



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:27 PM UTC

PDB ID : 3VQT / pdb_00003vqt
Title : Crystal structure analysis of the translation factor RF3
Authors : Kihira, K.; Shomura, Y.; Shibata, N.; Kitamura, M.; Higuchi, Y.
Deposited on : 2012-03-30
Resolution : 1.80 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

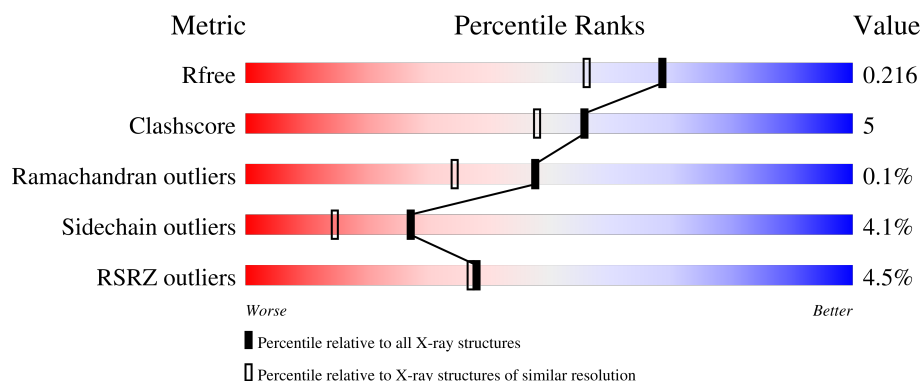
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	548	4% 77% 11% • 10%
1	B	548	4% 80% 9% • 11%
1	C	548	4% 76% 11% • 10%
1	D	548	4% 77% 11% • 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16607 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 Peptide chain release factor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	0	0
			3899	2471	683	724	21			
1	B	490	Total	C	N	O	S	0	0	0
			3860	2451	674	715	20			
1	C	491	Total	C	N	O	S	0	0	0
			3869	2456	675	718	20			
1	D	494	Total	C	N	O	S	0	0	0
			3900	2471	686	723	20			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP B8DIL5
A	-17	SER	-	expression tag	UNP B8DIL5
A	-16	SER	-	expression tag	UNP B8DIL5
A	-15	HIS	-	expression tag	UNP B8DIL5
A	-14	HIS	-	expression tag	UNP B8DIL5
A	-13	HIS	-	expression tag	UNP B8DIL5
A	-12	HIS	-	expression tag	UNP B8DIL5
A	-11	HIS	-	expression tag	UNP B8DIL5
A	-10	HIS	-	expression tag	UNP B8DIL5
A	-9	SER	-	expression tag	UNP B8DIL5
A	-8	SER	-	expression tag	UNP B8DIL5
A	-7	GLY	-	expression tag	UNP B8DIL5
A	-6	LEU	-	expression tag	UNP B8DIL5
A	-5	VAL	-	expression tag	UNP B8DIL5
A	-4	PRO	-	expression tag	UNP B8DIL5
A	-3	ARG	-	expression tag	UNP B8DIL5
A	-2	GLY	-	expression tag	UNP B8DIL5
A	-1	SER	-	expression tag	UNP B8DIL5
A	0	HIS	-	expression tag	UNP B8DIL5
B	-18	GLY	-	expression tag	UNP B8DIL5
B	-17	SER	-	expression tag	UNP B8DIL5

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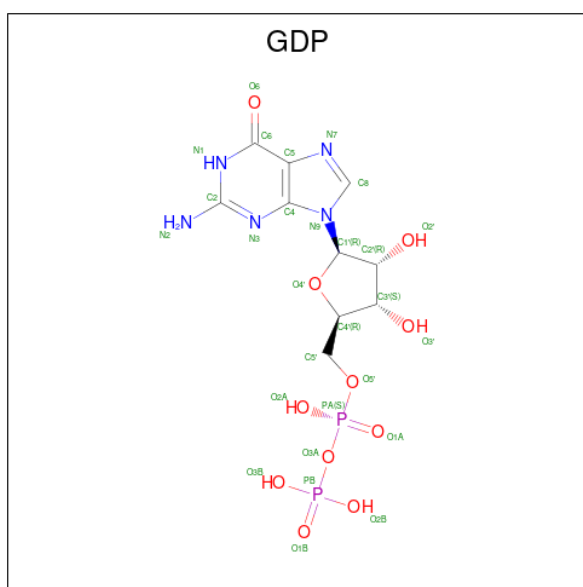
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP B8DIL5
B	-15	HIS	-	expression tag	UNP B8DIL5
B	-14	HIS	-	expression tag	UNP B8DIL5
B	-13	HIS	-	expression tag	UNP B8DIL5
B	-12	HIS	-	expression tag	UNP B8DIL5
B	-11	HIS	-	expression tag	UNP B8DIL5
B	-10	HIS	-	expression tag	UNP B8DIL5
B	-9	SER	-	expression tag	UNP B8DIL5
B	-8	SER	-	expression tag	UNP B8DIL5
B	-7	GLY	-	expression tag	UNP B8DIL5
B	-6	LEU	-	expression tag	UNP B8DIL5
B	-5	VAL	-	expression tag	UNP B8DIL5
B	-4	PRO	-	expression tag	UNP B8DIL5
B	-3	ARG	-	expression tag	UNP B8DIL5
B	-2	GLY	-	expression tag	UNP B8DIL5
B	-1	SER	-	expression tag	UNP B8DIL5
B	0	HIS	-	expression tag	UNP B8DIL5
C	-18	GLY	-	expression tag	UNP B8DIL5
C	-17	SER	-	expression tag	UNP B8DIL5
C	-16	SER	-	expression tag	UNP B8DIL5
C	-15	HIS	-	expression tag	UNP B8DIL5
C	-14	HIS	-	expression tag	UNP B8DIL5
C	-13	HIS	-	expression tag	UNP B8DIL5
C	-12	HIS	-	expression tag	UNP B8DIL5
C	-11	HIS	-	expression tag	UNP B8DIL5
C	-10	HIS	-	expression tag	UNP B8DIL5
C	-9	SER	-	expression tag	UNP B8DIL5
C	-8	SER	-	expression tag	UNP B8DIL5
C	-7	GLY	-	expression tag	UNP B8DIL5
C	-6	LEU	-	expression tag	UNP B8DIL5
C	-5	VAL	-	expression tag	UNP B8DIL5
C	-4	PRO	-	expression tag	UNP B8DIL5
C	-3	ARG	-	expression tag	UNP B8DIL5
C	-2	GLY	-	expression tag	UNP B8DIL5
C	-1	SER	-	expression tag	UNP B8DIL5
C	0	HIS	-	expression tag	UNP B8DIL5
D	-18	GLY	-	expression tag	UNP B8DIL5
D	-17	SER	-	expression tag	UNP B8DIL5
D	-16	SER	-	expression tag	UNP B8DIL5
D	-15	HIS	-	expression tag	UNP B8DIL5
D	-14	HIS	-	expression tag	UNP B8DIL5
D	-13	HIS	-	expression tag	UNP B8DIL5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP B8DIL5
D	-11	HIS	-	expression tag	UNP B8DIL5
D	-10	HIS	-	expression tag	UNP B8DIL5
D	-9	SER	-	expression tag	UNP B8DIL5
D	-8	SER	-	expression tag	UNP B8DIL5
D	-7	GLY	-	expression tag	UNP B8DIL5
D	-6	LEU	-	expression tag	UNP B8DIL5
D	-5	VAL	-	expression tag	UNP B8DIL5
D	-4	PRO	-	expression tag	UNP B8DIL5
D	-3	ARG	-	expression tag	UNP B8DIL5
D	-2	GLY	-	expression tag	UNP B8DIL5
D	-1	SER	-	expression tag	UNP B8DIL5
D	0	HIS	-	expression tag	UNP B8DIL5

- 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
2	A	1	Total 28	C 10	N 5	O 11	P 2	0	0
2	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
2	C	1	Total 28	C 10	N 5	O 11	P 2	0	0
2	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

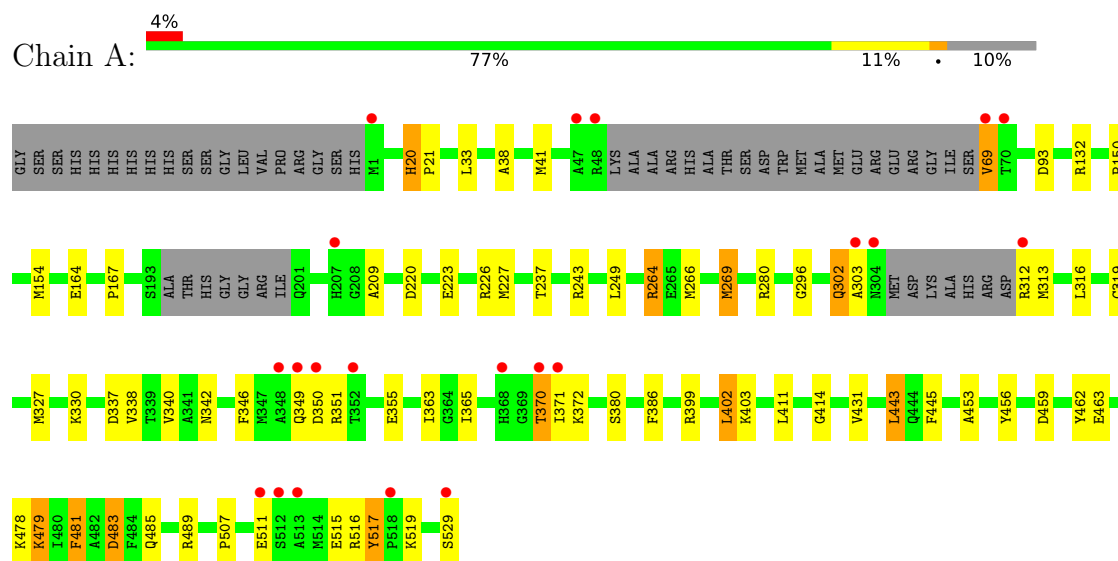
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	266	Total 266	O 266	0	0
3	B	227	Total 227	O 227	0	0
3	C	224	Total 224	O 224	0	0
3	D	250	Total 250	O 250	0	0

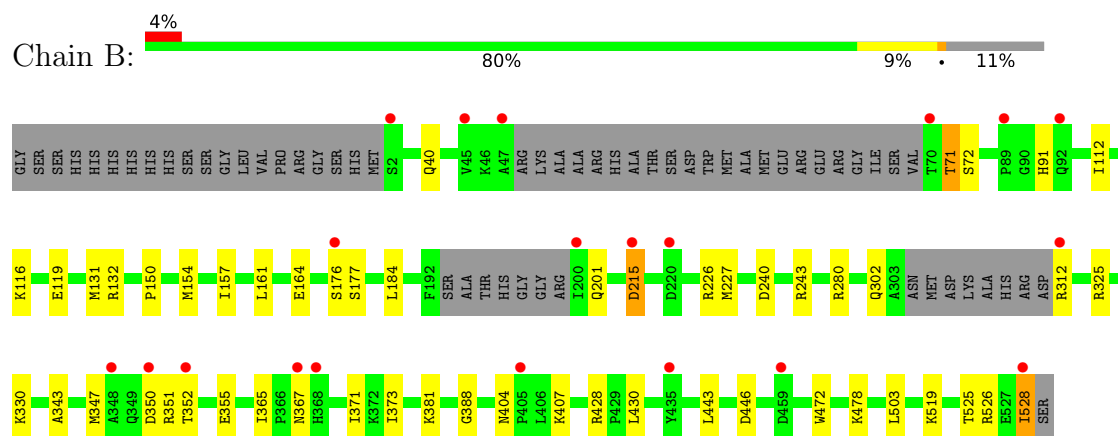
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

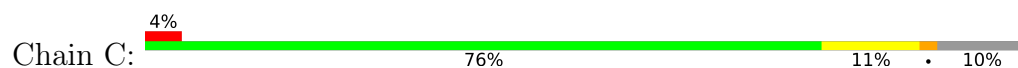
- Molecule 1: Peptide chain release factor 3

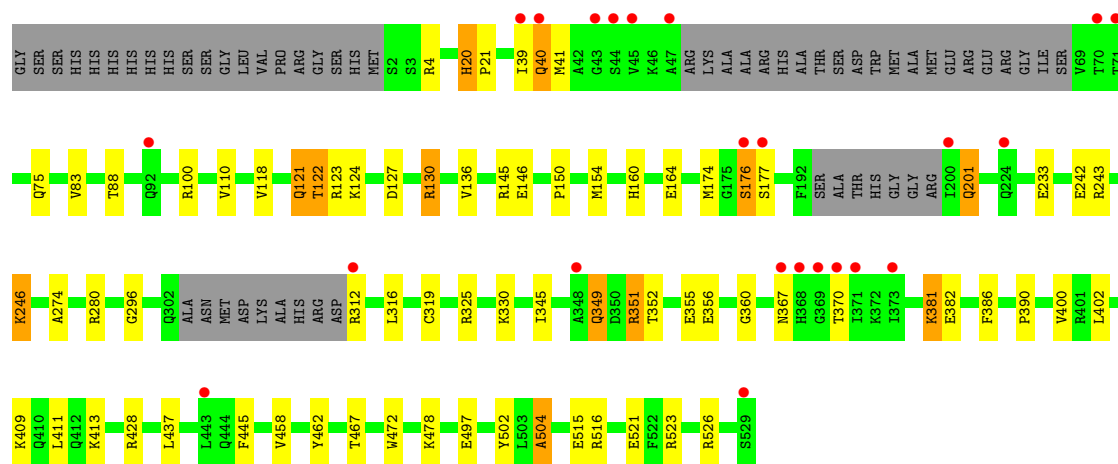


- Molecule 1: Peptide chain release factor 3

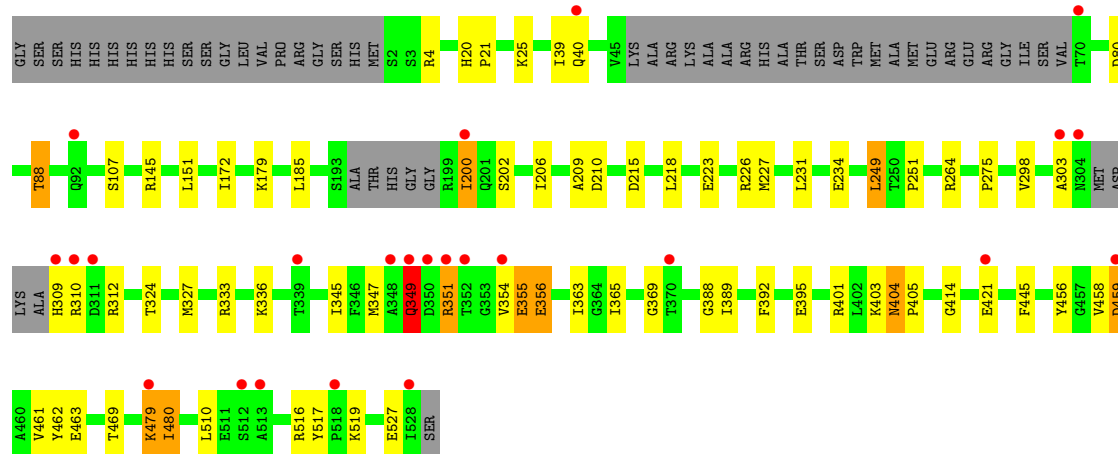
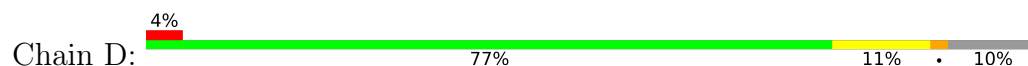


- Molecule 1: Peptide chain release factor 3





• Molecule 1: Peptide chain release factor 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	47.39Å 82.80Å 148.29Å 104.21° 89.78° 89.63°	Depositor
Resolution (Å)	33.87 – 1.80 33.87 – 1.80	Depositor EDS
% Data completeness (in resolution range)	93.5 (33.87-1.80) 93.5 (33.87-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.177 , 0.218 0.177 , 0.216	Depositor DCC
R_{free} test set	9597 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l 0.037 for -h,k,-k-l 0.003 for -h,-k,k+l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16607	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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: 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	1.26	7/3978 (0.2%)	1.16	8/5376 (0.1%)
1	B	1.23	4/3939 (0.1%)	1.14	4/5326 (0.1%)
1	C	1.27	9/3948 (0.2%)	1.17	15/5337 (0.3%)
1	D	1.27	7/3980 (0.2%)	1.19	17/5381 (0.3%)
All	All	1.26	27/15845 (0.2%)	1.17	44/21420 (0.2%)

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	C	0	1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	177	SER	N-CA	11.11	1.60	1.46
1	A	519	LYS	N-CA	9.41	1.58	1.46
1	B	365	ILE	CA-CB	8.30	1.62	1.53
1	A	479	LYS	CE-NZ	8.28	1.74	1.49
1	B	177	SER	N-CA	7.49	1.56	1.46
1	D	519	LYS	CA-C	6.54	1.61	1.52
1	C	458	VAL	CA-CB	6.20	1.61	1.54
1	A	38	ALA	CA-CB	-6.18	1.45	1.52
1	C	504	ALA	CA-CB	5.80	1.61	1.54
1	D	298	VAL	CA-CB	5.79	1.61	1.54
1	A	399	ARG	C-O	5.74	1.30	1.23
1	A	519	LYS	CA-C	5.73	1.60	1.52
1	C	176	SER	CA-CB	5.68	1.63	1.53
1	B	176	SER	CB-OG	5.64	1.53	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	215	ASP	C-O	5.62	1.31	1.24
1	A	453	ALA	N-CA	5.54	1.52	1.46
1	C	160	HIS	ND1-CE1	5.48	1.38	1.32
1	A	302	GLN	CD-OE1	5.45	1.33	1.23
1	D	354	VAL	CA-CB	5.30	1.59	1.54
1	D	206	ILE	CA-CB	5.27	1.60	1.54
1	C	274	ALA	CA-CB	5.14	1.60	1.53
1	C	176	SER	C-O	-5.13	1.17	1.24
1	C	176	SER	CB-OG	-5.08	1.31	1.42
1	D	392	PHE	C-O	-5.06	1.17	1.23
1	D	479	LYS	C-O	-5.06	1.18	1.24
1	D	4	ARG	CA-C	5.05	1.59	1.52
1	C	467	THR	C-O	-5.01	1.17	1.23

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	100	ARG	NE-CZ-NH1	9.12	130.62	121.50
1	D	480	ILE	N-CA-C	-8.43	102.20	110.72
1	C	100	ARG	NE-CZ-NH2	-8.01	111.99	119.20
1	D	517	TYR	CA-C-N	7.96	127.60	119.56
1	D	517	TYR	C-N-CA	7.96	127.60	119.56
1	C	201	GLN	N-CA-C	7.76	121.54	109.52
1	B	177	SER	N-CA-C	7.51	122.09	113.15
1	C	177	SER	N-CA-C	-7.22	104.21	113.16
1	D	404	ASN	CA-C-N	6.98	126.95	119.28
1	D	404	ASN	C-N-CA	6.98	126.95	119.28
1	C	160	HIS	CB-CG-CD2	-6.84	122.31	131.20
1	A	350	ASP	N-CA-C	6.75	118.52	111.03
1	A	517	TYR	CA-C-N	6.70	126.39	119.56
1	A	517	TYR	C-N-CA	6.70	126.39	119.56
1	D	249	LEU	CA-CB-CG	6.66	139.62	116.30
1	D	519	LYS	N-CA-C	6.51	120.49	112.54
1	A	371	ILE	N-CA-C	6.41	118.72	108.85
1	A	20	HIS	N-CA-C	-6.37	102.10	110.39
1	C	100	ARG	CD-NE-CZ	6.30	133.23	124.40
1	D	327	MET	N-CA-C	6.20	119.69	110.52
1	D	145	ARG	CG-CD-NE	-5.86	99.11	112.00
1	A	355	GLU	N-CA-C	5.86	117.59	109.15
1	B	201	GLN	N-CA-C	5.84	118.74	110.50
1	C	349	GLN	CA-C-N	5.83	128.37	120.44
1	C	349	GLN	C-N-CA	5.83	128.37	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	356	GLU	N-CA-C	-5.81	100.24	109.07
1	C	400	VAL	CB-CA-C	-5.80	103.26	111.21
1	C	160	HIS	CB-CG-ND1	5.78	131.37	122.70
1	C	130	ARG	NE-CZ-NH2	-5.77	114.01	119.20
1	C	478	LYS	N-CA-C	5.76	118.33	111.71
1	C	122	THR	CB-CA-C	-5.62	102.05	110.88
1	D	310	ARG	N-CA-C	5.58	119.09	111.39
1	D	185	LEU	N-CA-C	5.56	117.42	111.36
1	D	251	PRO	N-CA-C	-5.45	102.57	110.80
1	B	184	LEU	N-CA-C	5.43	116.88	111.07
1	A	370	THR	N-CA-C	5.40	119.62	113.19
1	A	313	MET	CG-SD-CE	-5.39	89.04	100.90
1	B	350	ASP	N-CA-C	5.35	117.55	111.02
1	D	458	VAL	CA-C-N	-5.34	115.57	123.05
1	D	458	VAL	C-N-CA	-5.34	115.57	123.05
1	D	349	GLN	CA-C-N	5.33	127.42	120.28
1	D	349	GLN	C-N-CA	5.33	127.42	120.28
1	C	20	HIS	N-CA-C	-5.19	103.13	110.29
1	C	360	GLY	N-CA-C	-5.01	108.73	114.69

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	351	ARG	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	3899	0	3871	45	0
1	B	3860	0	3832	30	1
1	C	3869	0	3841	33	0
1	D	3900	0	3862	40	0
2	A	28	0	12	0	0
2	B	28	0	12	1	0
2	C	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	28	0	12	0	0
3	A	266	0	0	7	0
3	B	227	0	0	2	0
3	C	224	0	0	6	0
3	D	250	0	0	3	0
All	All	16607	0	15454	146	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (146) 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:479:LYS:CE	1:A:479:LYS:NZ	1.74	1.47
1:A:264:ARG:HH11	1:A:264:ARG:CG	1.61	1.12
1:A:264:ARG:HG2	1:A:264:ARG:NH1	1.48	1.04
1:A:463:GLU:HG2	1:B:227:MET:HE1	1.42	1.00
1:A:478:LYS:HE2	3:A:852:HOH:O	1.73	0.88
1:C:130:ARG:HD3	3:C:872:HOH:O	1.73	0.88
1:B:526:ARG:NH1	1:B:528:ILE:HG22	1.88	0.88
1:B:526:ARG:HH12	1:B:528:ILE:HG22	1.40	0.86
1:C:145:ARG:NH1	3:C:762:HOH:O	2.10	0.82
1:C:164:GLU:OE1	1:C:243:ARG:NH2	2.11	0.82
1:A:269:MET:CE	3:A:760:HOH:O	2.32	0.77
1:A:269:MET:HE3	3:A:760:HOH:O	1.83	0.77
1:B:215:ASP:OD1	1:B:226:ARG:NH2	2.20	0.74
1:B:404:ASN:HD22	1:B:407:LYS:HE3	1.53	0.72
1:C:150:PRO:O	1:C:154:MET:HG2	1.90	0.71
1:B:164:GLU:CD	1:B:243:ARG:HH22	1.99	0.70
1:A:164:GLU:OE1	1:A:243:ARG:NH2	2.25	0.70
1:A:264:ARG:HH11	1:A:264:ARG:HG2	0.67	0.69
1:B:91:HIS:NE2	2:B:601:GDP:O1B	2.27	0.67
1:B:325:ARG:HD2	1:B:355:GLU:OE1	1.94	0.67
1:A:93:ASP:HA	1:A:443:LEU:HD22	1.77	0.66
1:D:403:LYS:HB2	1:D:459:ASP:OD1	1.96	0.66
1:C:516:ARG:HD2	3:C:901:HOH:O	1.94	0.65
1:D:40:GLN:OE1	1:D:349:GLN:NE2	2.30	0.65
1:D:347:MET:HE1	1:D:355:GLU:OE1	1.98	0.64
1:A:164:GLU:CD	1:A:243:ARG:HH22	2.05	0.64
1:D:351:ARG:NH2	3:D:1017:HOH:O	2.18	0.63
1:C:312:ARG:HB2	1:C:367:ASN:OD1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:LYS:CE	3:A:852:HOH:O	2.38	0.62
1:A:463:GLU:HG2	1:B:227:MET:CE	2.26	0.61
1:D:312:ARG:NH1	1:D:369:GLY:HA2	2.16	0.61
1:A:280:ARG:HG2	1:A:386:PHE:CD2	2.37	0.60
1:C:296:GLY:HA3	1:C:316:LEU:HD21	1.85	0.59
1:B:325:ARG:NH2	1:B:343:ALA:O	2.36	0.58
1:D:312:ARG:CZ	1:D:369:GLY:HA2	2.33	0.58
1:D:403:LYS:HE3	1:D:461:VAL:CG1	2.34	0.58
1:D:403:LYS:HE3	1:D:461:VAL:HG11	1.86	0.58
1:D:395:GLU:HB2	3:D:1233:HOH:O	2.04	0.57
1:A:264:ARG:CG	1:A:264:ARG:NH1	2.31	0.57
1:A:93:ASP:HA	1:A:443:LEU:CD2	2.34	0.57
1:C:127:ASP:OD1	1:C:130:ARG:NH2	2.37	0.57
1:B:150:PRO:O	1:B:154:MET:HG2	2.05	0.56
1:C:330:LYS:HE3	1:C:381:LYS:HG2	1.86	0.56
1:D:209:ALA:O	1:D:226:ARG:HD3	2.06	0.56
1:A:249:LEU:C	1:A:249:LEU:HD23	2.31	0.56
1:D:445:PHE:HB3	1:D:462:TYR:CE1	2.41	0.55
1:B:164:GLU:OE2	1:B:243:ARG:NH2	2.33	0.55
1:A:479:LYS:NZ	1:A:479:LYS:CD	2.65	0.55
1:B:215:ASP:CG	1:B:226:ARG:HH22	2.14	0.55
1:C:118:VAL:HG12	1:C:123:ARG:HG3	1.88	0.54
1:C:325:ARG:NH2	3:C:835:HOH:O	2.40	0.54
1:D:401:ARG:HH11	1:D:401:ARG:HG2	1.71	0.54
1:A:209:ALA:O	1:A:226:ARG:HD3	2.08	0.53
1:A:402:LEU:O	3:A:962:HOH:O	2.19	0.53
1:A:402:LEU:HD13	1:A:411:LEU:HD22	1.90	0.53
1:A:403:LYS:HD3	1:A:459:ASP:HB3	1.90	0.53
1:C:110:VAL:HG23	1:C:136:VAL:CG1	2.38	0.53
1:D:324:THR:HG22	1:D:356:GLU:HG2	1.90	0.53
1:C:312:ARG:CB	1:C:367:ASN:OD1	2.57	0.52
1:C:40:GLN:HG3	1:C:41:MET:N	2.24	0.52
1:D:312:ARG:HH12	1:D:421:GLU:CD	2.17	0.52
1:D:172:ILE:HG21	1:D:218:LEU:HD22	1.91	0.51
1:B:351:ARG:NH2	3:B:741:HOH:O	2.44	0.51
1:D:401:ARG:HG2	1:D:401:ARG:NH1	2.26	0.51
1:C:110:VAL:HG23	1:C:136:VAL:HG11	1.92	0.51
1:C:280:ARG:HD3	1:C:319:CYS:SG	2.51	0.51
1:C:280:ARG:HG2	1:C:386:PHE:CD2	2.46	0.51
1:A:346:PHE:O	3:A:914:HOH:O	2.19	0.50
1:A:511:GLU:O	1:A:515:GLU:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:GLN:HG2	1:C:349:GLN:CG	2.41	0.50
1:D:333:ARG:HG2	1:D:333:ARG:HH21	1.76	0.50
1:A:296:GLY:HA3	1:A:316:LEU:HD21	1.93	0.50
1:A:150:PRO:O	1:A:154:MET:HG2	2.11	0.50
1:A:264:ARG:NH1	3:A:807:HOH:O	2.29	0.49
1:C:146:GLU:HA	1:C:174:MET:HE3	1.94	0.49
1:A:280:ARG:HD3	1:A:319:CYS:SG	2.53	0.49
1:B:132:ARG:NH1	1:B:388:GLY:O	2.44	0.49
1:D:312:ARG:NH1	1:D:421:GLU:CD	2.71	0.49
1:A:164:GLU:HG2	1:A:237:THR:HG21	1.93	0.49
1:C:402:LEU:HD21	1:C:411:LEU:HB2	1.93	0.49
1:A:20:HIS:CG	1:A:21:PRO:HD2	2.47	0.48
1:A:363:ILE:HD12	1:A:365:ILE:HD11	1.95	0.48
1:C:502:TYR:HE2	1:C:504:ALA:HB2	1.78	0.48
1:D:215:ASP:OD1	1:D:226:ARG:NH2	2.43	0.48
1:A:431:VAL:CG1	1:A:489:ARG:HG2	2.43	0.48
1:A:483:ASP:OD1	1:A:483:ASP:C	2.57	0.48
1:B:443:LEU:HD12	1:B:446:ASP:HB2	1.94	0.48
1:C:40:GLN:HG2	1:C:349:GLN:CD	2.39	0.48
1:D:303:ALA:HA	1:D:312:ARG:HG2	1.95	0.48
1:A:372:LYS:HE2	1:A:529:SER:OXT	2.15	0.47
1:A:516:ARG:HG2	1:A:517:TYR:CE2	2.50	0.47
1:C:428:ARG:NH2	3:C:903:HOH:O	2.46	0.47
1:A:445:PHE:HB3	1:A:462:TYR:CE1	2.49	0.47
1:B:71:THR:CG2	1:B:71:THR:O	2.62	0.46
1:B:240:ASP:OD1	1:B:243:ARG:HG3	2.16	0.46
1:B:131:MET:HE1	1:B:525:THR:HG21	1.98	0.46
1:C:164:GLU:OE1	1:C:243:ARG:CZ	2.63	0.46
1:C:121:GLN:HG2	3:C:743:HOH:O	2.15	0.46
1:C:445:PHE:HB3	1:C:462:TYR:CE1	2.51	0.46
1:D:347:MET:HE1	1:D:355:GLU:HG3	1.98	0.46
1:D:388:GLY:H	1:D:527:GLU:CD	2.24	0.46
1:A:481:PHE:O	1:A:485:GLN:HG3	2.16	0.45
1:D:345:ILE:HG21	1:D:347:MET:HE3	1.98	0.45
1:D:363:ILE:HD12	1:D:365:ILE:HD11	1.99	0.45
1:A:303:ALA:HA	1:A:312:ARG:HG2	2.00	0.44
1:C:497:GLU:HG3	1:C:526:ARG:CZ	2.48	0.44
1:D:25:LYS:NZ	1:D:88:THR:O	2.50	0.44
1:D:414:GLY:HA2	1:D:456:TYR:CZ	2.53	0.44
1:B:157:ILE:HG23	1:B:161:LEU:HD12	2.00	0.44
1:B:312:ARG:N	1:B:367:ASN:HD22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:GLN:HA	1:C:83:VAL:O	2.19	0.43
1:D:107:SER:HB3	1:D:275:PRO:HD2	2.01	0.43
1:A:33:LEU:HD13	1:A:41:MET:HG3	2.00	0.43
1:A:154:MET:HE1	1:A:167:PRO:HD3	2.01	0.43
1:D:345:ILE:HG22	1:D:347:MET:HG3	1.99	0.43
1:D:404:ASN:HA	1:D:405:PRO:HD2	1.77	0.42
1:B:381:LYS:HB3	1:B:381:LYS:HE3	1.75	0.42
1:D:179:LYS:HA	1:D:179:LYS:HD2	1.75	0.42
1:A:327:MET:O	1:A:340:VAL:HG22	2.20	0.42
1:D:231:LEU:C	1:D:231:LEU:HD23	2.44	0.42
1:B:373:ILE:HG22	1:B:528:ILE:HD11	2.01	0.42
1:A:69:VAL:HG12	1:A:302:GLN:OE1	2.20	0.42
1:D:200:ILE:HD13	1:D:264:ARG:HH21	1.85	0.42
1:D:389:ILE:HG21	1:D:389:ILE:HD13	1.76	0.42
1:C:472:TRP:CD2	1:C:526:ARG:HB2	2.54	0.42
1:C:521:GLU:CD	1:C:523:ARG:HE	2.27	0.42
1:B:428:ARG:HB3	1:B:428:ARG:CZ	2.48	0.42
1:D:151:LEU:HD23	1:D:151:LEU:HA	1.81	0.42
1:C:20:HIS:CG	1:C:21:PRO:HD2	2.55	0.42
1:D:349:GLN:H	1:D:349:GLN:HG3	1.69	0.42
1:A:330:LYS:HD2	1:A:380:SER:O	2.19	0.41
1:C:345:ILE:HD12	1:C:355:GLU:HG2	2.02	0.41
1:D:336:LYS:HD2	3:D:1053:HOH:O	2.20	0.41
1:B:367:ASN:HB2	1:B:371:ILE:HD12	2.02	0.41
1:D:401:ARG:HG3	1:D:463:GLU:CD	2.45	0.41
1:B:131:MET:HE2	1:B:131:MET:HB3	1.74	0.41
1:C:242:GLU:O	1:C:246:LYS:HD3	2.21	0.41
1:B:280:ARG:NH1	3:B:859:HOH:O	2.50	0.41
1:A:414:GLY:HA2	1:A:456:TYR:CZ	2.56	0.41
1:D:223:GLU:HG3	1:D:227:MET:HE2	2.02	0.41
1:A:266:MET:HE3	1:A:266:MET:HB3	1.91	0.41
1:B:472:TRP:CD2	1:B:526:ARG:HB2	2.56	0.41
1:D:20:HIS:CG	1:D:21:PRO:HD2	2.56	0.41
1:D:469:THR:HG21	1:D:510:LEU:HD22	2.03	0.41
1:B:116:LYS:HD3	1:B:119:GLU:OE2	2.21	0.40
1:B:528:ILE:HD13	1:B:528:ILE:HG21	1.59	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:ASP:OD2	1:B:478:LYS:NZ[1_655]	2.14	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	487/548 (89%)	475 (98%)	12 (2%)	0	100	100
1	B	482/548 (88%)	475 (98%)	7 (2%)	0	100	100
1	C	483/548 (88%)	475 (98%)	7 (1%)	1 (0%)	43	31
1	D	486/548 (89%)	478 (98%)	8 (2%)	0	100	100
All	All	1938/2192 (88%)	1903 (98%)	34 (2%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	390	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	412/453 (91%)	394 (96%)	18 (4%)	25	13
1	B	407/453 (90%)	395 (97%)	12 (3%)	37	25
1	C	409/453 (90%)	388 (95%)	21 (5%)	21	9
1	D	412/453 (91%)	396 (96%)	16 (4%)	28	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1640/1812 (90%)	1573 (96%)	67 (4%)	27 15

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

Mol	Chain	Res	Type
1	A	69	VAL
1	A	132	ARG
1	A	220	ASP
1	A	223	GLU
1	A	227	MET
1	A	264	ARG
1	A	269	MET
1	A	337	ASP
1	A	338	VAL
1	A	342	ASN
1	A	349	GLN
1	A	351	ARG
1	A	370	THR
1	A	402	LEU
1	A	443	LEU
1	A	481	PHE
1	A	483	ASP
1	A	507	PRO
1	B	40	GLN
1	B	71	THR
1	B	72	SER
1	B	112	ILE
1	B	302	GLN
1	B	330	LYS
1	B	347	MET
1	B	352	THR
1	B	430	LEU
1	B	503	LEU
1	B	519	LYS
1	B	528	ILE
1	C	4	ARG
1	C	39	ILE
1	C	40	GLN
1	C	88	THR
1	C	121	GLN
1	C	122	THR
1	C	124	LYS

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Mol	Chain	Res	Type
1	C	176	SER
1	C	201	GLN
1	C	233	GLU
1	C	246	LYS
1	C	351	ARG
1	C	352	THR
1	C	356	GLU
1	C	370	THR
1	C	381	LYS
1	C	382	GLU
1	C	409	LYS
1	C	413	LYS
1	C	437	LEU
1	C	515	GLU
1	D	39	ILE
1	D	80	ASP
1	D	88	THR
1	D	200	ILE
1	D	202	SER
1	D	210	ASP
1	D	234	GLU
1	D	249	LEU
1	D	309	HIS
1	D	349	GLN
1	D	351	ARG
1	D	355	GLU
1	D	459	ASP
1	D	479	LYS
1	D	480	ILE
1	D	516	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
1	A	186	HIS
1	A	349	GLN
1	A	425	GLN
1	B	40	GLN
1	B	425	GLN
1	C	207	HIS
1	C	302	GLN

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Mol	Chain	Res	Type
1	C	425	GLN
1	D	186	HIS
1	D	213	GLN
1	D	278	GLN
1	D	417	GLN
1	D	425	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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	601	-	29,30,30	1.00	2 (6%)	45,47,47	2.01	13 (28%)
2	GDP	B	601	-	29,30,30	1.15	2 (6%)	45,47,47	1.80	11 (24%)
2	GDP	D	601	-	29,30,30	1.19	3 (10%)	45,47,47	1.75	12 (26%)
2	GDP	C	601	-	29,30,30	1.32	3 (10%)	45,47,47	1.93	13 (28%)

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	601	-	-	4/16/32/32	0/3/3/3
2	GDP	B	601	-	-	2/16/32/32	0/3/3/3
2	GDP	D	601	-	-	2/16/32/32	0/3/3/3
2	GDP	C	601	-	-	2/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	GDP	C5-C4	4.09	1.50	1.38
2	B	601	GDP	C5-C4	3.68	1.48	1.38
2	D	601	GDP	C4-N9	-2.95	1.30	1.38
2	D	601	GDP	C5-C4	2.90	1.46	1.38
2	D	601	GDP	C4-N3	2.62	1.40	1.34
2	B	601	GDP	C4-N9	-2.55	1.31	1.38
2	A	601	GDP	C4-N9	-2.28	1.32	1.38
2	C	601	GDP	PB-O3B	-2.25	1.46	1.54
2	C	601	GDP	O6-C6	2.06	1.27	1.23
2	A	601	GDP	C5-C4	2.06	1.44	1.38

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	GDP	C2-N3-C4	5.55	121.85	112.30
2	A	601	GDP	C5-C4-N3	-5.44	119.74	128.39
2	C	601	GDP	C5-C4-N3	-4.94	120.52	128.39
2	B	601	GDP	C5-C4-N3	-4.60	121.07	128.39
2	C	601	GDP	C2-N3-C4	4.52	120.09	112.30
2	D	601	GDP	N9-C4-N3	4.46	134.86	125.95
2	C	601	GDP	N9-C4-N3	4.31	134.58	125.95
2	B	601	GDP	C2-N3-C4	4.28	119.68	112.30
2	A	601	GDP	N9-C4-N3	4.25	134.44	125.95
2	A	601	GDP	O2A-PA-O3A	4.17	118.56	107.27
2	D	601	GDP	C5-C4-N3	-4.06	121.92	128.39
2	B	601	GDP	C6-C5-N7	3.87	137.34	130.29
2	C	601	GDP	C6-C5-N7	3.85	137.30	130.29
2	B	601	GDP	O2A-PA-O3A	3.84	117.64	107.27
2	B	601	GDP	N9-C4-N3	3.72	133.39	125.95
2	A	601	GDP	C6-C5-N7	3.64	136.92	130.29
2	D	601	GDP	C2-N3-C4	3.62	118.53	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	GDP	O2A-PA-O3A	3.56	116.90	107.27
2	C	601	GDP	O3B-PB-O2B	3.53	121.02	107.80
2	D	601	GDP	C8-N9-C4	3.25	112.11	106.03
2	C	601	GDP	O2B-PB-O1B	-2.86	99.70	110.83
2	A	601	GDP	O2'-C2'-C3'	2.82	120.87	111.82
2	A	601	GDP	C2-N1-C6	-2.73	120.17	125.11
2	A	601	GDP	N9-C8-N7	-2.72	108.35	113.40
2	D	601	GDP	C6-C5-N7	2.60	135.03	130.29
2	D	601	GDP	O3A-PB-O1B	-2.55	97.60	111.04
2	D	601	GDP	O2A-PA-O3A	2.54	114.13	107.27
2	C	601	GDP	C8-N9-C4	2.47	110.65	106.03
2	A	601	GDP	C8-N7-C5	2.45	108.63	104.26
2	B	601	GDP	O6-C6-C5	-2.43	120.12	126.53
2	A	601	GDP	C4-C5-N7	-2.42	106.83	110.67
2	C	601	GDP	C4-C5-N7	-2.38	106.90	110.67
2	A	601	GDP	C8-N9-C4	2.32	110.37	106.03
2	B	601	GDP	C4-C5-N7	-2.31	107.01	110.67
2	B	601	GDP	C8-N9-C4	2.31	110.35	106.03
2	D	601	GDP	O3B-PB-O2B	2.28	116.35	107.80
2	B	601	GDP	O3B-PB-O2B	2.28	116.34	107.80
2	A	601	GDP	C5-C6-N1	2.26	119.00	113.25
2	D	601	GDP	N9-C8-N7	-2.19	109.33	113.40
2	D	601	GDP	O6-C6-C5	-2.19	120.75	126.53
2	A	601	GDP	O6-C6-C5	-2.17	120.80	126.53
2	D	601	GDP	C6-C5-C4	-2.15	115.59	118.83
2	B	601	GDP	C6-C5-C4	-2.11	115.65	118.83
2	C	601	GDP	C8-N7-C5	2.10	108.00	104.26
2	C	601	GDP	O3B-PB-O3A	2.09	111.64	104.64
2	C	601	GDP	N9-C8-N7	-2.08	109.54	113.40
2	C	601	GDP	C6-C5-C4	-2.02	115.79	118.83
2	B	601	GDP	C5-C6-N1	2.01	118.38	113.25
2	D	601	GDP	C5-C6-N1	2.00	118.35	113.25

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GDP	PA-O3A-PB-O2B
2	A	601	GDP	PA-O3A-PB-O3B
2	C	601	GDP	PA-O3A-PB-O3B
2	D	601	GDP	PA-O3A-PB-O3B
2	D	601	GDP	PA-O3A-PB-O1B

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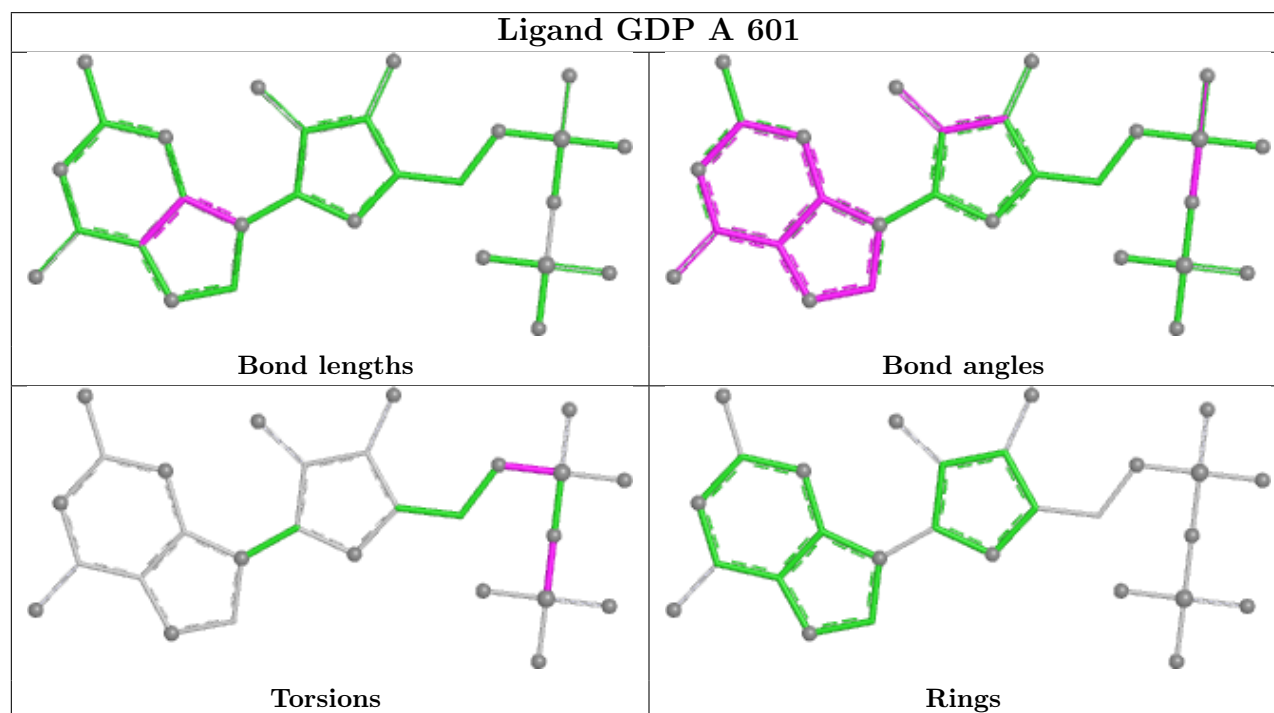
Mol	Chain	Res	Type	Atoms
2	B	601	GDP	PA-O3A-PB-O3B
2	A	601	GDP	C5'-O5'-PA-O1A
2	B	601	GDP	C5'-O5'-PA-O1A
2	A	601	GDP	PA-O3A-PB-O1B
2	C	601	GDP	PA-O3A-PB-O1B

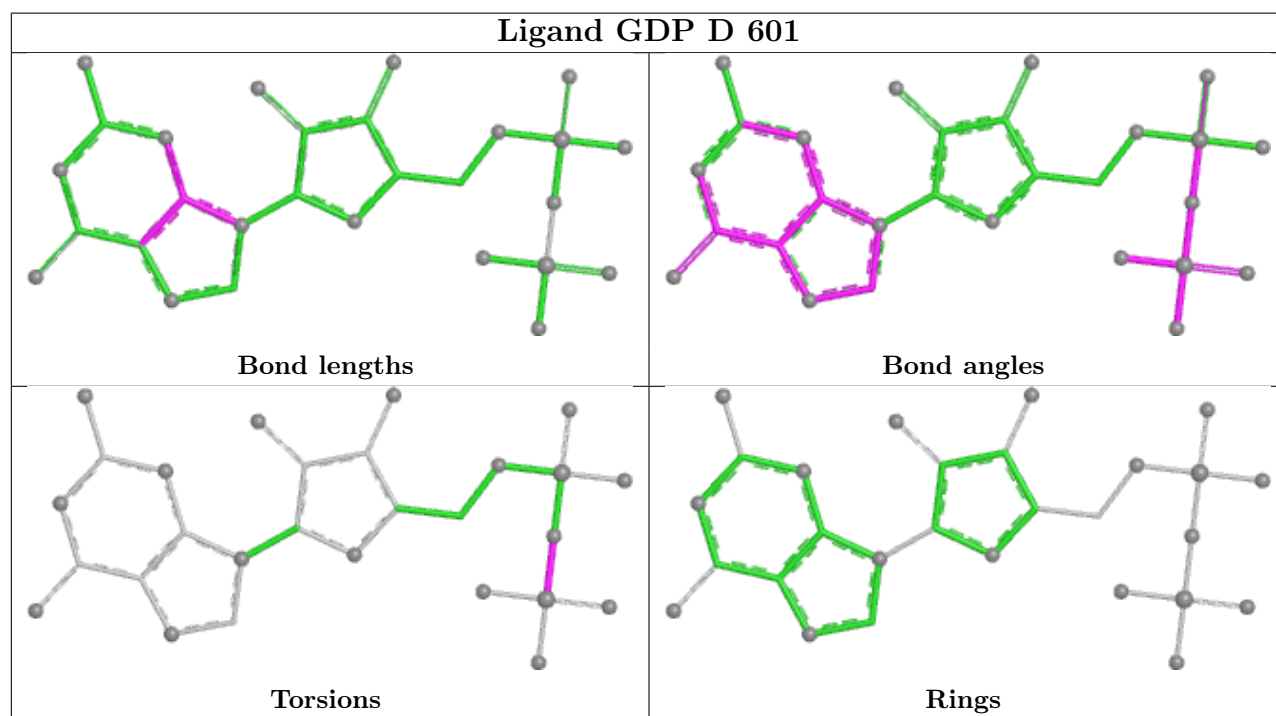
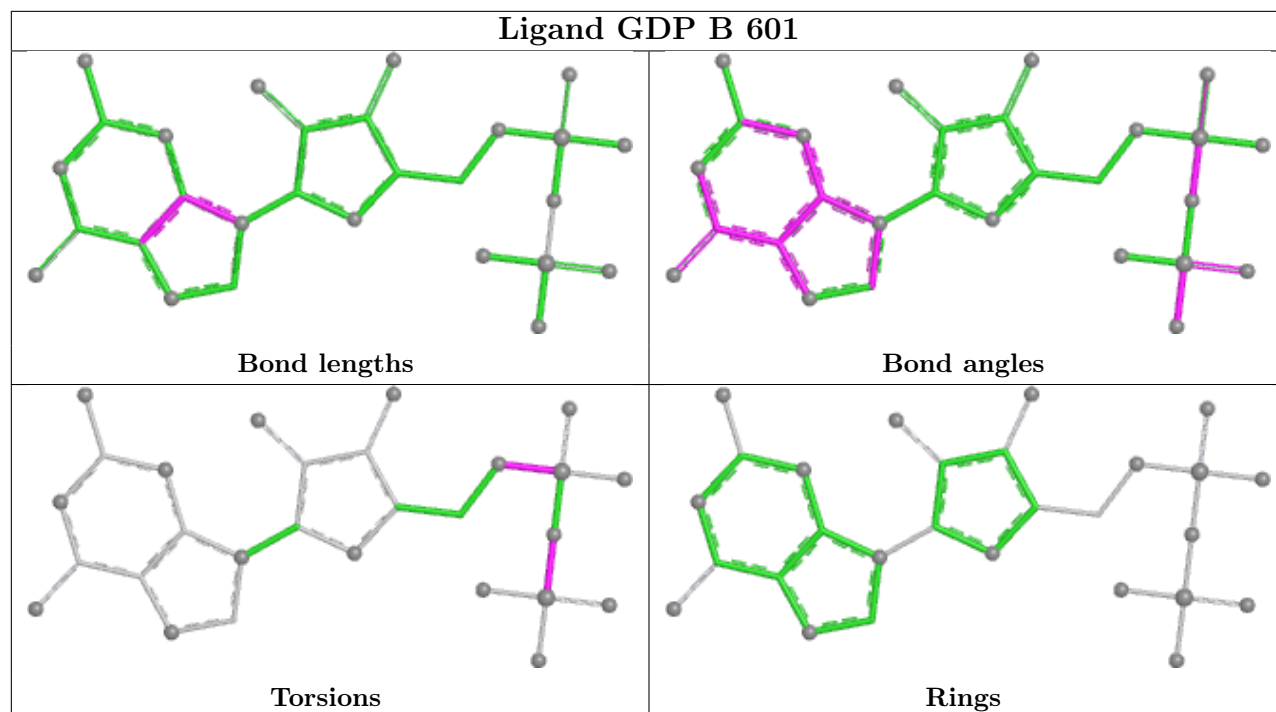
There are no ring outliers.

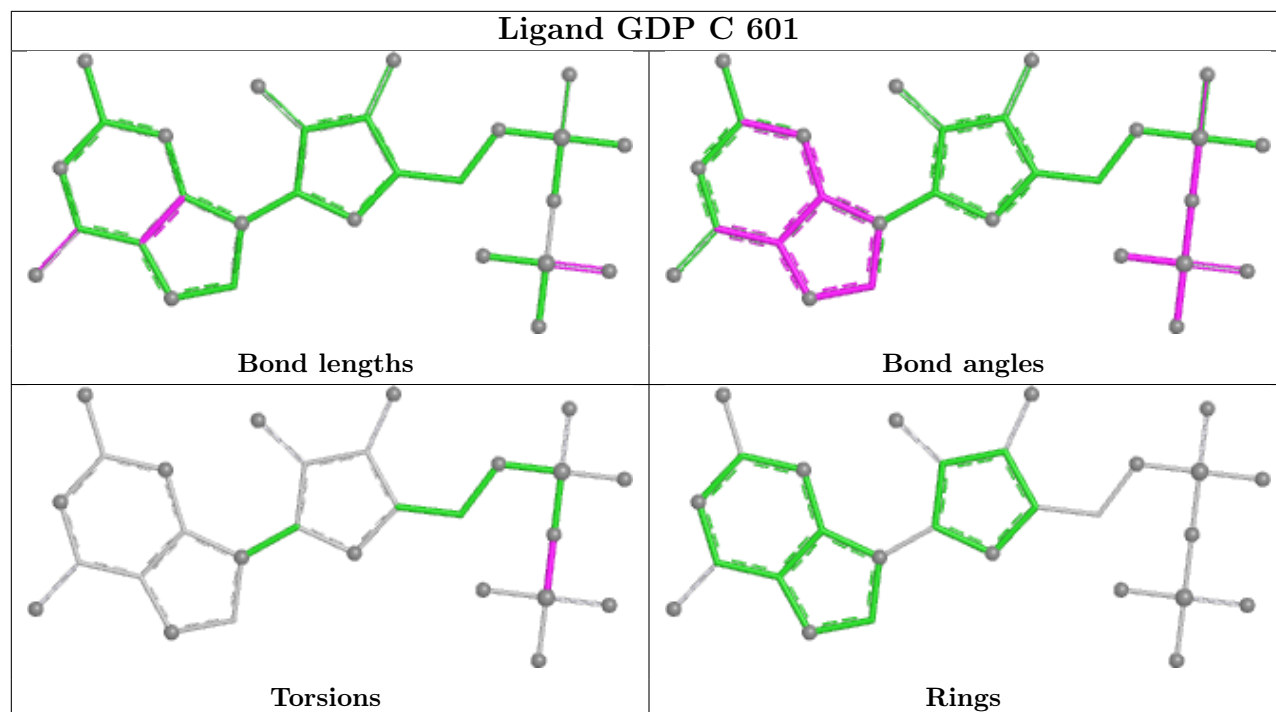
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	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	495/548 (90%)	0.12	21 (4%) 40 40	15, 28, 53, 73	0
1	B	490/548 (89%)	0.18	20 (4%) 41 41	16, 31, 51, 71	0
1	C	491/548 (89%)	0.22	23 (4%) 36 35	16, 30, 53, 70	0
1	D	494/548 (90%)	0.10	24 (4%) 35 33	15, 28, 52, 75	0
All	All	1970/2192 (89%)	0.16	88 (4%) 38 37	15, 29, 53, 75	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	47	ALA	6.5
1	C	370	THR	6.1
1	B	200	ILE	5.9
1	C	368	HIS	5.6
1	D	70	THR	5.2
1	C	92	GLN	4.7
1	C	369	GLY	4.7
1	C	367	ASN	4.6
1	C	176	SER	4.5
1	B	176	SER	4.5
1	B	92	GLN	4.4
1	A	512	SER	4.3
1	C	47	ALA	4.2
1	A	70	THR	4.0
1	D	200	ILE	3.8
1	B	528	ILE	3.7
1	D	309	HIS	3.7
1	C	200	ILE	3.7
1	B	350	ASP	3.6
1	B	348	ALA	3.6
1	B	70	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	303	ALA	3.5
1	A	304	ASN	3.4
1	C	70	THR	3.4
1	A	303	ALA	3.4
1	A	529	SER	3.3
1	B	312	ARG	3.3
1	A	370	THR	3.2
1	B	352	THR	3.2
1	C	177	SER	3.0
1	A	371	ILE	3.0
1	A	349	GLN	3.0
1	D	339	THR	3.0
1	D	350	ASP	2.9
1	D	421	GLU	2.9
1	A	48	ARG	2.9
1	B	45	VAL	2.9
1	D	348	ALA	2.9
1	D	518	PRO	2.8
1	A	312	ARG	2.8
1	D	349	GLN	2.8
1	C	529	SER	2.7
1	C	45	VAL	2.7
1	A	350	ASP	2.7
1	D	479	LYS	2.7
1	C	39	ILE	2.6
1	C	371	ILE	2.6
1	A	47	ALA	2.6
1	D	310	ARG	2.6
1	A	69	VAL	2.6
1	D	512	SER	2.6
1	D	370	THR	2.5
1	D	92	GLN	2.5
1	D	304	ASN	2.5
1	C	40	GLN	2.5
1	B	405	PRO	2.5
1	C	43	GLY	2.5
1	C	348	ALA	2.4
1	D	40	GLN	2.4
1	A	1	MET	2.4
1	D	459	ASP	2.4
1	A	352	THR	2.4
1	D	513	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	368	HIS	2.4
1	B	368	HIS	2.3
1	D	528	ILE	2.3
1	B	220	ASP	2.3
1	D	311	ASP	2.3
1	D	354	VAL	2.3
1	B	367	ASN	2.3
1	D	351	ARG	2.3
1	B	215	ASP	2.2
1	A	518	PRO	2.2
1	A	513	ALA	2.2
1	B	459	ASP	2.2
1	A	207	HIS	2.1
1	C	373	ILE	2.1
1	B	89	PRO	2.1
1	B	2	SER	2.1
1	C	443	LEU	2.1
1	C	44	SER	2.0
1	C	224	GLN	2.0
1	A	348	ALA	2.0
1	C	312	ARG	2.0
1	A	511	GLU	2.0
1	C	71	THR	2.0
1	D	352	THR	2.0
1	B	435	TYR	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 ⓘ

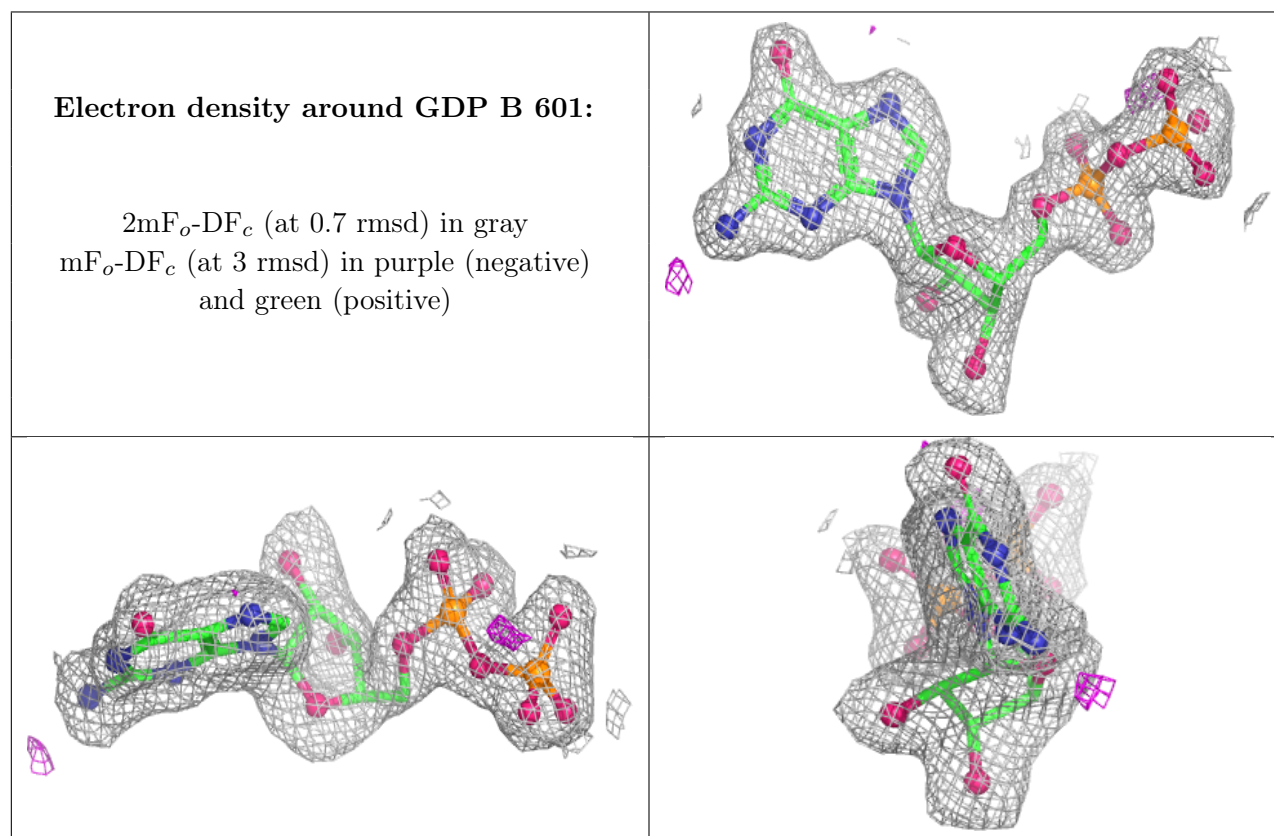
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

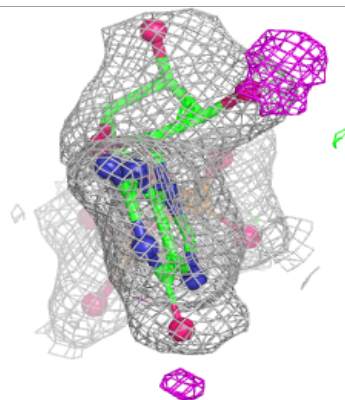
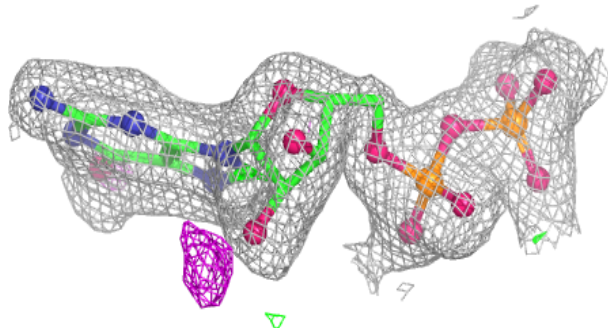
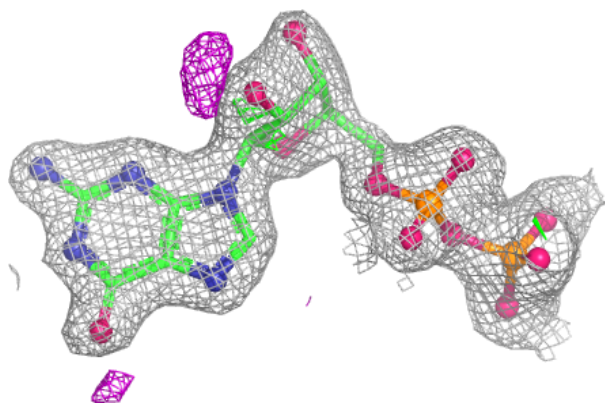
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GDP	B	601	28/28	0.96	0.07	26,35,37,41	0
2	GDP	C	601	28/28	0.96	0.08	24,34,39,44	0
2	GDP	A	601	28/28	0.98	0.06	22,27,31,33	0
2	GDP	D	601	28/28	0.98	0.05	21,26,30,32	0

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.

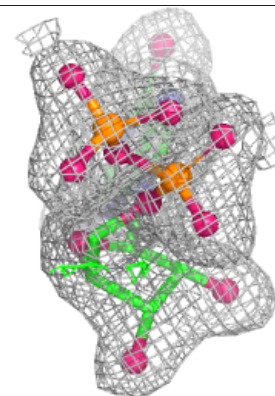
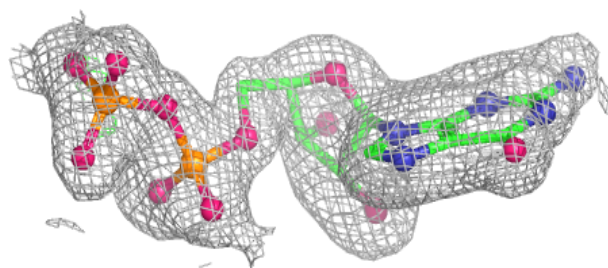
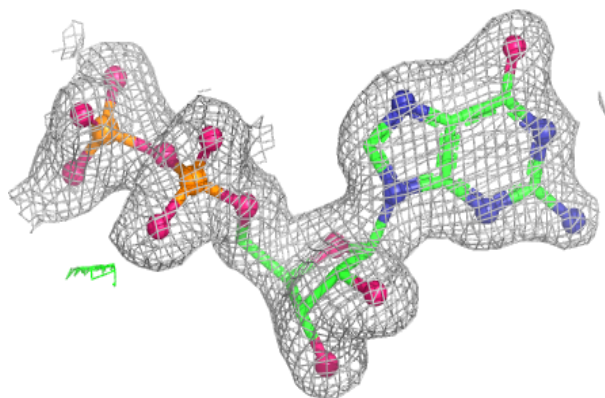


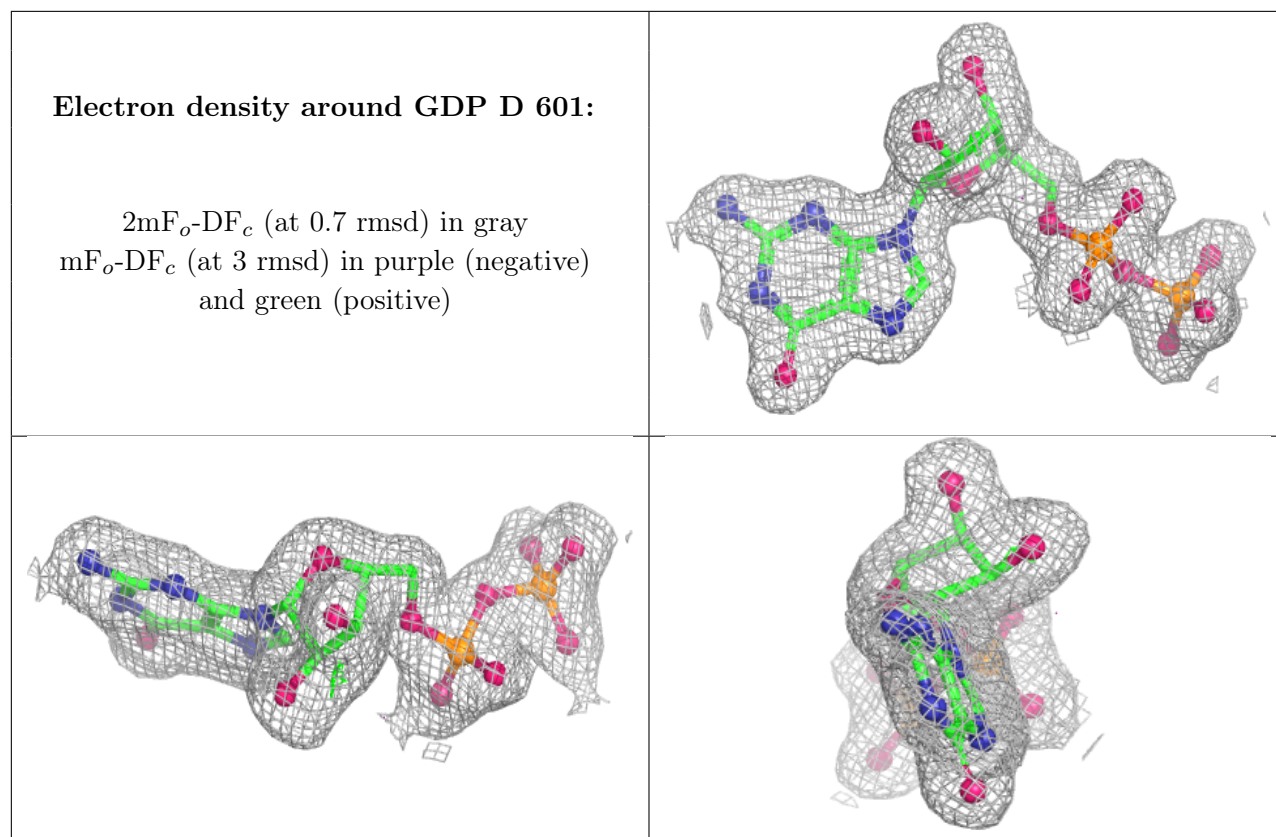
Electron density around GDP C 601:

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

**Electron density around GDP A 601:**

$2mF_o-DF_c$ (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.