.36	0.40
1:A:110:GLN:HB2	5:A:601:HOH:O	2.21	0.40

There are no symmetry-related clashes.

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	284/328 (87%)	252 (89%)	27 (10%)	5 (2%)	6 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	286/328 (87%)	250 (87%)	24 (8%)	12 (4%)	2	16
All	All	570/656 (87%)	502 (88%)	51 (9%)	17 (3%)	3	23

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	LYS
1	A	219	PHE
1	A	220	ASN
1	B	155	LYS
1	B	219	PHE
1	B	63	LYS
1	B	210	LYS
1	B	240	ARG
1	B	231	PRO
1	B	307	GLY
1	B	195	PRO
1	B	220	ASN
1	A	290	GLY
1	B	172	VAL
1	B	212	THR
1	B	290	GLY
1	A	307	GLY

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	257/293 (88%)	228 (89%)	29 (11%)	5	24
1	B	259/293 (88%)	221 (85%)	38 (15%)	3	16
All	All	516/586 (88%)	449 (87%)	67 (13%)	4	20

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	7	MET
1	A	26	GLU
1	A	29	LYS
1	A	44	VAL
1	A	47	TYR
1	A	49	THR
1	A	62	LYS
1	A	63	LYS
1	A	67	LEU
1	A	69	SER
1	A	70	THR
1	A	139	MET
1	A	146	THR
1	A	149	THR
1	A	155	LYS
1	A	186	SER
1	A	208	LEU
1	A	210	LYS
1	A	212	THR
1	A	214	GLN
1	A	217	GLU
1	A	218	THR
1	A	233	LYS
1	A	242	VAL
1	A	245	ARG
1	A	281	THR
1	A	305	SER
1	A	306	SER
1	B	7	MET
1	B	8	THR
1	B	14	ILE
1	B	17	THR
1	B	20	ARG
1	B	29	LYS
1	B	44	VAL
1	B	47	TYR
1	B	49	THR
1	B	55	MET
1	B	61	LYS
1	B	66	SER
1	B	67	LEU
1	B	84	PRO

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Mol	Chain	Res	Type
1	B	135	ASN
1	B	139	MET
1	B	146	THR
1	B	149	THR
1	B	154	SER
1	B	171	PHE
1	B	194	GLN
1	B	207	LYS
1	B	209	LYS
1	B	210	LYS
1	B	213	SER
1	B	215	LYS
1	B	228	LYS
1	B	232	LYS
1	B	244	ARG
1	B	245	ARG
1	B	246	LYS
1	B	249	GLN
1	B	254	GLN
1	B	256	GLU
1	B	281	THR
1	B	295	SER
1	B	304	ILE
1	B	306	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	A	137	GLN
1	A	243	HIS
1	B	18	ASN
1	B	111	ASN
1	B	136	GLN
1	B	141	GLN
1	B	194	GLN
1	B	243	HIS

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z > 2$
3	GDP	A	593	4,2	29,30,30	2.06	8 (27%)	45,47,47	1.60	8 (17%)
4	AF3	A	594	2,3,5	0,3,3	-	-	-		
4	AF3	B	594	2,3,5	0,3,3	-	-	-		
3	GDP	B	593	4,2	29,30,30	2.06	8 (27%)	45,47,47	1.59	8 (17%)

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
3	GDP	A	593	4,2	-	2/16/32/32	0/3/3/3
3	GDP	B	593	4,2	-	2/16/32/32	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	593	GDP	PA-O3A	5.85	1.65	1.59
3	B	593	GDP	PA-O3A	5.62	1.65	1.59
3	B	593	GDP	PB-O2B	-4.09	1.39	1.54
3	A	593	GDP	PB-O2B	-4.08	1.39	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	593	GDP	PB-O3B	-3.96	1.40	1.54
3	A	593	GDP	O4'-C4'	3.66	1.53	1.45
3	B	593	GDP	O4'-C4'	3.39	1.52	1.45
3	A	593	GDP	PB-O1B	-3.29	1.40	1.50
3	A	593	GDP	O4'-C1'	3.21	1.49	1.42
3	A	593	GDP	C5-N7	-3.12	1.32	1.39
3	B	593	GDP	O4'-C1'	3.05	1.49	1.42
3	B	593	GDP	C5-N7	-2.85	1.33	1.39
3	B	593	GDP	PB-O1B	-2.84	1.41	1.50
3	A	593	GDP	PB-O3B	-2.57	1.45	1.54
3	B	593	GDP	C4-N9	-2.41	1.31	1.38
3	A	593	GDP	C4-N9	-2.20	1.32	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	593	GDP	C5-C4-N3	-5.00	120.42	128.39
3	B	593	GDP	C2-N3-C4	4.91	120.75	112.30
3	B	593	GDP	C5-C4-N3	-4.90	120.59	128.39
3	A	593	GDP	C2-N3-C4	4.87	120.68	112.30
3	A	593	GDP	C2-N1-C6	-3.22	119.28	125.11
3	B	593	GDP	C2-N1-C6	-3.11	119.47	125.11
3	A	593	GDP	N9-C4-N3	2.80	131.56	125.95
3	B	593	GDP	N9-C8-N7	-2.75	108.30	113.40
3	A	593	GDP	N9-C8-N7	-2.72	108.36	113.40
3	B	593	GDP	N9-C4-N3	2.71	131.37	125.95
3	A	593	GDP	C5-C6-N1	2.44	119.47	113.25
3	B	593	GDP	O6-C6-C5	-2.36	120.29	126.53
3	B	593	GDP	C5-C6-N1	2.33	119.19	113.25
3	A	593	GDP	O6-C6-C5	-2.31	120.42	126.53
3	A	593	GDP	C8-N7-C5	2.05	107.91	104.26
3	B	593	GDP	C8-N7-C5	2.00	107.83	104.26

There are no chirality outliers.

All (4) torsion outliers are listed below:

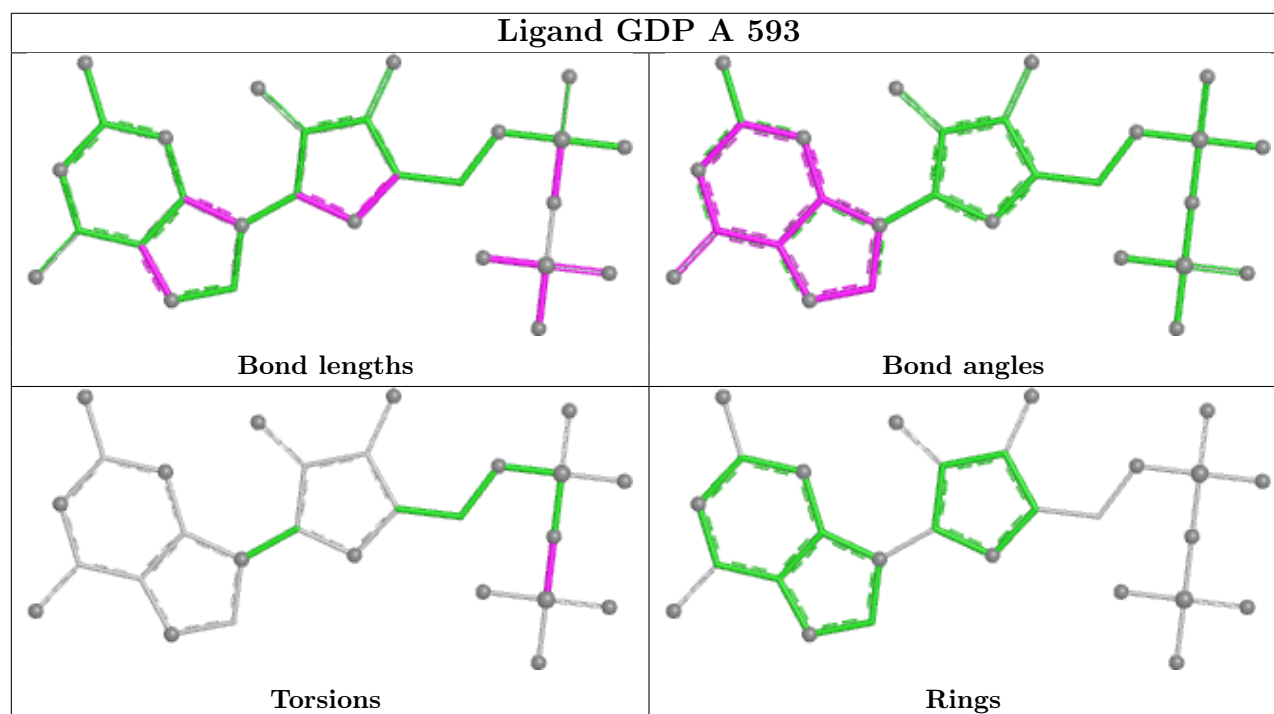
Mol	Chain	Res	Type	Atoms
3	A	593	GDP	PA-O3A-PB-O2B
3	B	593	GDP	PA-O3A-PB-O2B
3	A	593	GDP	PA-O3A-PB-O1B
3	B	593	GDP	PA-O3A-PB-O3B

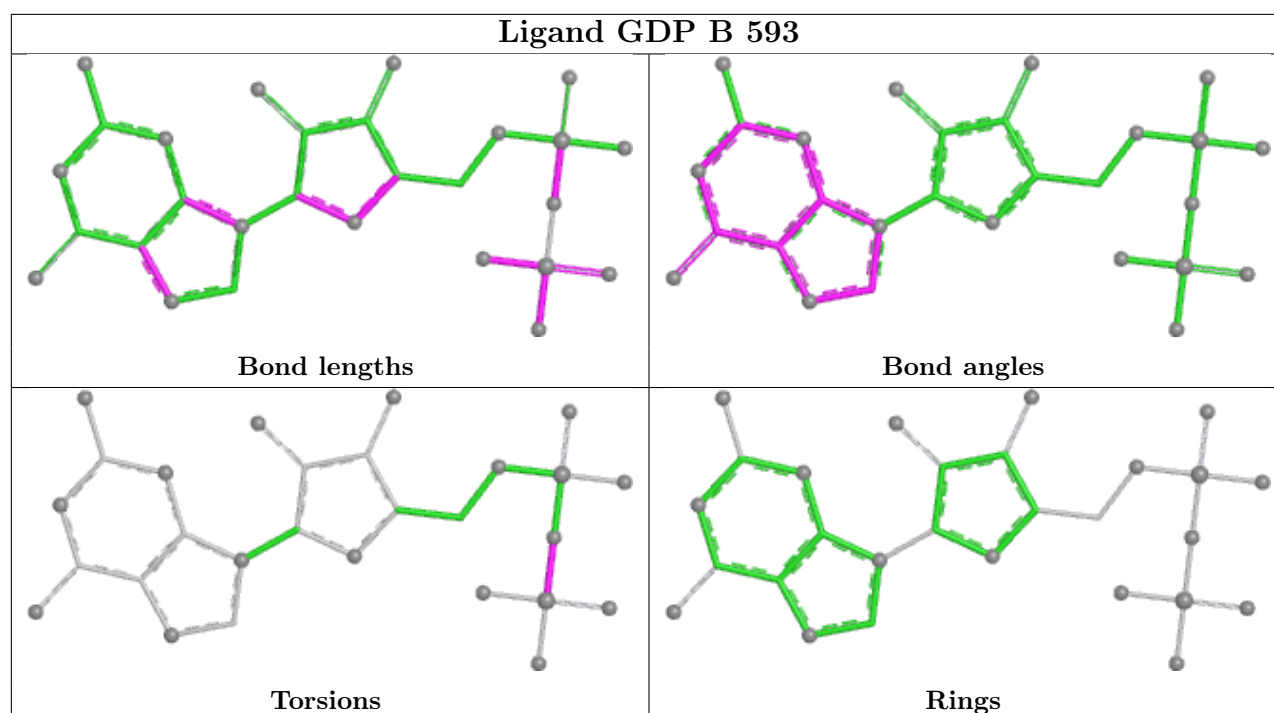
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	593	GDP	1	0
3	B	593	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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	288/328 (87%)	-0.32	2 (0%) 84 69	33, 58, 90, 98	0
1	B	290/328 (88%)	-0.23	4 (1%) 73 54	32, 58, 90, 99	0
All	All	578/656 (88%)	-0.28	6 (1%) 79 63	32, 58, 90, 99	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	242	VAL	2.9
1	A	172	VAL	2.9
1	A	173	SER	2.6
1	B	173	SER	2.4
1	B	172	VAL	2.0
1	B	105	GLU	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](#)

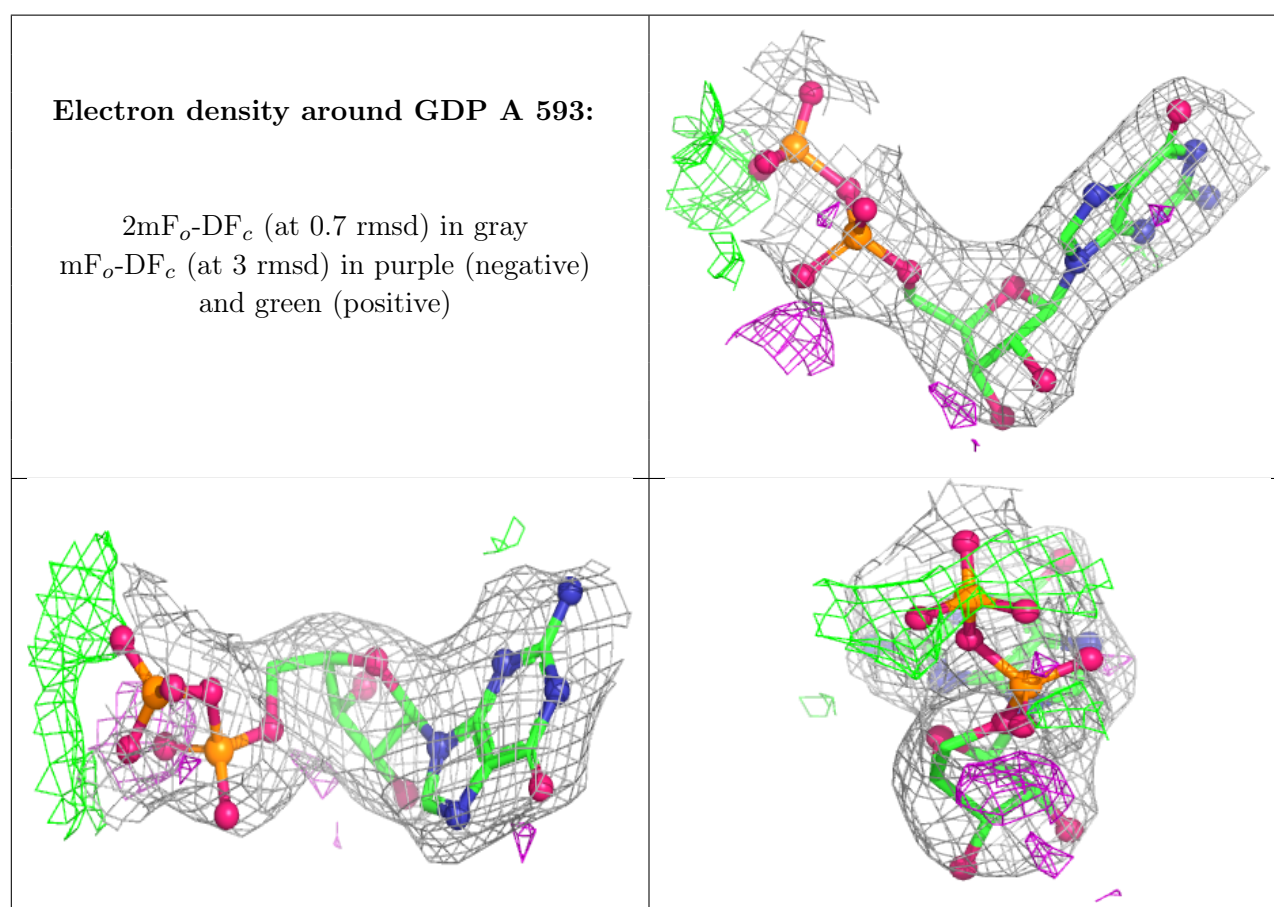
There are no oligosaccharides in this entry.

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.

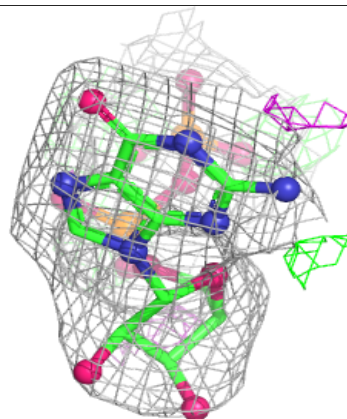
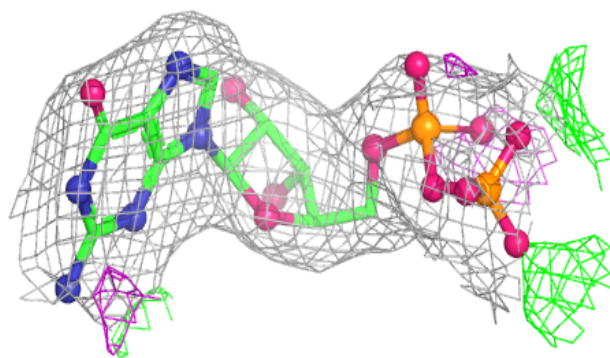
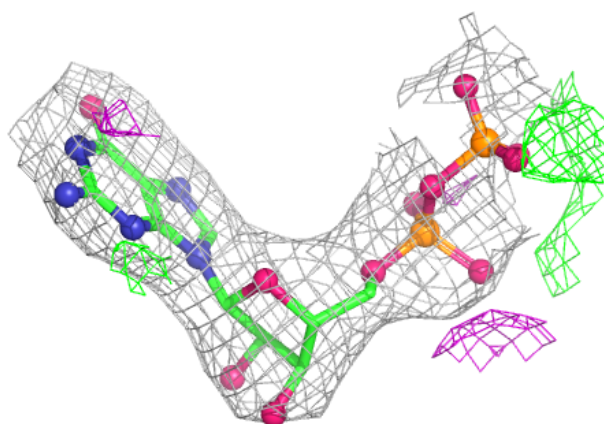
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	595	1/1	0.81	0.15	40,40,40,40	0
2	MG	B	595	1/1	0.81	0.20	43,43,43,43	0
3	GDP	A	593	28/28	0.96	0.08	46,49,55,59	0
3	GDP	B	593	28/28	0.96	0.08	47,51,55,56	0
4	AF3	A	594	4/4	0.97	0.12	32,37,38,38	0
4	AF3	B	594	4/4	0.97	0.11	30,34,36,37	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 B 593:

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.