



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:14 AM UTC

PDB ID : 9N2Q / pdb_00009n2q
Title : Structure of GDP-bound GM4951
Authors : Raj, R.; Beutler, B.
Deposited on : 2025-01-29
Resolution : 2.51 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

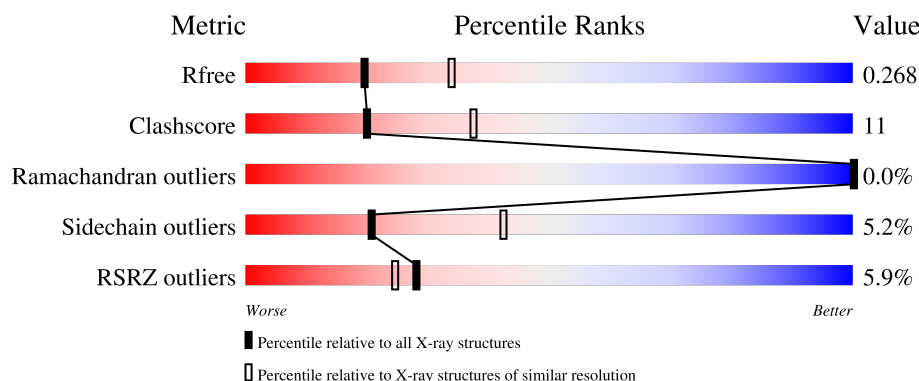
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	416	 6% 66% 26% • 6%
1	B	416	 7% 69% 24% • 5%
1	C	416	 4% 70% 23% • 6%
1	D	416	 6% 72% 21% • 5%
1	E	416	 5% 71% 22% • 5%

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Mol	Chain	Length	Quality of chain
1	F	416	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	504	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 19314 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 inducible GTPase 1C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	0	0
			3162	2022	527	597	16			
1	B	397	Total	C	N	O	S	0	0	0
			3180	2032	529	603	16			
1	C	393	Total	C	N	O	S	0	0	0
			3173	2031	526	600	16			
1	D	397	Total	C	N	O	S	0	0	0
			3187	2039	527	605	16			
1	E	397	Total	C	N	O	S	0	0	0
			3201	2047	531	607	16			
1	F	393	Total	C	N	O	S	0	0	0
			3171	2033	529	593	16			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	HIS	-	expression tag	UNP Q3UED7
A	-8	HIS	-	expression tag	UNP Q3UED7
A	-7	HIS	-	expression tag	UNP Q3UED7
A	-6	HIS	-	expression tag	UNP Q3UED7
A	-5	HIS	-	expression tag	UNP Q3UED7
A	-4	HIS	-	expression tag	UNP Q3UED7
A	-3	SER	-	expression tag	UNP Q3UED7
A	-2	GLN	-	expression tag	UNP Q3UED7
A	-1	ASP	-	expression tag	UNP Q3UED7
A	0	PRO	-	expression tag	UNP Q3UED7
B	-9	HIS	-	expression tag	UNP Q3UED7
B	-8	HIS	-	expression tag	UNP Q3UED7
B	-7	HIS	-	expression tag	UNP Q3UED7
B	-6	HIS	-	expression tag	UNP Q3UED7
B	-5	HIS	-	expression tag	UNP Q3UED7
B	-4	HIS	-	expression tag	UNP Q3UED7
B	-3	SER	-	expression tag	UNP Q3UED7

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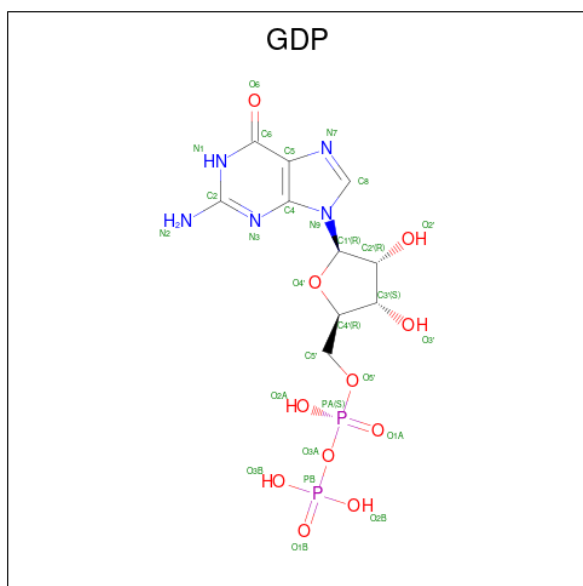
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLN	-	expression tag	UNP Q3UED7
B	-1	ASP	-	expression tag	UNP Q3UED7
B	0	PRO	-	expression tag	UNP Q3UED7
C	-9	HIS	-	expression tag	UNP Q3UED7
C	-8	HIS	-	expression tag	UNP Q3UED7
C	-7	HIS	-	expression tag	UNP Q3UED7
C	-6	HIS	-	expression tag	UNP Q3UED7
C	-5	HIS	-	expression tag	UNP Q3UED7
C	-4	HIS	-	expression tag	UNP Q3UED7
C	-3	SER	-	expression tag	UNP Q3UED7
C	-2	GLN	-	expression tag	UNP Q3UED7
C	-1	ASP	-	expression tag	UNP Q3UED7
C	0	PRO	-	expression tag	UNP Q3UED7
D	-9	HIS	-	expression tag	UNP Q3UED7
D	-8	HIS	-	expression tag	UNP Q3UED7
D	-7	HIS	-	expression tag	UNP Q3UED7
D	-6	HIS	-	expression tag	UNP Q3UED7
D	-5	HIS	-	expression tag	UNP Q3UED7
D	-4	HIS	-	expression tag	UNP Q3UED7
D	-3	SER	-	expression tag	UNP Q3UED7
D	-2	GLN	-	expression tag	UNP Q3UED7
D	-1	ASP	-	expression tag	UNP Q3UED7
D	0	PRO	-	expression tag	UNP Q3UED7
E	-9	HIS	-	expression tag	UNP Q3UED7
E	-8	HIS	-	expression tag	UNP Q3UED7
E	-7	HIS	-	expression tag	UNP Q3UED7
E	-6	HIS	-	expression tag	UNP Q3UED7
E	-5	HIS	-	expression tag	UNP Q3UED7
E	-4	HIS	-	expression tag	UNP Q3UED7
E	-3	SER	-	expression tag	UNP Q3UED7
E	-2	GLN	-	expression tag	UNP Q3UED7
E	-1	ASP	-	expression tag	UNP Q3UED7
E	0	PRO	-	expression tag	UNP Q3UED7
F	-9	HIS	-	expression tag	UNP Q3UED7
F	-8	HIS	-	expression tag	UNP Q3UED7
F	-7	HIS	-	expression tag	UNP Q3UED7
F	-6	HIS	-	expression tag	UNP Q3UED7
F	-5	HIS	-	expression tag	UNP Q3UED7
F	-4	HIS	-	expression tag	UNP Q3UED7
F	-3	SER	-	expression tag	UNP Q3UED7
F	-2	GLN	-	expression tag	UNP Q3UED7
F	-1	ASP	-	expression tag	UNP Q3UED7

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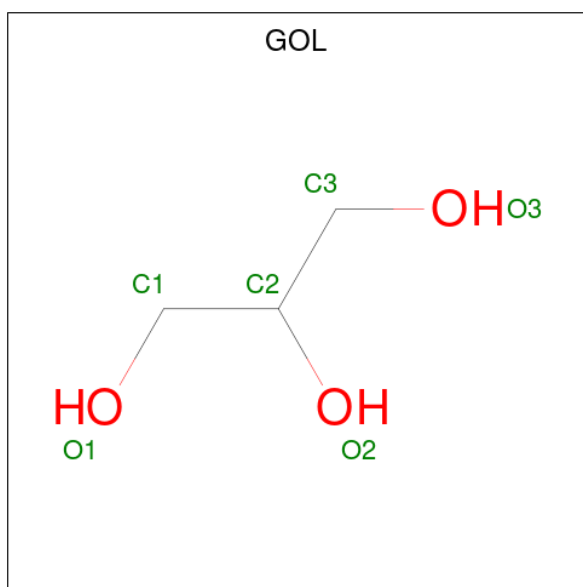
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	PRO	-	expression tag	UNP Q3UED7

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	B	4	Total	O	0	0
			4	4		
4	C	7	Total	O	0	0
			7	7		
4	D	7	Total	O	0	0
			7	7		
4	E	5	Total	O	0	0
			5	5		

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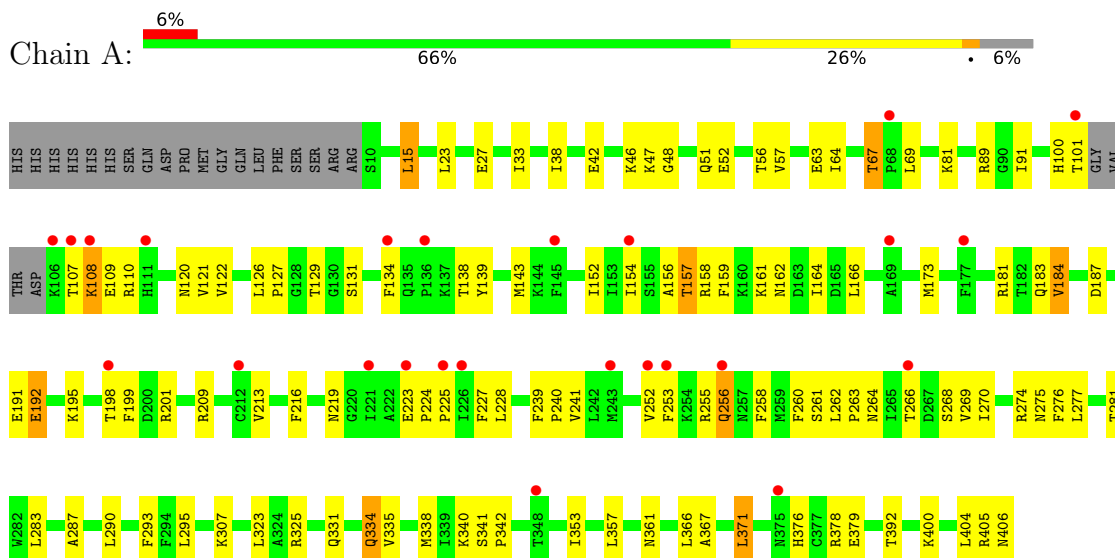
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	4	Total	O	0	0
			4	4		

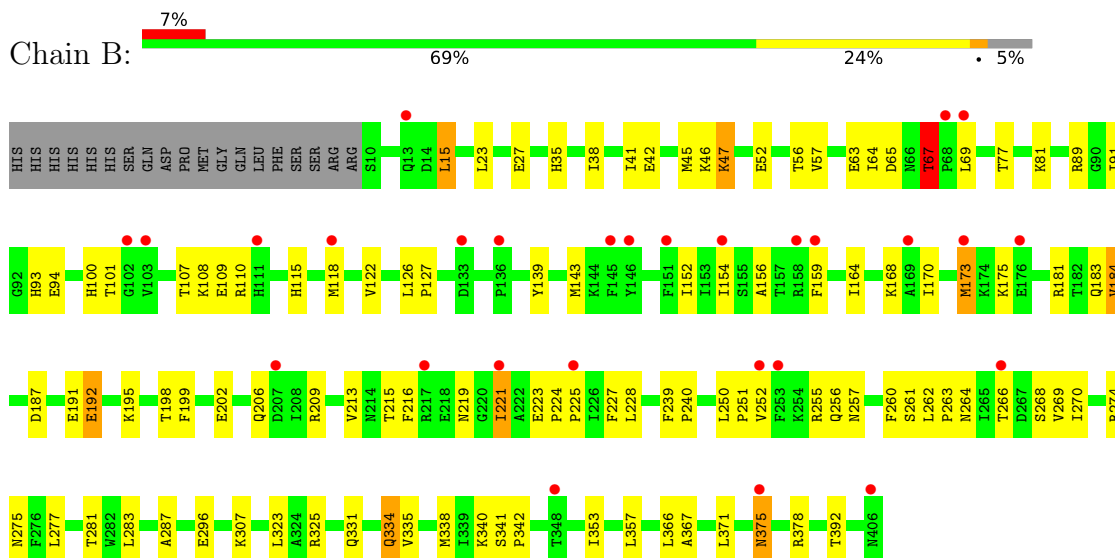
3 Residue-property plots

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 inducible GTPase 1C

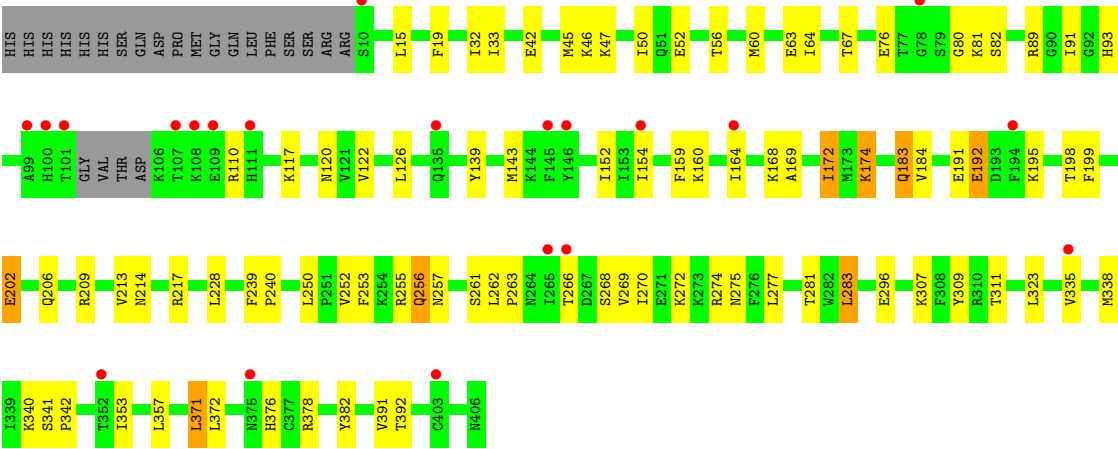


• Molecule 1: Interferon inducible GTPase 1C



• Molecule 1: Interferon inducible GTPase 1C





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.32Å 100.64Å 152.35Å 87.49° 78.52° 89.91°	Depositor
Resolution (Å)	49.72 – 2.51 49.72 – 2.51	Depositor EDS
% Data completeness (in resolution range)	90.6 (49.72-2.51) 90.7 (49.72-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0349	Depositor
R, R_{free}	0.230 , 0.274 (Not available) , 0.268	Depositor DCC
R_{free} test set	5324 reflections (4.43%)	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.450 for h,-k,h-l 0.005 for -h,k,-l 0.004 for -h,-k,-h+l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19314	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GOL

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	0.61	1/3230 (0.0%)	1.07	4/4367 (0.1%)
1	B	0.62	3/3248 (0.1%)	1.07	3/4395 (0.1%)
1	C	0.62	1/3241 (0.0%)	1.05	5/4381 (0.1%)
1	D	0.62	2/3255 (0.1%)	1.05	3/4401 (0.1%)
1	E	0.62	1/3269 (0.0%)	1.05	5/4419 (0.1%)
1	F	0.60	2/3239 (0.1%)	1.04	2/4375 (0.0%)
All	All	0.62	10/19482 (0.1%)	1.05	22/26338 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	376	HIS	CE1-NE2	7.68	1.40	1.32
1	C	376	HIS	CE1-NE2	7.57	1.40	1.32
1	E	376	HIS	CE1-NE2	6.29	1.38	1.32
1	A	376	HIS	CE1-NE2	5.38	1.38	1.32
1	B	35	HIS	CE1-NE2	5.35	1.37	1.32
1	B	93	HIS	CE1-NE2	5.31	1.37	1.32
1	F	93	HIS	CE1-NE2	5.21	1.37	1.32
1	D	376	HIS	CE1-NE2	5.19	1.37	1.32
1	D	236	HIS	CE1-NE2	5.11	1.37	1.32
1	B	115	HIS	CE1-NE2	5.06	1.37	1.32

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	128	GLY	N-CA-C	-7.37	101.24	112.89
1	E	103	VAL	N-CA-C	-6.64	106.66	113.10
1	C	202	GLU	CB-CG-CD	6.01	122.82	112.60
1	B	173	MET	N-CA-C	-5.79	102.47	110.35
1	F	159	PHE	CB-CA-C	5.72	119.24	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	311	THR	CA-CB-OG1	-5.67	101.10	109.60
1	D	311	THR	CA-CB-OG1	-5.58	101.24	109.60
1	D	375	ASN	CB-CA-C	-5.57	100.45	110.36
1	D	159	PHE	CB-CA-C	5.55	118.96	109.80
1	E	375	ASN	CB-CA-C	-5.55	100.48	110.36
1	A	67	THR	CA-CB-OG1	-5.49	101.36	109.60
1	C	133	ASP	CA-CB-CG	5.37	117.97	112.60
1	C	159	PHE	CB-CA-C	5.37	118.65	109.80
1	F	311	THR	CA-CB-OG1	-5.35	101.58	109.60
1	A	159	PHE	CB-CA-C	5.30	118.46	109.50
1	E	311	THR	CA-CB-OG1	-5.28	101.68	109.60
1	B	67	THR	CB-CA-C	5.19	117.82	109.41
1	E	107	THR	N-CA-C	-5.17	104.37	111.81
1	A	157	THR	O-C-N	5.15	124.64	120.83
1	A	47	LYS	N-CA-C	-5.14	101.89	109.86
1	E	93	HIS	CA-CB-CG	5.13	118.94	113.80
1	B	159	PHE	CB-CA-C	5.04	118.02	109.50

There are no chirality outliers.

There are no planarity outliers.

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	3162	0	3066	89	0
1	B	3180	0	3081	85	0
1	C	3173	0	3088	81	0
1	D	3187	0	3105	69	0
1	E	3201	0	3127	82	0
1	F	3171	0	3104	62	0
2	A	28	0	12	1	0
2	B	28	0	12	2	0
2	C	28	0	12	0	0
2	D	28	0	12	1	0
2	E	28	0	12	2	0
2	F	28	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	6	0	8	2	0
3	B	18	0	24	11	0
3	D	6	0	8	0	0
3	E	12	0	16	0	0
4	A	3	0	0	0	0
4	B	4	0	0	0	0
4	C	7	0	0	0	0
4	D	7	0	0	0	0
4	E	5	0	0	0	0
4	F	4	0	0	2	0
All	All	19314	0	18699	431	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 11.

All (431) 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:C:81:LYS:HB2	1:C:154:ILE:HD11	1.28	1.11
1:C:202:GLU:HG3	1:E:366:LEU:HD13	1.41	1.02
1:D:91:ILE:HD11	1:D:116:PRO:HG3	1.42	1.00
1:D:206:GLN:HE21	1:F:371:LEU:HD12	1.32	0.92
1:C:81:LYS:HB2	1:C:154:ILE:CD1	2.00	0.91
1:C:206:GLN:NE2	1:E:371:LEU:HA	1.84	0.91
1:A:256:GLN:HG2	1:A:276:PHE:CE1	2.06	0.90
1:E:158:ARG:HD3	1:E:211:ASN:HB3	1.52	0.89
1:B:64:ILE:CG2	3:B:504:GOL:H2	2.03	0.88
3:A:502:GOL:H11	1:D:101:THR:HA	1.56	0.86
1:D:366:LEU:HD13	1:F:202:GLU:HG2	1.55	0.86
1:D:405:ARG:O	1:D:406:ASN:C	2.19	0.85
1:C:81:LYS:CB	1:C:154:ILE:HD11	2.06	0.84
1:A:256:GLN:HG2	1:A:276:PHE:CZ	2.13	0.83
1:A:277:LEU:O	1:A:281:THR:HG23	1.82	0.80
1:D:206:GLN:HE22	1:F:371:LEU:HA	1.47	0.80
1:B:64:ILE:HG23	3:B:504:GOL:H2	1.63	0.79
1:B:277:LEU:O	1:B:281:THR:HG23	1.82	0.79
1:A:48:GLY:C	1:E:51:GLN:HE22	1.91	0.78
1:B:164:ILE:HD11	1:B:215:THR:HG22	1.64	0.78
1:C:206:GLN:HE21	1:E:371:LEU:HD12	1.48	0.78
1:B:168:LYS:HG2	1:B:221:ILE:HD11	1.63	0.78
1:D:206:GLN:NE2	1:F:371:LEU:HD12	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:277:LEU:O	1:F:281:THR:HG23	1.84	0.77
1:C:277:LEU:O	1:C:281:THR:HG23	1.84	0.76
1:C:371:LEU:HD11	1:E:213:VAL:HG21	1.66	0.76
1:D:277:LEU:O	1:D:281:THR:HG23	1.83	0.76
1:E:209:ARG:HG2	1:E:228:LEU:HD11	1.68	0.75
1:C:206:GLN:HE22	1:E:371:LEU:HA	1.50	0.75
1:B:164:ILE:CG2	1:B:221:ILE:HD12	2.18	0.74
1:D:206:GLN:NE2	1:F:371:LEU:HA	2.03	0.74
1:C:156:ALA:HB1	1:C:183:GLN:OE1	1.89	0.73
1:B:164:ILE:HG12	1:B:216:PHE:CE1	2.24	0.73
1:C:164:ILE:HD12	1:C:216:PHE:CE1	2.23	0.73
1:C:371:LEU:HA	1:E:206:GLN:NE2	2.03	0.72
1:A:201:ARG:NH2	3:A:502:GOL:O2	2.23	0.72
1:B:164:ILE:CD1	1:B:215:THR:HG22	2.21	0.70
1:F:168:LYS:O	1:F:172:ILE:HG23	1.92	0.70
1:D:213:VAL:HG21	1:F:371:LEU:CD2	2.23	0.69
1:B:64:ILE:HG22	3:B:504:GOL:H2	1.74	0.69
1:E:205:LEU:O	1:E:209:ARG:HG3	1.93	0.69
1:D:371:LEU:HD12	1:F:206:GLN:HE22	1.57	0.69
1:E:106:LYS:HD2	1:E:106:LYS:N	2.07	0.69
1:B:156:ALA:HB1	1:B:183:GLN:OE1	1.94	0.68
1:A:256:GLN:CG	1:A:276:PHE:CE1	2.77	0.68
1:E:106:LYS:HE2	1:E:128:GLY:H	1.59	0.67
1:D:366:LEU:HD13	1:F:202:GLU:CG	2.25	0.67
1:E:61:LEU:O	1:E:64:ILE:HG22	1.94	0.66
1:B:57:VAL:HG11	1:B:287:ALA:HB2	1.77	0.66
1:A:57:VAL:HG11	1:A:287:ALA:HB2	1.77	0.66
1:B:264:ASN:HB3	1:B:270:ILE:HD11	1.75	0.66
1:A:264:ASN:HB3	1:A:270:ILE:HD11	1.76	0.66
1:A:405:ARG:O	1:A:406:ASN:CB	2.44	0.66
1:A:164:ILE:HD12	1:A:216:PHE:HD1	1.61	0.65
1:D:154:ILE:HD11	1:D:182:THR:HG21	1.77	0.65
1:E:86:ASN:HD21	1:E:94:GLU:HB2	1.61	0.65
1:B:164:ILE:HG23	1:B:221:ILE:HD12	1.79	0.65
1:E:258:PHE:CZ	1:E:262:LEU:HD21	2.31	0.65
1:B:375:ASN:HD22	1:B:378:ARG:H	1.44	0.64
1:F:195:LYS:HB3	1:F:198:THR:HG22	1.78	0.64
1:A:252:VAL:O	1:A:256:GLN:NE2	2.31	0.64
1:C:252:VAL:O	1:C:256:GLN:NE2	2.31	0.64
1:D:258:PHE:CZ	1:D:262:LEU:HD21	2.33	0.63
1:A:127:PRO:HG2	1:A:139:TYR:HE1	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:PHE:CZ	1:A:138:THR:HG22	2.33	0.63
1:C:195:LYS:HB3	1:C:198:THR:HG22	1.79	0.63
1:F:252:VAL:O	1:F:256:GLN:NE2	2.31	0.63
1:C:371:LEU:HD23	1:E:206:GLN:HE21	1.64	0.63
1:F:169:ALA:O	1:F:172:ILE:HG12	1.97	0.63
1:D:137:LYS:HD3	1:D:137:LYS:H	1.64	0.62
1:D:264:ASN:HB3	1:D:270:ILE:HD11	1.81	0.62
1:B:77:THR:OG1	1:B:101:THR:HG21	1.99	0.62
1:D:371:LEU:HD12	1:F:206:GLN:NE2	2.14	0.62
1:D:89:ARG:HD2	1:D:123:PHE:HD2	1.65	0.62
1:A:405:ARG:O	1:A:406:ASN:HB3	1.99	0.62
1:C:371:LEU:HA	1:E:206:GLN:HE22	1.64	0.62
1:D:89:ARG:HD2	1:D:123:PHE:CD2	2.35	0.62
1:B:63:GLU:O	1:B:67:THR:HG22	2.00	0.62
1:F:82:SER:HB2	4:F:601:HOH:O	1.99	0.62
1:B:94:GLU:OE2	1:C:198:THR:HG22	2.00	0.62
1:D:252:VAL:O	1:D:256:GLN:NE2	2.32	0.62
1:F:184:VAL:HG21	1:F:228:LEU:HB3	1.81	0.61
1:B:127:PRO:HG2	1:B:139:TYR:HE1	1.65	0.61
1:E:252:VAL:O	1:E:256:GLN:NE2	2.32	0.61
1:C:81:LYS:CB	1:C:154:ILE:CD1	2.73	0.61
1:E:182:THR:HG22	1:E:229:ILE:HD11	1.83	0.61
1:B:164:ILE:HG12	1:B:216:PHE:HE1	1.62	0.61
1:E:135:GLN:HB2	1:E:138:THR:OG1	2.01	0.61
1:A:48:GLY:C	1:E:51:GLN:NE2	2.59	0.61
1:A:252:VAL:HG13	1:A:253:PHE:CD2	2.37	0.60
1:A:195:LYS:HB3	1:A:198:THR:HG22	1.82	0.60
1:A:223:GLU:N	1:A:224:PRO:HD3	2.16	0.60
1:A:184:VAL:HG21	1:A:228:LEU:HB3	1.84	0.60
1:C:184:VAL:HG21	1:C:228:LEU:HB3	1.83	0.60
1:E:63:GLU:O	1:E:67:THR:HG23	2.02	0.60
1:E:250:LEU:O	1:E:255:ARG:NH1	2.35	0.60
1:D:184:VAL:HG21	1:D:228:LEU:HB3	1.83	0.59
1:F:169:ALA:HA	1:F:172:ILE:HD13	1.85	0.59
1:C:25:GLU:OE1	1:C:30:ILE:HD11	2.02	0.59
1:D:63:GLU:O	1:D:67:THR:HG23	2.03	0.59
1:F:250:LEU:O	1:F:255:ARG:NH1	2.35	0.59
1:B:164:ILE:HD11	1:B:215:THR:CG2	2.33	0.59
1:C:250:LEU:O	1:C:255:ARG:NH1	2.35	0.59
1:C:371:LEU:CD1	1:E:213:VAL:HG21	2.31	0.59
1:F:309:TYR:HB3	1:F:391:VAL:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:TYR:HB3	1:D:391:VAL:HG21	1.84	0.59
1:D:206:GLN:NE2	1:F:372:LEU:H	2.01	0.58
1:A:164:ILE:HD12	1:A:216:PHE:CD1	2.38	0.58
1:C:366:LEU:C	1:C:366:LEU:HD23	2.29	0.58
1:A:64:ILE:HD13	1:A:253:PHE:HD1	1.69	0.58
1:E:195:LYS:HB3	1:E:198:THR:HG22	1.85	0.58
1:B:250:LEU:O	1:B:255:ARG:NH1	2.37	0.58
1:B:184:VAL:HG21	1:B:228:LEU:HB3	1.86	0.58
1:C:63:GLU:O	1:C:67:THR:HG23	2.03	0.58
1:D:250:LEU:O	1:D:255:ARG:NH1	2.36	0.58
1:D:145:PHE:HE2	1:D:175:LYS:HG3	1.66	0.58
1:E:309:TYR:HB3	1:E:391:VAL:HG21	1.84	0.58
1:C:309:TYR:HB3	1:C:391:VAL:HG21	1.86	0.57
1:F:110:ARG:HB3	1:F:143:MET:CE	2.34	0.57
1:A:366:LEU:C	1:A:366:LEU:HD23	2.28	0.57
1:B:152:ILE:HG22	1:B:154:ILE:HG13	1.86	0.57
1:F:63:GLU:O	1:F:67:THR:HG23	2.03	0.57
1:B:366:LEU:C	1:B:366:LEU:HD23	2.29	0.57
1:E:110:ARG:HB3	1:E:143:MET:CE	2.34	0.57
1:A:256:GLN:CG	1:A:276:PHE:CZ	2.87	0.57
1:E:76:GLU:OE2	1:E:106:LYS:HG3	2.04	0.57
1:E:266:THR:HG22	1:E:268:SER:H	1.70	0.57
1:F:80:GLY:N	2:F:501:GDP:O3B	2.37	0.57
1:E:135:GLN:HB2	1:E:138:THR:HG1	1.69	0.57
1:E:189:ARG:NH1	1:E:192:GLU:OE1	2.38	0.57
1:F:266:THR:HG22	1:F:268:SER:H	1.70	0.57
1:F:335:VAL:HA	1:F:338:MET:HE3	1.87	0.57
1:B:264:ASN:HB3	1:B:270:ILE:CD1	2.35	0.56
1:B:168:LYS:CG	1:B:221:ILE:HD11	2.34	0.56
1:C:266:THR:HG22	1:C:268:SER:H	1.70	0.56
1:C:168:LYS:O	1:C:172:ILE:HG23	2.04	0.56
1:A:63:GLU:O	1:A:67:THR:HG23	2.06	0.56
1:A:108:LYS:HD3	1:A:108:LYS:H	1.70	0.56
1:B:195:LYS:HB3	1:B:198:THR:HG22	1.86	0.56
1:A:152:ILE:HG22	1:A:154:ILE:HG13	1.88	0.56
1:C:206:GLN:HE21	1:E:371:LEU:HA	1.69	0.56
1:A:23:LEU:O	1:A:27:GLU:HG3	2.06	0.56
1:D:266:THR:HG22	1:D:268:SER:H	1.71	0.56
1:B:223:GLU:N	1:B:224:PRO:HD3	2.21	0.55
1:F:152:ILE:HG22	1:F:154:ILE:HG13	1.87	0.55
2:E:501:GDP:O2A	2:E:501:GDP:H3'	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ASN:HB3	1:A:270:ILE:CD1	2.37	0.55
1:A:164:ILE:HD13	1:A:219:ASN:HB2	1.88	0.55
1:B:64:ILE:HG23	3:B:504:GOL:C2	2.36	0.55
1:D:110:ARG:HB3	1:D:143:MET:CE	2.37	0.55
1:D:270:ILE:HG22	1:D:392:THR:HG23	1.88	0.55
1:B:266:THR:HG22	1:B:268:SER:H	1.72	0.54
1:C:169:ALA:O	1:C:172:ILE:HG12	2.08	0.54
1:A:266:THR:HG22	1:A:268:SER:H	1.72	0.54
1:D:335:VAL:HA	1:D:338:MET:HE3	1.88	0.54
1:A:110:ARG:HB3	1:A:143:MET:CE	2.38	0.54
1:A:255:ARG:HG3	1:A:256:GLN:OE1	2.07	0.54
1:B:335:VAL:HA	1:B:338:MET:HE3	1.87	0.54
1:C:110:ARG:HB3	1:C:143:MET:CE	2.38	0.54
1:E:335:VAL:HA	1:E:338:MET:HE3	1.89	0.54
1:B:110:ARG:HB3	1:B:143:MET:CE	2.38	0.54
1:A:335:VAL:HA	1:A:338:MET:HE3	1.88	0.53
1:B:65:ASP:HA	3:B:504:GOL:O1	2.08	0.53
1:E:159:PHE:O	1:E:215:THR:HG21	2.08	0.53
1:B:183:GLN:HG2	2:B:501:GDP:C5	2.43	0.53
1:C:335:VAL:HA	1:C:338:MET:HE3	1.90	0.53
1:D:239:PHE:HB3	1:D:240:PRO:HD3	1.90	0.53
1:F:183:GLN:HG3	2:F:501:GDP:C5	2.43	0.53
1:C:79:SER:HA	1:C:156:ALA:HB2	1.90	0.53
1:D:209:ARG:O	1:D:213:VAL:HG23	2.09	0.53
1:A:262:LEU:HB2	1:A:263:PRO:HD2	1.91	0.53
1:A:293:PHE:C	1:E:375:ASN:HD21	2.17	0.53
1:A:100:HIS:O	1:A:101:THR:CB	2.57	0.52
1:C:209:ARG:O	1:C:213:VAL:HG23	2.09	0.52
1:F:209:ARG:O	1:F:213:VAL:HG23	2.09	0.52
1:B:164:ILE:HD12	1:B:219:ASN:ND2	2.24	0.52
1:B:41:ILE:O	1:B:45:MET:HG2	2.10	0.52
1:B:107:THR:HG23	1:B:109:GLU:HB3	1.91	0.52
1:A:107:THR:C	1:A:109:GLU:H	2.17	0.52
1:A:134:PHE:HZ	1:A:138:THR:HG22	1.74	0.52
1:E:239:PHE:HB3	1:E:240:PRO:HD3	1.91	0.51
1:B:23:LEU:O	1:B:27:GLU:HG3	2.10	0.51
1:C:169:ALA:HA	1:C:172:ILE:HD13	1.91	0.51
1:A:38:ILE:HD13	1:A:378:ARG:HH22	1.75	0.51
1:C:262:LEU:HB2	1:C:263:PRO:HD2	1.91	0.51
1:B:371:LEU:N	3:B:503:GOL:H31	2.26	0.51
1:C:366:LEU:HD23	1:C:367:ALA:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:LEU:HD21	1:A:258:PHE:CD1	2.46	0.51
1:B:274:ARG:HH21	1:B:275:ASN:HD21	1.59	0.51
1:C:152:ILE:HG22	1:C:154:ILE:HG23	1.93	0.51
1:C:154:ILE:HG22	1:C:180:VAL:HB	1.92	0.51
1:A:57:VAL:CG1	1:A:287:ALA:HB2	2.40	0.50
1:F:262:LEU:HB2	1:F:263:PRO:HD2	1.92	0.50
1:E:93:HIS:CE1	1:E:95:GLU:HA	2.47	0.50
1:A:120:ASN:OD1	1:A:121:VAL:HG23	2.10	0.50
1:B:57:VAL:CG1	1:B:287:ALA:HB2	2.40	0.50
1:A:164:ILE:HD12	1:A:216:PHE:HA	1.93	0.50
1:F:19:PHE:CD1	1:F:283:LEU:HD21	2.47	0.50
1:B:260:PHE:HZ	1:B:277:LEU:HD21	1.76	0.50
1:F:239:PHE:HB3	1:F:240:PRO:HD3	1.93	0.50
1:B:64:ILE:CG2	3:B:504:GOL:C2	2.84	0.50
1:B:239:PHE:HB3	1:B:240:PRO:HD3	1.93	0.50
1:E:105:ASP:C	1:E:107:THR:N	2.69	0.50
1:B:164:ILE:HG22	1:B:221:ILE:HD12	1.92	0.50
1:B:371:LEU:H	3:B:503:GOL:H31	1.77	0.49
1:E:61:LEU:HA	1:E:64:ILE:HG22	1.94	0.49
1:A:274:ARG:HH21	1:A:275:ASN:HD21	1.60	0.49
1:B:331:GLN:O	1:B:334:GLN:HG2	2.12	0.49
1:C:206:GLN:NE2	1:E:372:LEU:H	2.11	0.49
1:B:270:ILE:HG22	1:B:392:THR:HG23	1.95	0.49
1:F:214:ASN:HA	1:F:217:ARG:HG3	1.94	0.49
1:A:331:GLN:O	1:A:334:GLN:HG2	2.13	0.49
1:A:156:ALA:HB1	1:A:183:GLN:HG3	1.94	0.49
1:A:270:ILE:HG22	1:A:392:THR:HG23	1.94	0.49
1:C:239:PHE:HB3	1:C:240:PRO:HD3	1.93	0.49
1:E:270:ILE:HG22	1:E:392:THR:HG23	1.95	0.49
1:A:239:PHE:HB3	1:A:240:PRO:HD3	1.95	0.48
1:B:192:GLU:HG2	1:B:199:PHE:CE2	2.48	0.48
1:E:158:ARG:CD	1:E:211:ASN:HB3	2.35	0.48
1:B:262:LEU:HB2	1:B:263:PRO:HD2	1.95	0.48
1:C:106:LYS:O	1:C:109:GLU:HB2	2.13	0.48
1:C:206:GLN:NE2	1:E:371:LEU:HD12	2.21	0.48
1:E:110:ARG:HG3	1:E:110:ARG:O	2.13	0.48
1:A:295:LEU:O	1:E:375:ASN:OD1	2.30	0.48
1:C:181:ARG:NH2	1:C:187:ASP:OD2	2.44	0.48
1:A:192:GLU:HG2	1:A:199:PHE:CE2	2.48	0.48
1:C:371:LEU:HD23	1:E:206:GLN:NE2	2.27	0.48
1:D:156:ALA:HB1	1:D:183:GLN:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:LEU:HD23	1:B:367:ALA:N	2.28	0.48
1:D:110:ARG:O	1:D:110:ARG:HG3	2.14	0.48
1:F:192:GLU:HG2	1:F:199:PHE:CE2	2.49	0.48
1:A:260:PHE:HZ	1:A:277:LEU:HD21	1.79	0.48
1:B:252:VAL:O	1:B:256:GLN:HG2	2.14	0.48
1:A:361:ASN:ND2	1:A:379:GLU:HG3	2.29	0.48
1:B:191:GLU:OE1	1:B:191:GLU:HA	2.14	0.47
1:C:89:ARG:NH1	1:C:91:ILE:HD11	2.29	0.47
1:D:213:VAL:HG21	1:F:371:LEU:HD22	1.95	0.47
1:E:76:GLU:HA	1:E:106:LYS:HZ3	1.78	0.47
1:E:170:ILE:HG23	1:E:175:LYS:HB3	1.96	0.47
1:D:264:ASN:HB3	1:D:270:ILE:CD1	2.44	0.47
1:F:110:ARG:O	1:F:110:ARG:HG3	2.14	0.47
1:B:257:ASN:ND2	3:B:504:GOL:H11	2.28	0.47
1:C:202:GLU:CD	1:E:366:LEU:HB2	2.38	0.47
1:A:129:THR:OG1	1:A:162:ASN:HB3	2.15	0.47
1:C:274:ARG:HH21	1:C:275:ASN:HD21	1.62	0.47
1:E:19:PHE:CD1	1:E:283:LEU:HD11	2.50	0.47
1:B:170:ILE:O	1:B:173:MET:O	2.32	0.47
1:B:164:ILE:HD12	1:B:219:ASN:HD22	1.80	0.47
1:A:52:GLU:O	1:A:56:THR:HG23	2.15	0.47
1:C:81:LYS:CA	1:C:154:ILE:CD1	2.93	0.47
1:F:89:ARG:NH1	1:F:91:ILE:HD11	2.30	0.47
1:A:64:ILE:HD13	1:A:253:PHE:CD1	2.48	0.46
1:D:89:ARG:CZ	1:D:113:TYR:HB3	2.45	0.46
1:F:76:GLU:OE2	1:F:160:LYS:NZ	2.48	0.46
1:C:19:PHE:CD1	1:C:283:LEU:HD11	2.49	0.46
1:C:81:LYS:NZ	1:C:126:LEU:O	2.48	0.46
1:C:340:LYS:C	1:C:342:PRO:HD2	2.41	0.46
1:D:340:LYS:C	1:D:342:PRO:HD2	2.41	0.46
1:E:340:LYS:C	1:E:342:PRO:HD2	2.41	0.46
1:A:191:GLU:OE1	1:A:191:GLU:HA	2.16	0.46
1:C:110:ARG:O	1:C:110:ARG:HG3	2.15	0.46
1:E:195:LYS:HB3	1:E:198:THR:CG2	2.46	0.46
1:F:340:LYS:C	1:F:342:PRO:HD2	2.41	0.46
1:C:331:GLN:O	1:C:334:GLN:HG2	2.14	0.46
1:B:375:ASN:ND2	1:B:378:ARG:H	2.13	0.46
1:B:42:GLU:O	1:B:46:LYS:HG2	2.16	0.46
1:A:366:LEU:HD23	1:A:367:ALA:N	2.30	0.46
1:B:375:ASN:HD22	1:B:378:ARG:N	2.13	0.46
1:D:174:LYS:HB2	1:D:174:LYS:HE3	1.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LYS:C	1:A:342:PRO:HD2	2.41	0.46
1:F:195:LYS:HB3	1:F:198:THR:CG2	2.44	0.46
1:B:216:PHE:HB3	1:B:221:ILE:HG22	1.97	0.46
1:D:60:MET:HE3	1:D:60:MET:HB2	1.81	0.46
1:E:105:ASP:O	1:E:108:LYS:HB3	2.15	0.46
1:F:174:LYS:HE2	1:F:174:LYS:HB3	1.53	0.46
1:B:52:GLU:O	1:B:56:THR:HG23	2.16	0.45
1:C:106:LYS:O	1:C:109:GLU:N	2.48	0.45
1:B:118:MET:HE1	1:B:261:SER:N	2.31	0.45
1:A:161:LYS:O	1:A:164:ILE:HG22	2.16	0.45
1:B:81:LYS:NZ	1:B:126:LEU:O	2.50	0.45
1:C:319:SER:HA	1:C:322:ARG:HE	1.81	0.45
1:F:81:LYS:NZ	1:F:126:LEU:O	2.50	0.45
1:A:51:GLN:HE21	1:E:51:GLN:H	1.64	0.45
1:A:371:LEU:HD13	1:A:371:LEU:HA	1.76	0.45
1:E:54:ASN:HD21	1:E:58:ARG:HE	1.65	0.45
1:A:81:LYS:NZ	1:A:126:LEU:O	2.50	0.45
1:A:89:ARG:NH1	1:A:91:ILE:HD11	2.31	0.45
1:A:195:LYS:HB3	1:A:198:THR:CG2	2.45	0.45
1:B:94:GLU:OE2	1:C:198:THR:CG2	2.64	0.45
1:F:274:ARG:HH21	1:F:275:ASN:HD21	1.64	0.45
1:B:340:LYS:C	1:B:342:PRO:HD2	2.42	0.45
1:D:91:ILE:O	1:D:91:ILE:HG22	2.17	0.45
1:B:202:GLU:HG3	1:B:206:GLN:HE21	1.81	0.45
1:B:89:ARG:NH1	1:B:91:ILE:HD11	2.32	0.44
1:C:191:GLU:HA	1:C:191:GLU:OE1	2.16	0.44
1:C:195:LYS:HB3	1:C:198:THR:CG2	2.46	0.44
1:F:42:GLU:O	1:F:46:LYS:HG2	2.16	0.44
1:E:52:GLU:O	1:E:56:THR:HG23	2.16	0.44
1:E:80:GLY:N	2:E:501:GDP:O3B	2.49	0.44
1:C:81:LYS:HA	1:C:154:ILE:CD1	2.47	0.44
1:D:52:GLU:O	1:D:56:THR:HG23	2.17	0.44
1:D:154:ILE:HD11	1:D:182:THR:CG2	2.43	0.44
1:B:195:LYS:HB3	1:B:198:THR:CG2	2.46	0.44
1:C:378:ARG:HD3	1:C:382:TYR:OH	2.17	0.44
1:F:353:ILE:O	1:F:357:LEU:HG	2.18	0.44
1:C:52:GLU:O	1:C:56:THR:HG23	2.18	0.44
1:C:353:ILE:O	1:C:357:LEU:HG	2.18	0.44
1:D:258:PHE:CE2	1:D:262:LEU:HD21	2.52	0.44
1:A:181:ARG:NH2	1:A:187:ASP:OD2	2.46	0.44
1:A:42:GLU:O	1:A:46:LYS:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:ARG:HD3	1:C:382:TYR:CZ	2.53	0.44
1:D:378:ARG:HD3	1:D:382:TYR:OH	2.18	0.44
1:B:181:ARG:NH2	1:B:187:ASP:OD2	2.47	0.44
1:D:91:ILE:HG22	1:D:93:HIS:O	2.17	0.44
1:A:134:PHE:HE2	1:A:139:TYR:HA	1.83	0.43
1:A:252:VAL:O	1:A:255:ARG:HG2	2.18	0.43
1:C:127:PRO:O	1:C:139:TYR:OH	2.35	0.43
1:E:258:PHE:CE2	1:E:262:LEU:HD21	2.52	0.43
1:C:353:ILE:HG23	1:C:354:GLN:OE1	2.18	0.43
1:F:52:GLU:O	1:F:56:THR:HG23	2.18	0.43
1:A:110:ARG:O	1:A:110:ARG:HG3	2.17	0.43
1:A:225:PRO:HB2	1:A:227:PHE:CE1	2.52	0.43
1:B:110:ARG:O	1:B:110:ARG:HG3	2.17	0.43
1:E:61:LEU:O	1:E:64:ILE:CG2	2.65	0.43
1:E:105:ASP:C	1:E:107:THR:H	2.25	0.43
1:F:378:ARG:HD3	1:F:382:TYR:OH	2.17	0.43
1:B:38:ILE:HD13	1:B:378:ARG:HH22	1.83	0.43
1:B:47:LYS:HB2	1:B:47:LYS:HE2	1.61	0.43
1:B:256:GLN:HB2	3:B:504:GOL:C3	2.48	0.43
1:D:15:LEU:HD23	1:D:15:LEU:HA	1.88	0.43
1:E:101:THR:HA	1:E:104:THR:HG23	2.00	0.43
1:A:15:LEU:HD23	1:A:15:LEU:HA	1.89	0.43
1:F:139:TYR:O	1:F:143:MET:HG2	2.19	0.43
1:A:134:PHE:CZ	1:A:138:THR:CG2	3.02	0.43
1:B:251:PRO:O	1:B:255:ARG:HB2	2.19	0.43
1:C:32:ILE:HG22	1:C:33:ILE:O	2.19	0.43
1:D:104:THR:C	1:D:106:LYS:H	2.26	0.43
1:D:172:ILE:C	1:D:174:LYS:H	2.26	0.43
1:A:157:THR:OG1	1:A:158:ARG:N	2.52	0.43
1:A:209:ARG:O	1:A:213:VAL:HG23	2.19	0.43
1:D:258:PHE:O	1:D:262:LEU:HG	2.18	0.43
1:D:353:ILE:O	1:D:357:LEU:HG	2.19	0.43
1:C:270:ILE:HG22	1:C:392:THR:HG23	2.01	0.43
1:C:351:GLU:HG3	1:C:355:GLU:OE2	2.19	0.43
1:E:174:LYS:HE3	1:E:174:LYS:HB2	1.53	0.43
2:B:501:GDP:H3'	2:B:501:GDP:O2A	2.18	0.43
1:C:139:TYR:O	1:C:143:MET:HG2	2.19	0.43
1:E:15:LEU:HD23	1:E:15:LEU:HA	1.86	0.43
1:D:274:ARG:HH21	1:D:275:ASN:HD21	1.65	0.42
1:A:183:GLN:HA	2:A:501:GDP:C6	2.53	0.42
1:E:120:ASN:H	1:E:120:ASN:HD22	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:TYR:O	1:B:143:MET:HG2	2.19	0.42
1:A:69:LEU:HD23	1:A:121:VAL:HG13	2.01	0.42
1:A:241:VAL:HG23	1:D:97:GLY:H	1.85	0.42
1:E:61:LEU:C	1:E:64:ILE:HG22	2.44	0.42
1:E:274:ARG:HH21	1:E:275:ASN:HD21	1.65	0.42
1:F:60:MET:HB2	1:F:60:MET:HE3	1.87	0.42
1:F:191:GLU:OE1	1:F:191:GLU:HA	2.18	0.42
1:A:139:TYR:O	1:A:143:MET:HG2	2.19	0.42
1:D:259:MET:HE3	1:D:259:MET:HB3	1.91	0.42
1:E:353:ILE:O	1:E:357:LEU:HG	2.20	0.42
1:A:107:THR:C	1:A:109:GLU:N	2.77	0.42
1:B:225:PRO:HB2	1:B:227:PHE:CE1	2.53	0.42
1:C:318:ALA:O	1:C:322:ARG:HG3	2.20	0.42
1:D:371:LEU:HA	1:F:206:GLN:HE22	1.84	0.42
1:E:209:ARG:O	1:E:213:VAL:HG23	2.19	0.42
1:E:258:PHE:O	1:E:262:LEU:HG	2.19	0.42
1:C:60:MET:HB2	1:C:60:MET:HE3	1.87	0.42
1:D:145:PHE:CE2	1:D:173:MET:HB3	2.55	0.42
1:E:45:MET:HE1	1:E:290:LEU:HD22	2.02	0.42
1:E:58:ARG:CZ	1:E:287:ALA:HB1	2.49	0.42
1:F:45:MET:HE2	1:F:50:ILE:HG12	2.02	0.42
1:A:353:ILE:O	1:A:357:LEU:HG	2.20	0.42
1:C:67:THR:HG21	1:C:253:PHE:HB3	2.02	0.42
1:D:80:GLY:N	2:D:501:GDP:O3B	2.52	0.42
1:D:81:LYS:NZ	1:D:126:LEU:O	2.52	0.42
1:D:120:ASN:H	1:D:120:ASN:HD22	1.67	0.42
1:E:81:LYS:NZ	1:E:126:LEU:O	2.52	0.42
1:F:67:THR:HG21	1:F:253:PHE:HB3	2.02	0.42
1:A:48:GLY:CA	1:E:51:GLN:NE2	2.82	0.42
1:A:131:SER:O	1:A:134:PHE:HB2	2.20	0.42
1:C:25:GLU:O	1:C:30:ILE:HG12	2.19	0.42
1:D:32:ILE:HG22	1:D:33:ILE:O	2.20	0.42
1:D:104:THR:C	1:D:106:LYS:N	2.76	0.42
1:D:139:TYR:O	1:D:143:MET:HG2	2.20	0.42
1:A:127:PRO:HG2	1:A:139:TYR:CE1	2.50	0.41
1:B:94:GLU:OE1	1:C:197:GLN:HG2	2.20	0.41
1:E:139:TYR:O	1:E:143:MET:HG2	2.20	0.41
1:F:183:GLN:HG3	2:F:501:GDP:C4	2.55	0.41
1:A:64:ILE:CD1	1:A:253:PHE:HD1	2.33	0.41
1:A:223:GLU:N	1:A:224:PRO:CD	2.83	0.41
1:B:353:ILE:O	1:B:357:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:SER:N	1:C:342:PRO:HD2	2.34	0.41
1:E:259:MET:HE3	1:E:259:MET:HB3	1.90	0.41
1:E:341:SER:N	1:E:342:PRO:HD2	2.35	0.41
1:F:15:LEU:HD12	1:F:15:LEU:HA	1.87	0.41
1:A:33:ILE:H	1:D:321:GLN:HE22	1.68	0.41
1:F:172:ILE:C	1:F:174:LYS:H	2.28	0.41
1:F:270:ILE:HG22	1:F:392:THR:HG23	2.03	0.41
1:F:378:ARG:HD3	1:F:382:TYR:CZ	2.55	0.41
1:B:209:ARG:O	1:B:213:VAL:HG23	2.21	0.41
1:C:100:HIS:O	1:C:101:THR:CB	2.68	0.41
1:A:341:SER:N	1:A:342:PRO:HD2	2.36	0.41
1:B:198:THR:HG22	1:C:94:GLU:OE2	2.21	0.41
1:D:341:SER:N	1:D:342:PRO:HD2	2.36	0.41
1:E:182:THR:HG22	1:E:229:ILE:CD1	2.51	0.41
1:E:268:SER:OG	1:E:272:LYS:NZ	2.53	0.41
1:F:120:ASN:HD21	1:F:257:ASN:ND2	2.19	0.41
1:A:293:PHE:O	1:E:375:ASN:ND2	2.53	0.41
1:C:259:MET:HE3	1:C:259:MET:HB3	1.90	0.41
1:F:32:ILE:HG22	1:F:33:ILE:O	2.21	0.41
1:B:15:LEU:HD23	1:B:15:LEU:HA	1.91	0.40
1:C:164:ILE:HD13	1:C:164:ILE:N	2.36	0.40
1:D:45:MET:HE1	1:D:290:LEU:HD22	2.03	0.40
1:D:135:GLN:HB2	1:D:138:THR:HB	2.03	0.40
1:D:251:PRO:O	1:D:255:ARG:HB2	2.21	0.40
1:D:268:SER:OG	1:D:272:LYS:NZ	2.54	0.40
1:E:400:LYS:O	1:E:404:LEU:HD13	2.21	0.40
1:F:268:SER:O	1:F:272:LYS:HG3	2.21	0.40
1:B:118:MET:HE1	1:B:260:PHE:HB3	2.03	0.40
1:B:341:SER:N	1:B:342:PRO:HD2	2.36	0.40
1:C:120:ASN:HD22	1:C:120:ASN:H	1.68	0.40
1:E:97:GLY:C	1:E:99:ALA:H	2.29	0.40
1:E:375:ASN:HB2	1:E:378:ARG:H	1.85	0.40
1:F:341:SER:N	1:F:342:PRO:HD2	2.36	0.40
1:D:375:ASN:HB2	1:D:378:ARG:H	1.86	0.40
1:F:82:SER:CB	4:F:601:HOH:O	2.62	0.40
1:A:400:LYS:O	1:A:404:LEU:HD13	2.22	0.40
1:B:250:LEU:O	1:B:255:ARG:CZ	2.70	0.40
1:B:371:LEU:HB2	3:B:503:GOL:H31	2.03	0.40
1:C:268:SER:O	1:C:272:LYS:HG3	2.22	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	389/416 (94%)	376 (97%)	13 (3%)	0	100	100
1	B	395/416 (95%)	378 (96%)	16 (4%)	1 (0%)	36	55
1	C	389/416 (94%)	378 (97%)	11 (3%)	0	100	100
1	D	395/416 (95%)	379 (96%)	16 (4%)	0	100	100
1	E	395/416 (95%)	382 (97%)	13 (3%)	0	100	100
1	F	389/416 (94%)	378 (97%)	11 (3%)	0	100	100
All	All	2352/2496 (94%)	2271 (97%)	80 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	108	LYS

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	345/382 (90%)	328 (95%)	17 (5%)	22	45
1	B	346/382 (91%)	328 (95%)	18 (5%)	21	42
1	C	348/382 (91%)	334 (96%)	14 (4%)	28	54
1	D	349/382 (91%)	330 (95%)	19 (5%)	20	41
1	E	352/382 (92%)	330 (94%)	22 (6%)	16	34
1	F	347/382 (91%)	329 (95%)	18 (5%)	21	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2087/2292 (91%)	1979 (95%)	108 (5%)	21	42

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	108	LYS
1	A	122	VAL
1	A	166	LEU
1	A	173	MET
1	A	184	VAL
1	A	192	GLU
1	A	256	GLN
1	A	261	SER
1	A	269	VAL
1	A	283	LEU
1	A	290	LEU
1	A	307	LYS
1	A	323	LEU
1	A	325	ARG
1	A	334	GLN
1	A	371	LEU
1	B	15	LEU
1	B	47	LYS
1	B	67	THR
1	B	69	LEU
1	B	100	HIS
1	B	122	VAL
1	B	175	LYS
1	B	184	VAL
1	B	192	GLU
1	B	221	ILE
1	B	269	VAL
1	B	283	LEU
1	B	296	GLU
1	B	307	LYS
1	B	323	LEU
1	B	325	ARG
1	B	334	GLN
1	B	375	ASN
1	C	107	THR
1	C	122	VAL

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Mol	Chain	Res	Type
1	C	164	ILE
1	C	172	ILE
1	C	184	VAL
1	C	203	LYS
1	C	256	GLN
1	C	261	SER
1	C	269	VAL
1	C	278	ARG
1	C	283	LEU
1	C	307	LYS
1	C	323	LEU
1	C	355	GLU
1	D	18	SER
1	D	108	LYS
1	D	122	VAL
1	D	137	LYS
1	D	145	PHE
1	D	164	ILE
1	D	174	LYS
1	D	184	VAL
1	D	192	GLU
1	D	198	THR
1	D	203	LYS
1	D	255	ARG
1	D	256	GLN
1	D	261	SER
1	D	269	VAL
1	D	296	GLU
1	D	307	LYS
1	D	323	LEU
1	D	371	LEU
1	E	18	SER
1	E	101	THR
1	E	103	VAL
1	E	106	LYS
1	E	107	THR
1	E	122	VAL
1	E	145	PHE
1	E	164	ILE
1	E	173	MET
1	E	174	LYS
1	E	175	LYS

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Mol	Chain	Res	Type
1	E	209	ARG
1	E	223	GLU
1	E	256	GLN
1	E	269	VAL
1	E	283	LEU
1	E	296	GLU
1	E	307	LYS
1	E	323	LEU
1	E	350	GLU
1	E	371	LEU
1	E	393	GLU
1	F	47	LYS
1	F	64	ILE
1	F	117	LYS
1	F	122	VAL
1	F	164	ILE
1	F	172	ILE
1	F	174	LYS
1	F	183	GLN
1	F	192	GLU
1	F	202	GLU
1	F	256	GLN
1	F	261	SER
1	F	269	VAL
1	F	283	LEU
1	F	296	GLU
1	F	307	LYS
1	F	323	LEU
1	F	371	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	206	GLN
1	A	233	ASN
1	A	236	HIS
1	A	275	ASN
1	B	100	HIS
1	B	206	GLN
1	B	236	HIS
1	B	256	GLN

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Mol	Chain	Res	Type
1	B	257	ASN
1	B	275	ASN
1	B	375	ASN
1	C	44	ASN
1	C	49	ASN
1	C	120	ASN
1	C	135	GLN
1	C	206	GLN
1	C	231	ASN
1	C	233	ASN
1	C	236	HIS
1	C	256	GLN
1	C	257	ASN
1	C	275	ASN
1	C	331	GLN
1	D	54	ASN
1	D	86	ASN
1	D	120	ASN
1	D	135	GLN
1	D	162	ASN
1	D	206	GLN
1	D	219	ASN
1	D	236	HIS
1	D	257	ASN
1	D	275	ASN
1	D	321	GLN
1	E	44	ASN
1	E	51	GLN
1	E	54	ASN
1	E	86	ASN
1	E	93	HIS
1	E	120	ASN
1	E	206	GLN
1	E	219	ASN
1	E	233	ASN
1	E	236	HIS
1	E	256	GLN
1	E	257	ASN
1	E	275	ASN
1	F	44	ASN
1	F	51	GLN
1	F	120	ASN

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Mol	Chain	Res	Type
1	F	206	GLN
1	F	219	ASN
1	F	236	HIS
1	F	256	GLN
1	F	275	ASN

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 ⓘ

13 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	C	501	-	29,30,30	0.61	0	45,47,47	0.75	1 (2%)
2	GDP	D	501	-	29,30,30	0.58	0	45,47,47	0.57	0
3	GOL	B	504	-	5,5,5	0.05	0	5,5,5	0.47	0
3	GOL	D	502	-	5,5,5	0.18	0	5,5,5	0.56	0
2	GDP	A	501	-	29,30,30	0.45	0	45,47,47	0.80	2 (4%)
3	GOL	A	502	-	5,5,5	0.16	0	5,5,5	0.42	0
2	GDP	B	501	-	29,30,30	0.44	0	45,47,47	0.95	2 (4%)
3	GOL	E	503	-	5,5,5	0.20	0	5,5,5	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GDP	F	501	-	29,30,30	0.63	0	45,47,47	0.83	1 (2%)
2	GDP	E	501	-	29,30,30	0.64	1 (3%)	45,47,47	0.67	0
3	GOL	B	502	-	5,5,5	0.08	0	5,5,5	0.34	0
3	GOL	B	503	-	5,5,5	0.22	0	5,5,5	0.51	0
3	GOL	E	502	-	5,5,5	0.19	0	5,5,5	0.59	0

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	C	501	-	-	2/16/32/32	0/3/3/3
2	GDP	D	501	-	-	1/16/32/32	0/3/3/3
3	GOL	B	504	-	-	0/4/4/4	-
3	GOL	D	502	-	-	4/4/4/4	-
2	GDP	A	501	-	-	1/16/32/32	0/3/3/3
3	GOL	A	502	-	-	4/4/4/4	-
2	GDP	B	501	-	-	1/16/32/32	0/3/3/3
3	GOL	E	503	-	-	4/4/4/4	-
2	GDP	F	501	-	-	1/16/32/32	0/3/3/3
2	GDP	E	501	-	-	3/16/32/32	0/3/3/3
3	GOL	B	502	-	-	2/4/4/4	-
3	GOL	B	503	-	-	2/4/4/4	-
3	GOL	E	502	-	-	3/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	GDP	PA-O3A	2.35	1.62	1.59

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	GDP	O3'-C3'-C2'	-3.38	100.98	111.82
2	C	501	GDP	O3'-C3'-C2'	-3.29	101.27	111.82
2	F	501	GDP	O3'-C3'-C2'	-2.82	102.78	111.82
2	B	501	GDP	C2'-C3'-C4'	2.63	107.69	102.61
2	A	501	GDP	O3'-C3'-C2'	-2.25	104.60	111.82
2	A	501	GDP	C2'-C3'-C4'	2.08	106.62	102.61

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	GOL	C1-C2-C3-O3
3	B	502	GOL	O1-C1-C2-C3
3	B	503	GOL	O1-C1-C2-C3
3	D	502	GOL	O1-C1-C2-C3
3	D	502	GOL	C1-C2-C3-O3
3	E	503	GOL	C1-C2-C3-O3
3	D	502	GOL	O1-C1-C2-O2
3	E	503	GOL	O2-C2-C3-O3
3	A	502	GOL	O1-C1-C2-C3
3	E	502	GOL	O1-C1-C2-C3
3	E	503	GOL	O1-C1-C2-C3
3	B	503	GOL	O1-C1-C2-O2
3	D	502	GOL	O2-C2-C3-O3
3	E	503	GOL	O1-C1-C2-O2
3	B	502	GOL	O1-C1-C2-O2
3	E	502	GOL	C1-C2-C3-O3
2	B	501	GDP	C4'-C5'-O5'-PA
2	E	501	GDP	C4'-C5'-O5'-PA
3	A	502	GOL	O1-C1-C2-O2
2	A	501	GDP	C4'-C5'-O5'-PA
2	D	501	GDP	C4'-C5'-O5'-PA
3	A	502	GOL	O2-C2-C3-O3
3	E	502	GOL	O1-C1-C2-O2
2	F	501	GDP	C4'-C5'-O5'-PA
2	C	501	GDP	C4'-C5'-O5'-PA
2	E	501	GDP	PB-O3A-PA-O1A
2	E	501	GDP	PB-O3A-PA-O2A
2	C	501	GDP	O4'-C4'-C5'-O5'

There are no ring outliers.

8 monomers are involved in 22 short contacts:

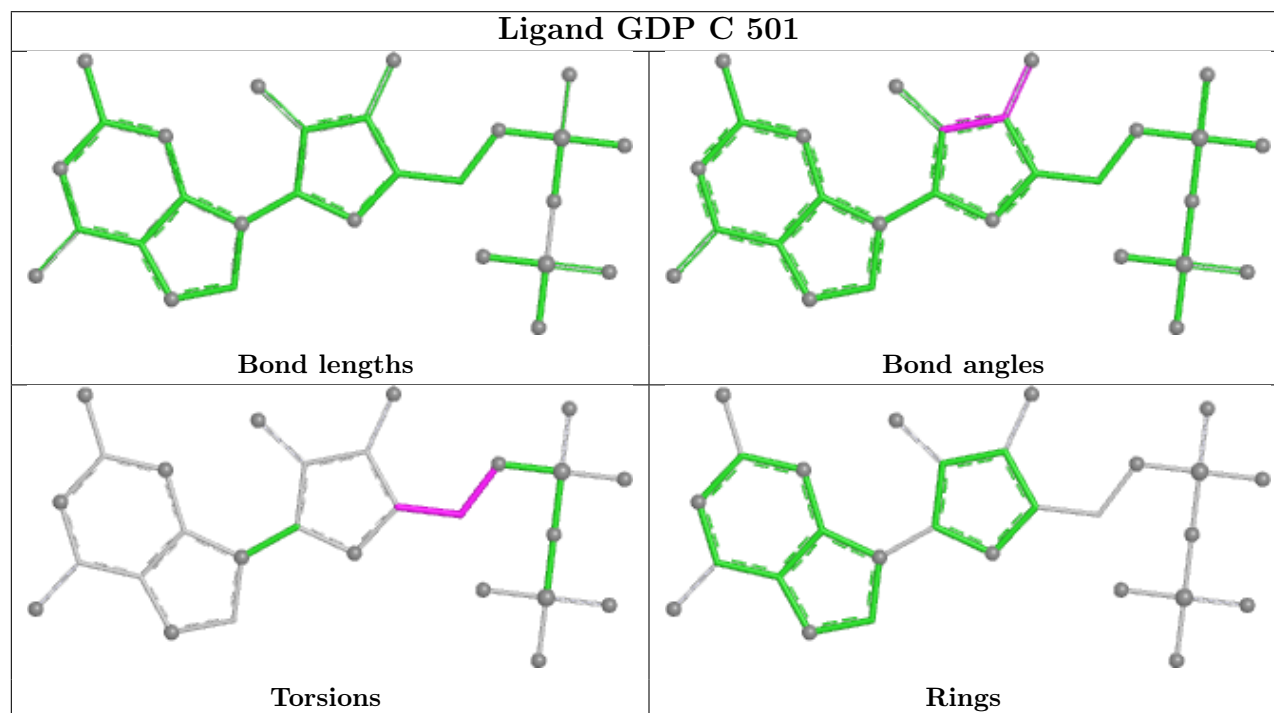
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	GDP	1	0
3	B	504	GOL	8	0
2	A	501	GDP	1	0
3	A	502	GOL	2	0
2	B	501	GDP	2	0
2	F	501	GDP	3	0
2	E	501	GDP	2	0

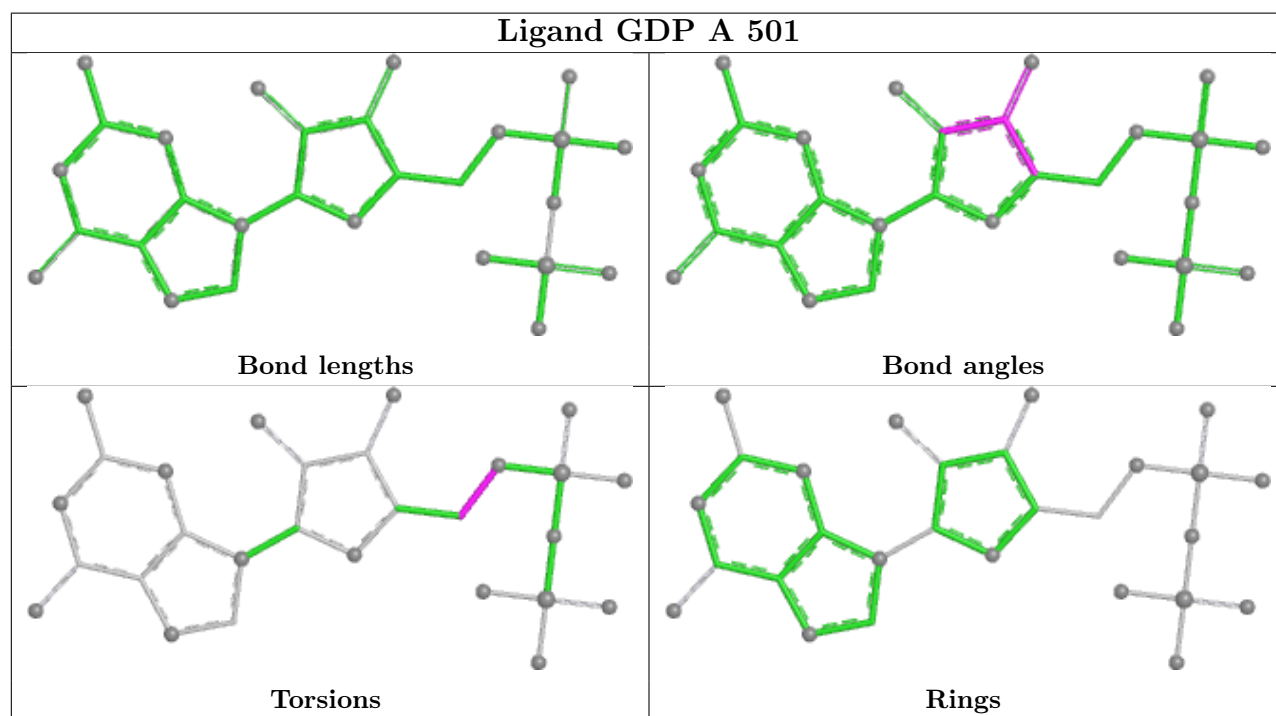
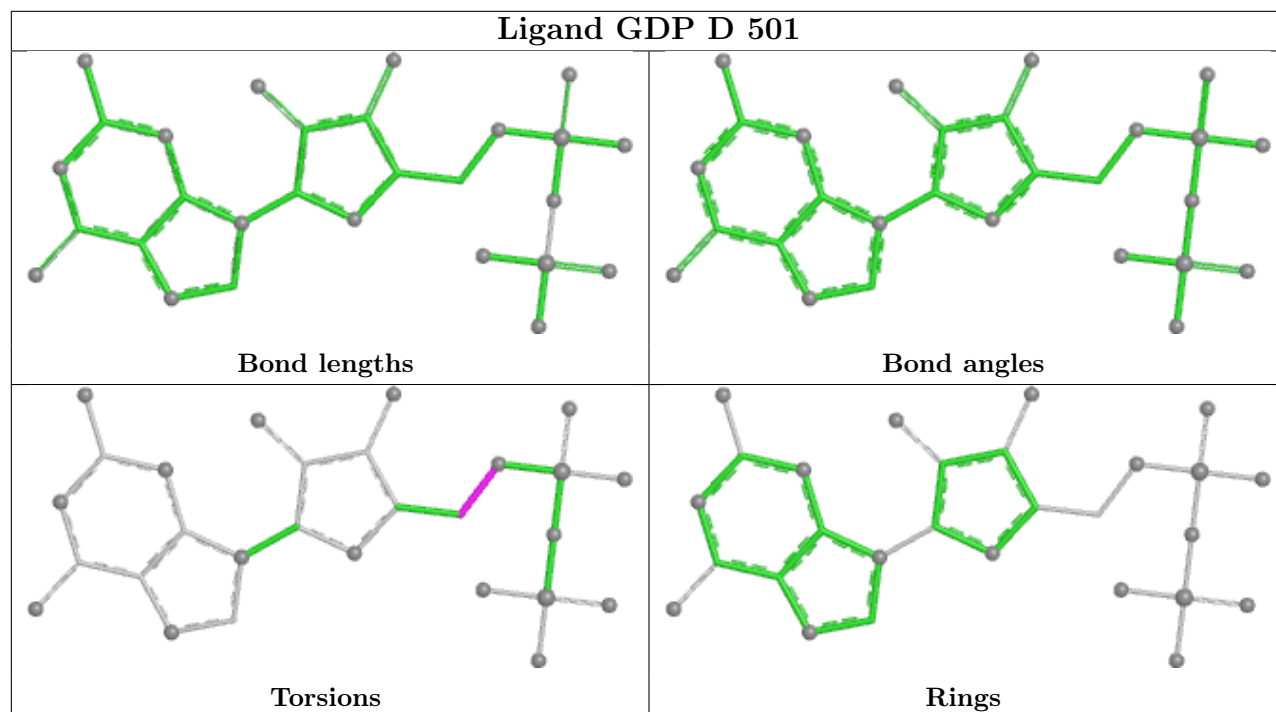
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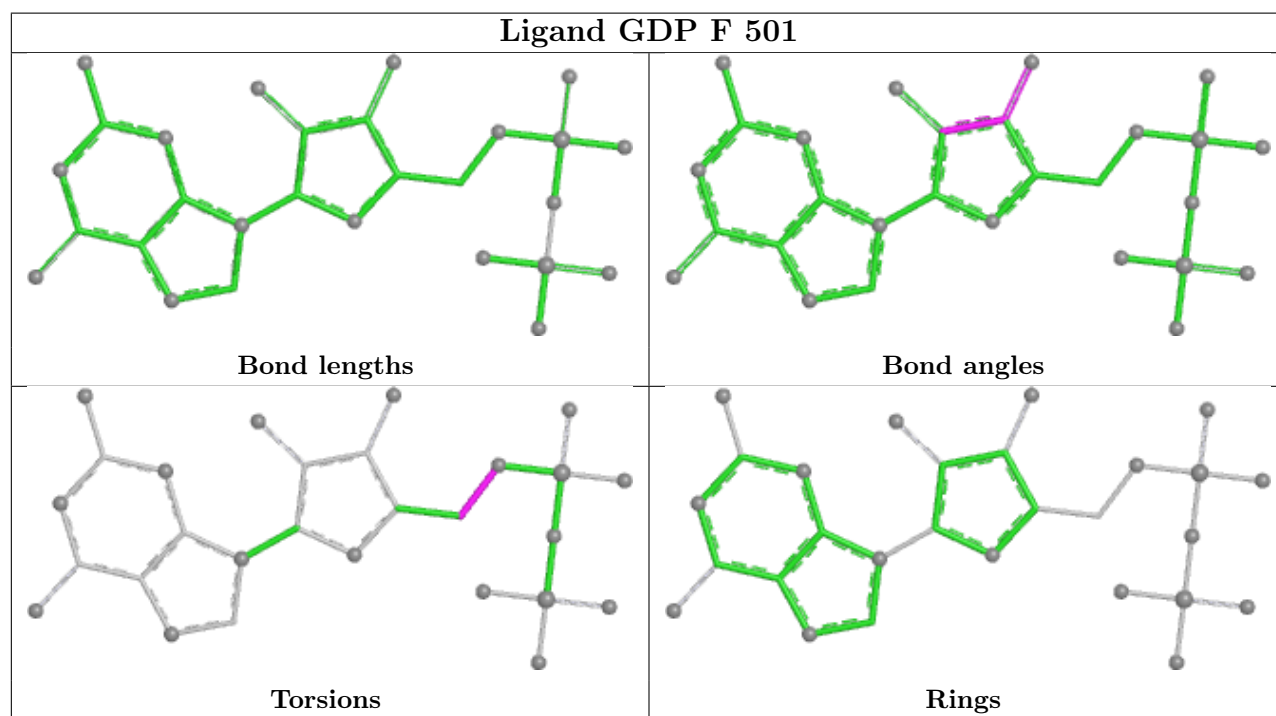
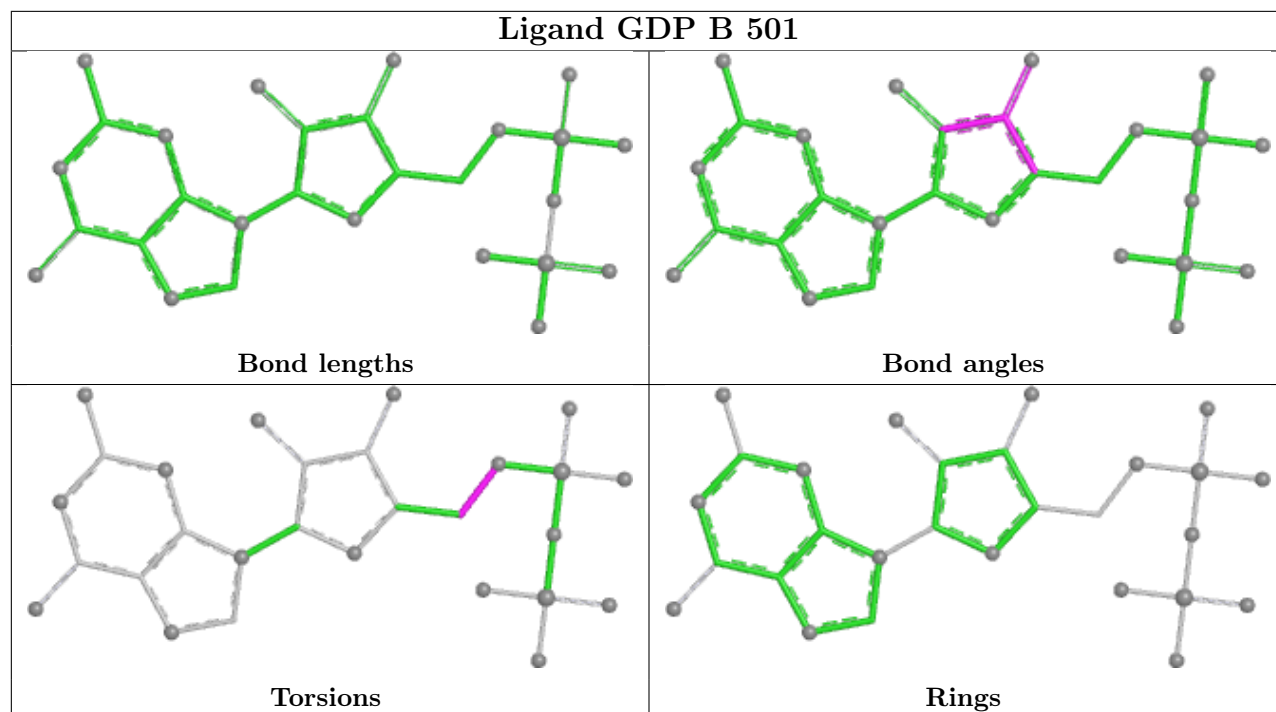
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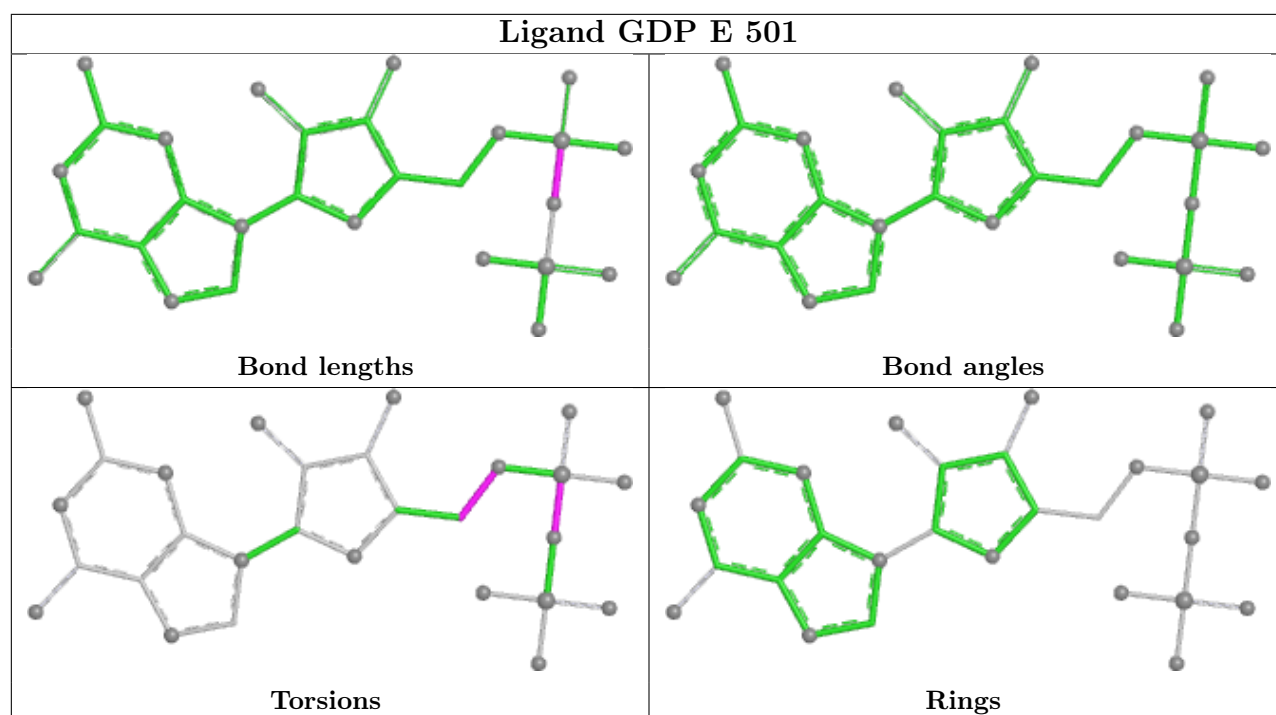
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	503	GOL	3	0

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	393/416 (94%)	0.58	25 (6%)	25	22	40, 81, 132, 173	0
1	B	397/416 (95%)	0.58	28 (7%)	22	19	40, 80, 131, 171	0
1	C	393/416 (94%)	0.46	17 (4%)	40	35	41, 75, 126, 146	0
1	D	397/416 (95%)	0.49	26 (6%)	25	22	30, 69, 127, 174	0
1	E	397/416 (95%)	0.47	22 (5%)	30	27	35, 69, 129, 183	0
1	F	393/416 (94%)	0.53	21 (5%)	32	28	41, 76, 122, 164	0
All	All	2370/2496 (94%)	0.52	139 (5%)	28	24	30, 74, 129, 183	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	93	HIS	7.6
1	D	102	GLY	6.3
1	E	98	ALA	6.2
1	F	101	THR	5.6
1	C	101	THR	5.5
1	E	183	GLN	5.2
1	E	103	VAL	4.7
1	E	102	GLY	4.7
1	E	100	HIS	4.2
1	E	194	PHE	4.2
1	B	221	ILE	4.0
1	B	253	PHE	4.0
1	A	253	PHE	3.9
1	D	103	VAL	3.9
1	B	133	ASP	3.7
1	A	101	THR	3.6
1	B	252	VAL	3.6
1	F	109	GLU	3.5
1	B	225	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	101	THR	3.4
1	D	91	ILE	3.4
1	E	136	PRO	3.3
1	A	145	PHE	3.2
1	D	92	GLY	3.2
1	F	145	PHE	3.2
1	C	145	PHE	3.1
1	A	225	PRO	3.1
1	C	335	VAL	3.1
1	E	107	THR	3.1
1	E	199	PHE	3.1
1	E	96	GLY	3.1
1	C	375	ASN	3.0
1	D	97	GLY	3.0
1	A	221	ILE	3.0
1	D	129	THR	3.0
1	B	145	PHE	3.0
1	F	78	GLY	3.0
1	A	243	MET	2.9
1	B	173	MET	2.9
1	F	375	ASN	2.9
1	B	158	ARG	2.9
1	D	368	ASN	2.8
1	D	145	PHE	2.8
1	F	107	THR	2.8
1	E	349	ASP	2.8
1	D	164	ILE	2.8
1	E	105	ASP	2.8
1	B	375	ASN	2.7
1	A	134	PHE	2.6
1	B	103	VAL	2.6
1	B	68	PRO	2.6
1	A	375	ASN	2.6
1	D	94	GLU	2.6
1	A	169	ALA	2.6
1	B	406	ASN	2.6
1	D	10	SER	2.6
1	F	164	ILE	2.5
1	F	99	ALA	2.5
1	A	198	THR	2.5
1	C	221	ILE	2.5
1	D	252	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	348	THR	2.5
1	C	107	THR	2.5
1	E	93	HIS	2.5
1	A	223	GLU	2.4
1	A	226	ILE	2.4
1	F	100	HIS	2.4
1	A	252	VAL	2.4
1	A	106	LYS	2.4
1	A	111	HIS	2.4
1	F	146	TYR	2.4
1	D	173	MET	2.4
1	A	212	CYS	2.4
1	E	145	PHE	2.4
1	B	176	GLU	2.4
1	B	217	ARG	2.3
1	B	13	GLN	2.3
1	C	202	GLU	2.3
1	B	136	PRO	2.3
1	A	107	THR	2.3
1	C	100	HIS	2.3
1	A	108	LYS	2.3
1	E	216	PHE	2.3
1	F	108	LYS	2.3
1	D	99	ALA	2.3
1	A	266	THR	2.3
1	A	256	GLN	2.3
1	F	135	GLN	2.3
1	F	335	VAL	2.3
1	B	169	ALA	2.3
1	F	266	THR	2.3
1	F	10	SER	2.3
1	A	154	ILE	2.3
1	B	348	THR	2.2
1	F	352	THR	2.2
1	E	10	SER	2.2
1	F	265	ILE	2.2
1	B	207	ASP	2.2
1	D	216	PHE	2.2
1	F	111	HIS	2.2
1	B	159	PHE	2.2
1	D	101	THR	2.2
1	D	104	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	235	CYS	2.2
1	C	12	ASP	2.2
1	D	12	ASP	2.2
1	D	349	ASP	2.2
1	B	151	PHE	2.2
1	D	194	PHE	2.2
1	C	99	ALA	2.2
1	B	69	LEU	2.2
1	C	329	ILE	2.2
1	A	136	PRO	2.2
1	E	252	VAL	2.1
1	B	118	MET	2.1
1	C	266	THR	2.1
1	E	404	LEU	2.1
1	A	177	PHE	2.1
1	D	197	GLN	2.1
1	B	154	ILE	2.1
1	D	137	LYS	2.1
1	F	403	CYS	2.1
1	D	221	ILE	2.1
1	C	146	TYR	2.1
1	D	330	ASP	2.1
1	F	194	PHE	2.0
1	D	222	ALA	2.0
1	B	102	GLY	2.0
1	B	266	THR	2.0
1	F	154	ILE	2.0
1	C	292	SER	2.0
1	B	111	HIS	2.0
1	C	403	CYS	2.0
1	C	315	VAL	2.0
1	E	97	GLY	2.0
1	E	266	THR	2.0
1	A	68	PRO	2.0
1	C	165	ASP	2.0
1	B	146	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

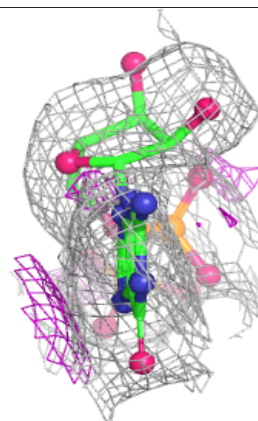
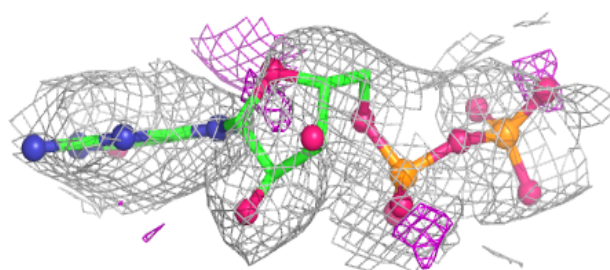
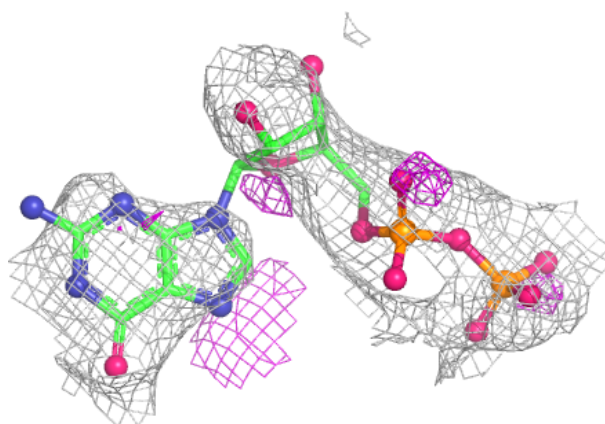
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	GOL	B	504	6/6	0.74	0.19	84,105,108,109	0
3	GOL	E	503	6/6	0.85	0.18	81,100,107,114	0
2	GDP	E	501	28/28	0.88	0.11	94,118,148,153	0
3	GOL	D	502	6/6	0.89	0.12	59,66,72,77	0
3	GOL	A	502	6/6	0.89	0.11	70,87,98,106	0
3	GOL	B	503	6/6	0.90	0.12	79,83,89,99	0
2	GDP	D	501	28/28	0.90	0.09	80,97,122,125	0
3	GOL	E	502	6/6	0.91	0.11	54,57,62,63	0
2	GDP	A	501	28/28	0.94	0.09	55,79,91,105	0
2	GDP	B	501	28/28	0.94	0.08	57,74,86,110	0
3	GOL	B	502	6/6	0.95	0.08	79,87,93,107	0
2	GDP	F	501	28/28	0.95	0.09	55,81,96,101	0
2	GDP	C	501	28/28	0.95	0.08	59,83,94,103	0

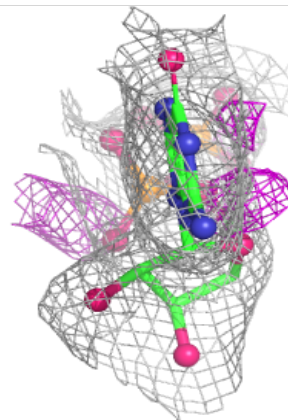
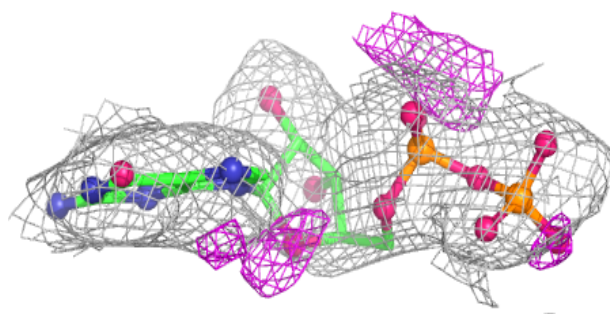
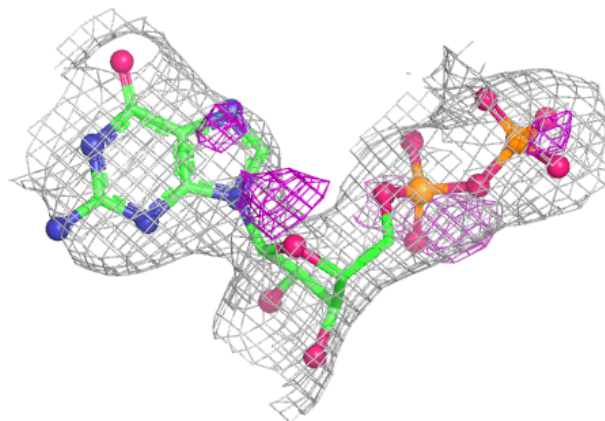
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GDP E 501:

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

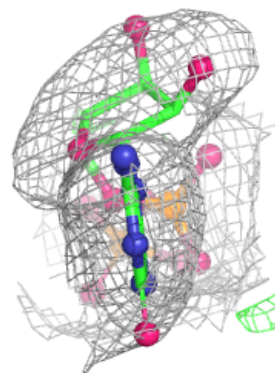
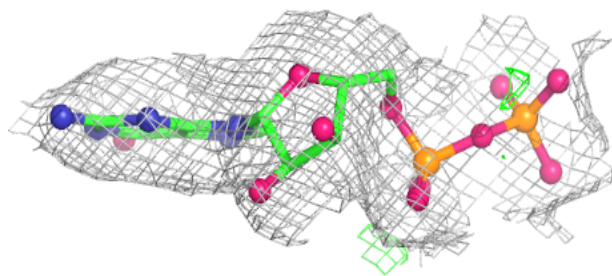
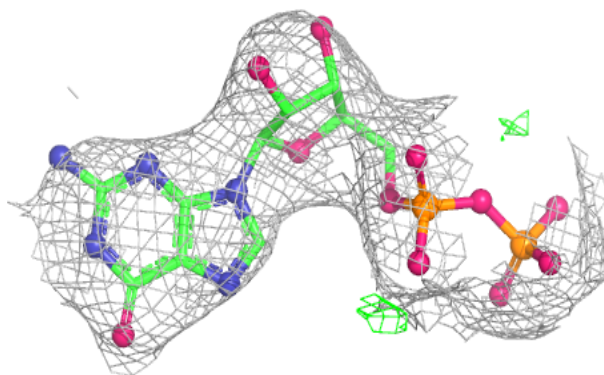
**Electron density around GDP D 501:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

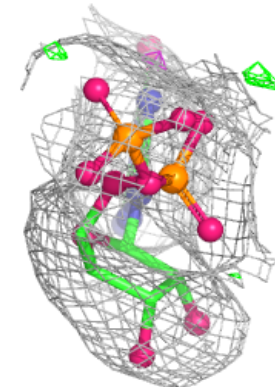
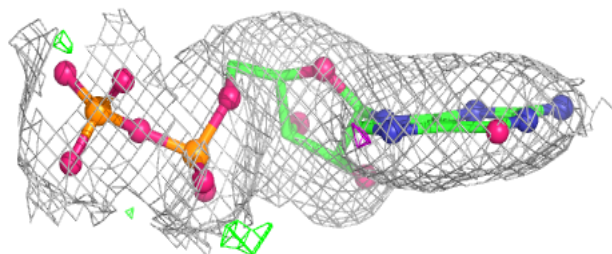
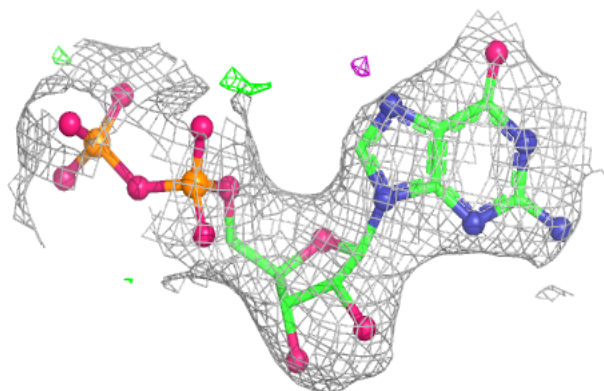


Electron density around GDP A 501:

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

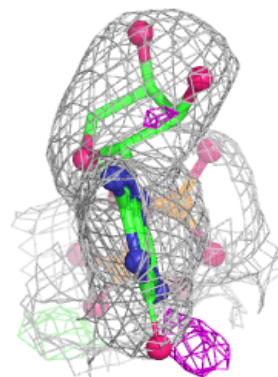
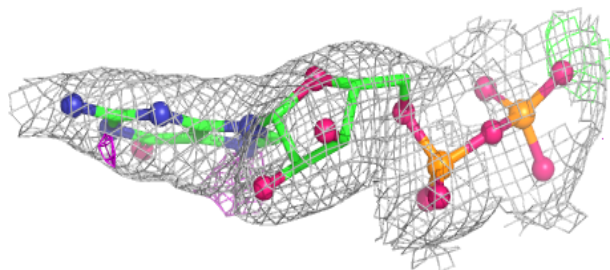
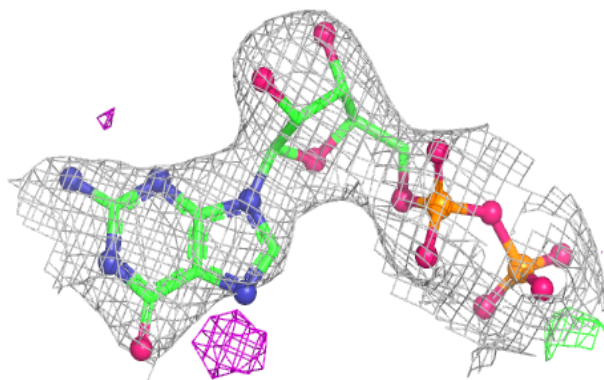
**Electron density around GDP B 501:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

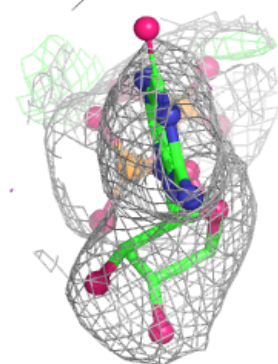
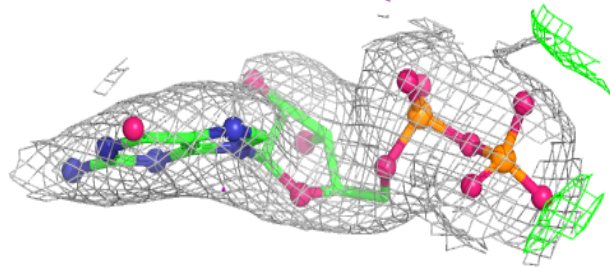
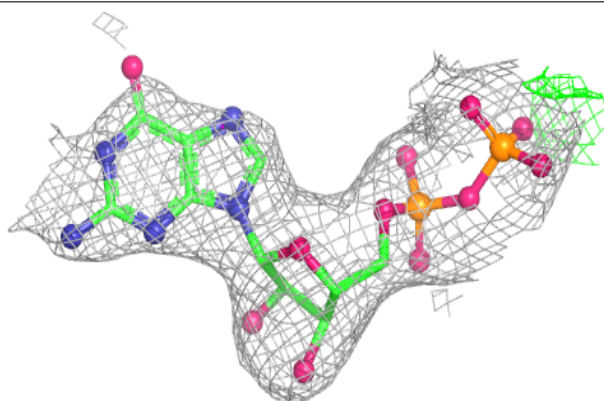


Electron density around GDP F 501:

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

**Electron density around GDP C 501:**

$2mF_o - DF_c$ (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.