



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 08:59 AM EDT

PDB ID : 3SYN / pdb_00003syn
Title : Crystal structure of FlhF in complex with its activator
Authors : Bange, G.; Kuemmerer, N.; Wild, K.; Sinning, I.
Deposited on : 2011-07-18
Resolution : 3.06 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:

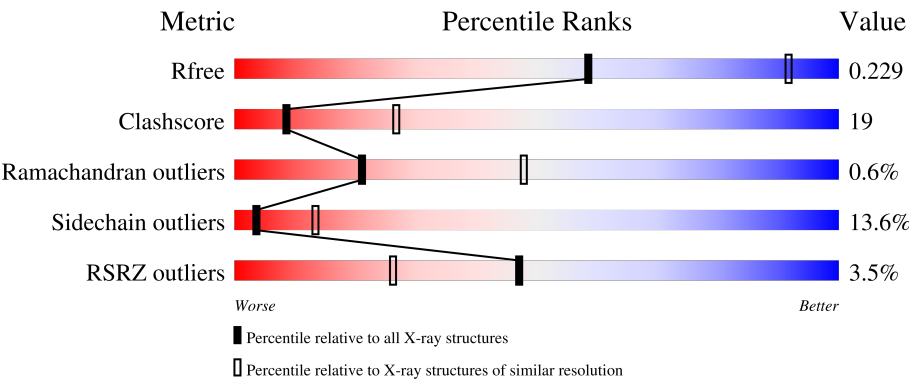
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	296	3% 52%29%6%13%
1	B	296	2% 53%28%6%13%
1	C	296	2% 52%30%.13%
1	D	296	3% 54%27%6%13%
2	E	23	9% 39%26%.30%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	23	
2	G	23	
2	H	23	

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
6	SO4	A	10	-	-	X	-
6	SO4	A	13	-	-	X	-
6	SO4	A	5	-	-	X	-
6	SO4	B	1	-	-	X	-
6	SO4	B	14	-	-	X	-
6	SO4	B	8	-	-	X	-
6	SO4	C	4	-	-	X	-
6	SO4	C	9	-	-	X	-
6	SO4	D	6	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9010 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 Flagellar biosynthesis protein flhF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			2042	1310	331	393	8			
1	B	258	Total	C	N	O	S	0	0	0
			2042	1310	331	393	8			
1	C	258	Total	C	N	O	S	0	0	0
			2042	1310	331	393	8			
1	D	258	Total	C	N	O	S	0	0	0
			2042	1310	331	393	8			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	71	MET	-	expression tag	UNP Q01960
A	72	GLY	-	expression tag	UNP Q01960
A	73	HIS	-	expression tag	UNP Q01960
A	74	HIS	-	expression tag	UNP Q01960
A	75	HIS	-	expression tag	UNP Q01960
A	76	HIS	-	expression tag	UNP Q01960
A	77	HIS	-	expression tag	UNP Q01960
A	78	HIS	-	expression tag	UNP Q01960
B	71	MET	-	expression tag	UNP Q01960
B	72	GLY	-	expression tag	UNP Q01960
B	73	HIS	-	expression tag	UNP Q01960
B	74	HIS	-	expression tag	UNP Q01960
B	75	HIS	-	expression tag	UNP Q01960
B	76	HIS	-	expression tag	UNP Q01960
B	77	HIS	-	expression tag	UNP Q01960
B	78	HIS	-	expression tag	UNP Q01960
C	71	MET	-	expression tag	UNP Q01960
C	72	GLY	-	expression tag	UNP Q01960
C	73	HIS	-	expression tag	UNP Q01960
C	74	HIS	-	expression tag	UNP Q01960
C	75	HIS	-	expression tag	UNP Q01960

Continued on next page...

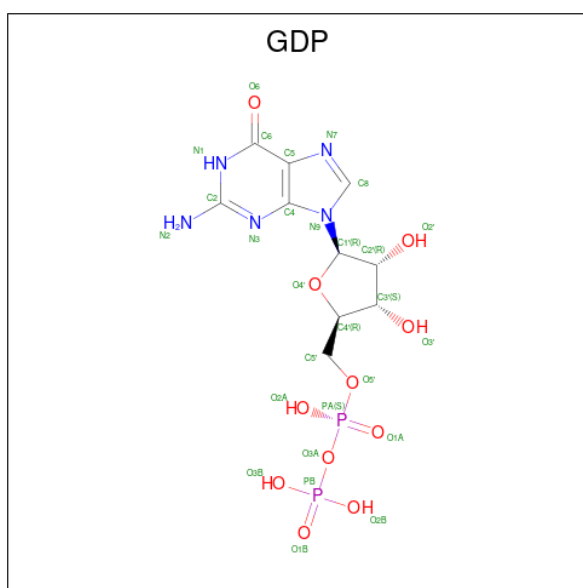
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	76	HIS	-	expression tag	UNP Q01960
C	77	HIS	-	expression tag	UNP Q01960
C	78	HIS	-	expression tag	UNP Q01960
D	71	MET	-	expression tag	UNP Q01960
D	72	GLY	-	expression tag	UNP Q01960
D	73	HIS	-	expression tag	UNP Q01960
D	74	HIS	-	expression tag	UNP Q01960
D	75	HIS	-	expression tag	UNP Q01960
D	76	HIS	-	expression tag	UNP Q01960
D	77	HIS	-	expression tag	UNP Q01960
D	78	HIS	-	expression tag	UNP Q01960

- Molecule 2 is a protein called ATP-binding protein YlxH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	16	Total	C	N	O	S	0	0	0
			136	82	28	25	1			
2	F	16	Total	C	N	O	S	0	0	0
			136	82	28	25	1			
2	G	16	Total	C	N	O	S	0	0	0
			136	82	28	25	1			
2	H	16	Total	C	N	O	S	0	0	0
			136	82	28	25	1			

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

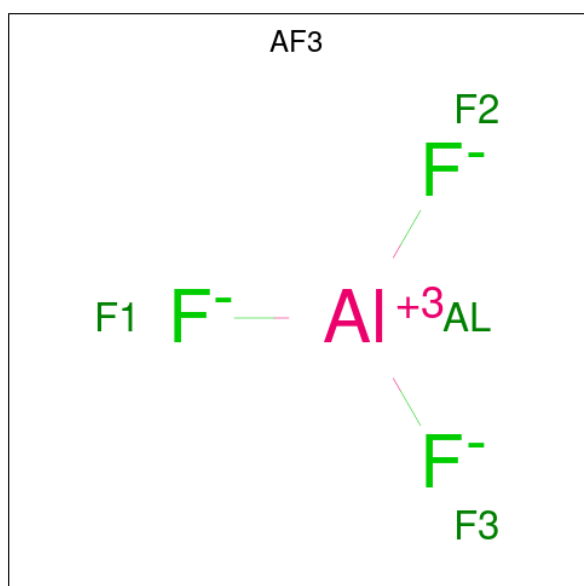


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

- Molecule 5 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF₃).



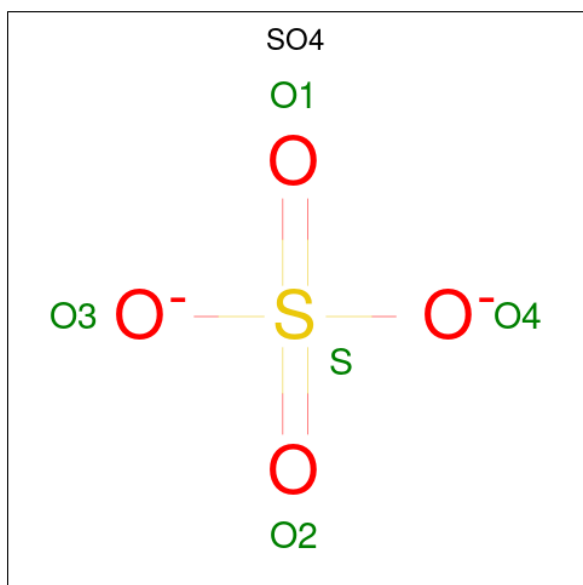
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Al	F	0	0
			4	1	3		
5	B	1	Total	Al	F	0	0
			4	1	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	Al	F	0	0
			4	1	3		
5	D	1	Total	Al	F	0	0
			4	1	3		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

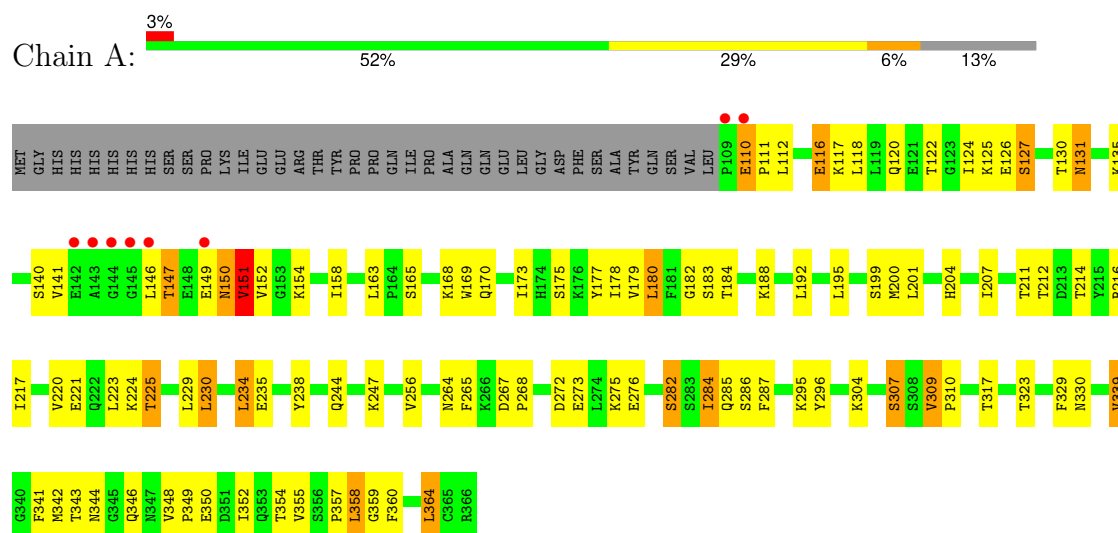
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	20	Total	O	0	0
			20	20		
7	B	21	Total	O	0	0
			21	21		
7	C	20	Total	O	0	0
			20	20		
7	D	26	Total	O	0	0
			26	26		
7	E	2	Total	O	0	0
			2	2		
7	F	1	Total	O	0	0
			1	1		
7	G	1	Total	O	0	0
			1	1		

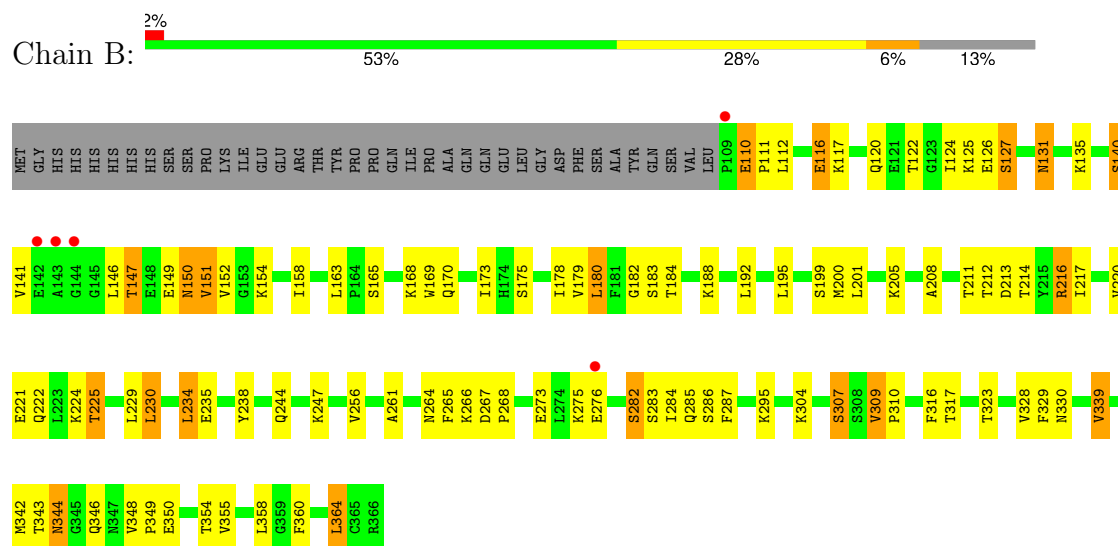
3 Residue-property plots

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: Flagellar biosynthesis protein fhfF

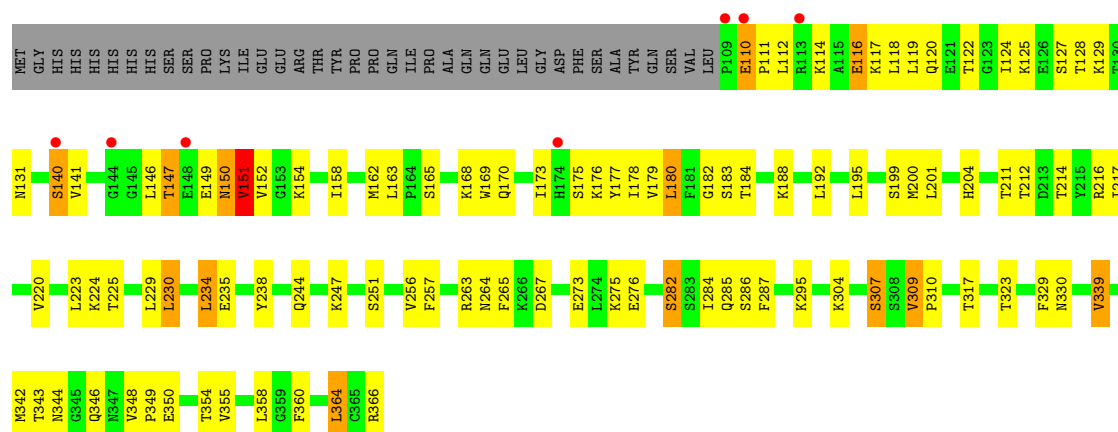


• Molecule 1: Flagellar biosynthesis protein fhfF

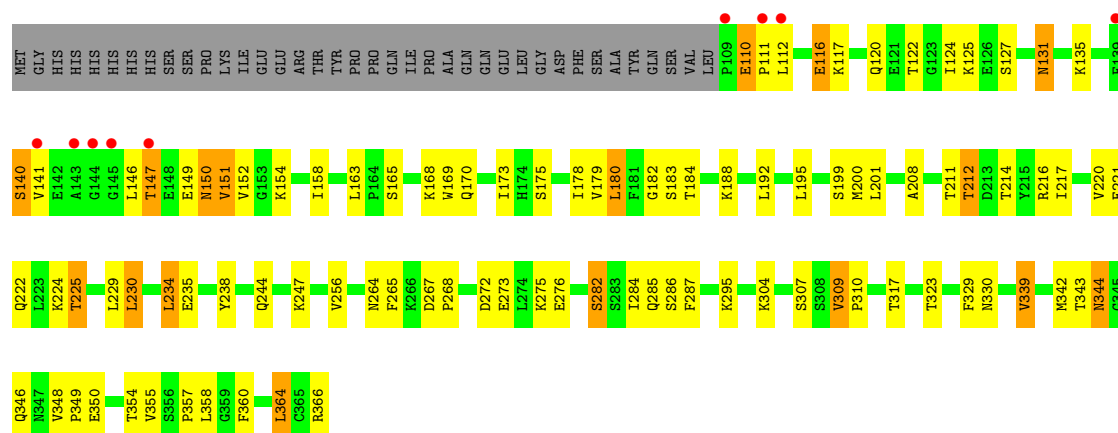


• Molecule 1: Flagellar biosynthesis protein fhfF

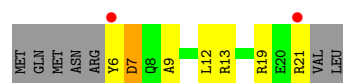




• Molecule 1: Flagellar biosynthesis protein flhF



• Molecule 2: ATP-binding protein YlxH

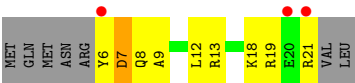


• Molecule 2: ATP-binding protein YlxH

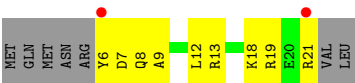


• Molecule 2: ATP-binding protein YlxH





● Molecule 2: ATP-binding protein YlxH



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	50.79Å 63.36Å 114.50Å 92.26° 100.96° 94.25°	Depositor
Resolution (Å)	63.09 – 3.06 63.09 – 3.06	Depositor EDS
% Data completeness (in resolution range)	92.9 (63.09-3.06) 92.9 (63.09-3.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.28 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, R_{free}	0.181 , 0.239 0.174 , 0.229	Depositor DCC
R_{free} test set	1259 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9010	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.59% 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: MG, GDP, SO4, AF3

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	0.59	0/2079	0.89	2/2805 (0.1%)
1	B	0.58	0/2079	0.87	0/2805
1	C	0.55	0/2079	0.88	1/2805 (0.0%)
1	D	0.56	0/2079	0.87	1/2805 (0.0%)
2	E	0.67	0/136	0.86	0/178
2	F	0.57	0/136	0.88	0/178
2	G	0.50	0/136	0.89	0/178
2	H	0.58	0/136	0.84	0/178
All	All	0.57	0/8860	0.88	4/11932 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	VAL	CB-CA-C	-6.02	104.29	111.81
1	C	151	VAL	CB-CA-C	-6.01	104.29	111.81
1	D	212	THR	N-CA-C	-5.33	106.66	114.39
1	A	284	ILE	N-CA-C	5.01	115.14	108.27

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2042	0	2079	87	0
1	B	2042	0	2080	85	0
1	C	2042	0	2080	79	0
1	D	2042	0	2080	80	0
2	E	136	0	139	6	0
2	F	136	0	139	10	0
2	G	136	0	139	9	0
2	H	136	0	139	11	0
3	A	28	0	12	0	0
3	B	28	0	12	0	0
3	C	28	0	12	1	0
3	D	28	0	12	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
5	C	4	0	0	0	0
5	D	4	0	0	1	0
6	A	25	0	0	9	0
6	B	15	0	0	8	0
6	C	20	0	0	4	0
6	D	15	0	0	3	0
7	A	20	0	0	2	0
7	B	21	0	0	2	0
7	C	20	0	0	1	0
7	D	26	0	0	0	0
7	E	2	0	0	0	0
7	F	1	0	0	0	0
7	G	1	0	0	0	0
All	All	9010	0	8923	337	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 19.

All (337) 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:D:179:VAL:HG21	1:D:284:ILE:HD11	1.52	0.93
1:B:179:VAL:HG21	1:B:284:ILE:HD11	1.52	0.92
1:D:110:GLU:HB2	1:D:111:PRO:HD3	1.53	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:GLU:HB2	1:C:111:PRO:HD3	1.53	0.90
1:A:110:GLU:HB2	1:A:111:PRO:HD3	1.52	0.89
1:A:179:VAL:HG21	1:A:284:ILE:HD11	1.54	0.89
1:B:110:GLU:HB2	1:B:111:PRO:HD3	1.54	0.88
1:C:179:VAL:HG21	1:C:284:ILE:HD11	1.54	0.86
1:A:188:LYS:HE2	7:A:9:HOH:O	1.80	0.81
1:B:179:VAL:CG2	1:B:284:ILE:HD11	2.12	0.79
1:D:179:VAL:CG2	1:D:284:ILE:HD11	2.13	0.79
1:C:179:VAL:CG2	1:C:284:ILE:HD11	2.15	0.76
1:A:147:THR:H	1:A:150:ASN:ND2	1.85	0.74
1:A:179:VAL:CG2	1:A:284:ILE:HD11	2.17	0.73
1:C:147:THR:H	1:C:150:ASN:ND2	1.87	0.72
1:B:214:THR:HG21	1:B:238:TYR:CE2	2.26	0.70
1:B:283:SER:HB3	6:B:14:SO4:O1	1.91	0.70
1:A:217:ILE:HD11	2:F:9:ALA:HB2	1.73	0.70
1:B:147:THR:H	1:B:150:ASN:ND2	1.91	0.69
1:D:214:THR:HG21	1:D:238:TYR:CE2	2.28	0.69
1:C:146:LEU:HD13	1:C:151:VAL:HG13	1.74	0.69
1:D:147:THR:H	1:D:150:ASN:ND2	1.92	0.68
1:C:217:ILE:HD11	2:H:9:ALA:HB2	1.74	0.68
1:B:146:LEU:HD13	1:B:151:VAL:HG13	1.75	0.68
1:B:154:LYS:O	1:B:158:ILE:HG13	1.94	0.68
1:D:122:THR:HB	1:D:364:LEU:HD22	1.76	0.68
1:C:214:THR:HG21	1:C:238:TYR:CE2	2.29	0.68
1:D:229:LEU:HD21	2:H:13:ARG:HG3	1.75	0.67
1:A:214:THR:HG21	1:A:238:TYR:CE2	2.30	0.67
1:C:122:THR:HB	1:C:364:LEU:HD22	1.75	0.66
1:A:296:TYR:N	6:A:5:SO4:O1	2.28	0.66
1:B:122:THR:HB	1:B:364:LEU:HD22	1.76	0.66
1:C:229:LEU:HD21	2:G:13:ARG:HG3	1.77	0.66
1:A:146:LEU:HD13	1:A:151:VAL:HG13	1.78	0.65
1:C:110:GLU:CB	1:C:111:PRO:HD3	2.27	0.64
1:D:116:GLU:O	1:D:120:GLN:HG2	1.97	0.64
1:A:110:GLU:CB	1:A:111:PRO:HD3	2.28	0.64
1:A:229:LEU:HD21	2:E:13:ARG:HG3	1.80	0.64
1:B:116:GLU:O	1:B:120:GLN:HG2	1.98	0.63
1:A:214:THR:HB	2:F:6:TYR:HE2	1.64	0.63
1:A:122:THR:HB	1:A:364:LEU:HD22	1.78	0.63
1:B:264:ASN:N	6:B:1:SO4:O1	2.31	0.63
1:C:214:THR:HB	2:H:6:TYR:HE2	1.64	0.63
1:D:234:LEU:HD23	1:D:235:GLU:N	2.14	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:GLU:HB2	1:C:111:PRO:CD	2.28	0.62
1:B:229:LEU:HD21	2:F:13:ARG:HG3	1.80	0.62
1:C:116:GLU:O	1:C:120:GLN:HG2	1.99	0.62
1:D:295:LYS:HA	6:D:6:SO4:O1	2.00	0.62
1:B:217:ILE:HD11	2:E:9:ALA:HB2	1.82	0.62
1:D:146:LEU:HD13	1:D:151:VAL:HG13	1.80	0.62
1:A:116:GLU:O	1:A:120:GLN:HG2	1.99	0.61
1:C:147:THR:N	1:C:150:ASN:ND2	2.49	0.61
1:A:357:PRO:HD2	6:A:10:SO4:O4	1.99	0.61
1:D:217:ILE:HD11	2:G:9:ALA:HB2	1.82	0.61
1:D:154:LYS:O	1:D:158:ILE:HG13	2.01	0.61
1:D:110:GLU:CB	1:D:111:PRO:HD3	2.27	0.61
1:A:147:THR:N	1:A:150:ASN:ND2	2.49	0.61
1:B:117:LYS:O	1:B:120:GLN:HB2	2.01	0.61
1:C:244:GLN:O	1:C:247:LYS:HB2	2.01	0.61
1:D:117:LYS:O	1:D:120:GLN:HB2	2.01	0.61
1:D:244:GLN:O	1:D:247:LYS:HB2	2.01	0.60
1:C:175:SER:HB2	1:C:285:GLN:HG3	1.83	0.60
1:A:175:SER:HB2	1:A:285:GLN:HG3	1.84	0.60
1:A:244:GLN:O	1:A:247:LYS:HB2	2.02	0.60
1:D:188:LYS:N	3:D:4:GDP:O1B	2.31	0.59
1:A:163:LEU:HD21	1:A:329:PHE:CE2	2.38	0.59
1:D:110:GLU:HB2	1:D:111:PRO:CD	2.30	0.59
1:B:110:GLU:CB	1:B:111:PRO:HD3	2.29	0.59
1:D:264:ASN:N	6:D:2:SO4:O3	2.35	0.59
1:B:110:GLU:HB2	1:B:111:PRO:CD	2.31	0.59
1:B:234:LEU:HD23	1:B:235:GLU:N	2.17	0.59
1:D:163:LEU:HD21	1:D:329:PHE:CE2	2.38	0.59
1:A:217:ILE:HD11	2:F:9:ALA:CB	2.32	0.58
1:C:217:ILE:HD11	2:H:9:ALA:CB	2.33	0.58
1:A:117:LYS:O	1:A:120:GLN:HB2	2.03	0.58
1:B:244:GLN:O	1:B:247:LYS:HB2	2.02	0.58
1:D:230:LEU:HD11	2:H:12:LEU:HD11	1.85	0.58
1:A:110:GLU:HB2	1:A:111:PRO:CD	2.30	0.58
1:B:112:LEU:HD11	1:B:146:LEU:HD21	1.85	0.58
1:B:214:THR:HB	2:E:6:TYR:HE2	1.68	0.58
1:A:154:LYS:O	1:A:158:ILE:HG13	2.03	0.58
1:B:282:SER:HB3	6:B:14:SO4:O3	2.04	0.58
1:C:179:VAL:C	1:C:180:LEU:HD23	2.29	0.58
1:C:295:LYS:HA	6:C:9:SO4:O2	2.03	0.58
1:B:147:THR:O	1:B:151:VAL:HG22	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:THR:N	1:B:150:ASN:ND2	2.52	0.58
1:D:112:LEU:HD11	1:D:146:LEU:HD21	1.86	0.58
1:D:317:THR:HA	1:D:343:THR:OG1	2.03	0.58
1:C:234:LEU:HD23	1:C:235:GLU:N	2.19	0.57
6:C:9:SO4:O2	1:D:295:LYS:HG2	2.03	0.57
1:A:282:SER:HB3	6:A:13:SO4:O2	2.04	0.57
1:D:147:THR:N	1:D:150:ASN:ND2	2.52	0.57
1:A:112:LEU:HD11	1:A:146:LEU:HD21	1.86	0.57
1:C:117:LYS:O	1:C:120:GLN:HB2	2.05	0.57
1:C:211:THR:HG21	1:C:220:VAL:HG22	1.87	0.57
1:C:264:ASN:N	6:C:4:SO4:O4	2.37	0.56
6:A:5:SO4:O4	1:B:295:LYS:HG2	2.06	0.56
1:A:234:LEU:HD23	1:A:235:GLU:N	2.21	0.56
1:D:342:MET:HE1	1:D:360:PHE:CD1	2.40	0.56
1:C:112:LEU:HD11	1:C:146:LEU:HD21	1.88	0.56
1:B:175:SER:HB2	1:B:285:GLN:HG3	1.88	0.56
1:A:125:LYS:HE2	7:A:56:HOH:O	2.06	0.56
1:C:154:LYS:O	1:C:158:ILE:HG13	2.06	0.55
1:D:273:GLU:O	1:D:276:GLU:HG2	2.06	0.55
1:A:317:THR:HA	1:A:343:THR:OG1	2.06	0.55
1:B:179:VAL:C	1:B:180:LEU:HD23	2.31	0.55
1:D:211:THR:HG21	1:D:220:VAL:HG22	1.88	0.55
1:A:179:VAL:C	1:A:180:LEU:HD23	2.31	0.55
1:D:147:THR:O	1:D:151:VAL:HG22	2.07	0.55
1:B:110:GLU:HA	1:B:110:GLU:OE1	2.07	0.55
1:B:214:THR:HG21	1:B:238:TYR:HE2	1.70	0.55
1:D:110:GLU:OE1	1:D:110:GLU:HA	2.07	0.55
1:D:221:GLU:O	1:D:225:THR:HG23	2.07	0.54
1:A:346:GLN:NE2	6:B:1:SO4:O4	2.41	0.54
1:B:170:GLN:HG2	1:B:354:THR:HB	1.89	0.54
1:C:147:THR:O	1:C:151:VAL:HG22	2.07	0.54
1:B:317:THR:HA	1:B:343:THR:OG1	2.08	0.54
1:D:234:LEU:C	1:D:234:LEU:CD2	2.81	0.54
1:A:211:THR:HG21	1:A:220:VAL:HG22	1.90	0.53
1:A:224:LYS:HA	1:A:234:LEU:HD12	1.91	0.53
1:A:358:LEU:HB2	6:A:10:SO4:O2	2.08	0.53
1:D:217:ILE:HD11	2:G:9:ALA:CB	2.37	0.53
1:D:175:SER:HB2	1:D:285:GLN:HG3	1.91	0.53
1:C:147:THR:HB	1:C:149:GLU:H	1.74	0.53
1:B:221:GLU:O	1:B:225:THR:HG23	2.09	0.53
1:C:214:THR:HG21	1:C:238:TYR:HE2	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:GLU:O	1:C:276:GLU:HG2	2.09	0.53
1:C:224:LYS:HA	1:C:234:LEU:HD12	1.92	0.52
1:A:110:GLU:OE1	1:A:110:GLU:HA	2.08	0.52
1:D:214:THR:HG21	1:D:238:TYR:HE2	1.73	0.52
1:B:342:MET:HE1	1:B:360:PHE:CD1	2.44	0.52
1:C:180:LEU:HD23	1:C:180:LEU:N	2.25	0.52
1:D:147:THR:HB	1:D:149:GLU:H	1.75	0.52
1:A:170:GLN:HG2	1:A:354:THR:HB	1.91	0.52
1:B:169:TRP:CZ3	1:B:339:VAL:HG13	2.44	0.52
1:B:273:GLU:O	1:B:276:GLU:HG2	2.10	0.52
1:C:170:GLN:HG2	1:C:354:THR:HB	1.90	0.52
1:A:295:LYS:HG2	6:B:8:SO4:O4	2.10	0.52
1:B:146:LEU:CD1	1:B:151:VAL:HG13	2.39	0.52
1:C:234:LEU:C	1:C:234:LEU:CD2	2.83	0.51
1:B:234:LEU:C	1:B:234:LEU:CD2	2.83	0.51
1:A:200:MET:HG2	1:A:201:LEU:HD23	1.93	0.51
1:B:295:LYS:HA	6:B:8:SO4:O4	2.10	0.51
1:A:342:MET:HE1	1:A:360:PHE:CD1	2.46	0.51
1:D:169:TRP:CE3	1:D:339:VAL:HG13	2.46	0.51
1:C:342:MET:HE1	1:C:360:PHE:CD1	2.46	0.51
1:B:180:LEU:HD22	1:B:287:PHE:HB2	1.93	0.51
1:B:217:ILE:HD11	2:E:9:ALA:CB	2.40	0.51
1:D:140:SER:CB	1:D:146:LEU:HD23	2.41	0.51
1:D:179:VAL:C	1:D:180:LEU:HD23	2.36	0.51
1:A:169:TRP:CE3	1:A:339:VAL:HG13	2.46	0.51
1:C:110:GLU:OE1	1:C:110:GLU:HA	2.10	0.51
1:A:234:LEU:C	1:A:234:LEU:CD2	2.84	0.50
1:B:140:SER:CB	1:B:146:LEU:HD23	2.41	0.50
1:B:169:TRP:CE3	1:B:339:VAL:HG13	2.47	0.50
1:C:147:THR:N	1:C:150:ASN:HD21	2.08	0.50
1:D:214:THR:HB	2:G:6:TYR:HE2	1.75	0.50
1:B:211:THR:HG21	1:B:220:VAL:HG22	1.94	0.50
1:C:230:LEU:HD11	2:G:12:LEU:HD11	1.93	0.50
1:D:180:LEU:HD22	1:D:287:PHE:HB2	1.94	0.50
1:B:182:GLY:N	1:B:188:LYS:HD3	2.26	0.50
1:B:200:MET:HG2	1:B:201:LEU:HD23	1.92	0.50
1:C:163:LEU:HD21	1:C:329:PHE:CE2	2.47	0.50
1:C:140:SER:CB	1:C:146:LEU:HD23	2.41	0.50
1:D:169:TRP:CE2	1:D:357:PRO:HG3	2.47	0.50
1:B:304:LYS:O	1:B:307:SER:HB3	2.12	0.50
1:C:200:MET:HG2	1:C:201:LEU:HD23	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:THR:O	1:A:151:VAL:HG22	2.12	0.49
1:C:182:GLY:O	1:C:265:PHE:HE1	1.95	0.49
1:D:182:GLY:O	1:D:265:PHE:HE1	1.95	0.49
1:A:273:GLU:O	1:A:276:GLU:HG2	2.12	0.49
1:A:140:SER:CB	1:A:146:LEU:HD23	2.42	0.49
1:A:169:TRP:CZ3	1:A:339:VAL:HG13	2.47	0.49
1:B:230:LEU:HD11	2:F:12:LEU:HD11	1.93	0.49
1:D:170:GLN:HG2	1:D:354:THR:HB	1.93	0.49
1:A:304:LYS:O	1:A:307:SER:HB3	2.13	0.49
1:B:182:GLY:O	1:B:265:PHE:HE1	1.96	0.49
1:C:146:LEU:CD1	1:C:151:VAL:HG13	2.41	0.49
1:A:230:LEU:HD11	2:E:12:LEU:HD11	1.95	0.49
1:B:180:LEU:HD23	1:B:180:LEU:N	2.28	0.49
1:D:182:GLY:N	1:D:188:LYS:HD3	2.27	0.49
1:B:147:THR:HB	1:B:149:GLU:H	1.78	0.49
1:A:147:THR:N	1:A:150:ASN:HD21	2.10	0.49
1:C:169:TRP:CE3	1:C:339:VAL:HG13	2.48	0.49
1:A:125:LYS:HG2	1:A:330:ASN:ND2	2.28	0.48
1:B:224:LYS:HA	1:B:234:LEU:HD12	1.94	0.48
1:D:169:TRP:CZ3	1:D:339:VAL:HG13	2.47	0.48
1:D:180:LEU:HG	1:D:192:LEU:HD13	1.95	0.48
1:B:163:LEU:HD21	1:B:329:PHE:CE2	2.48	0.48
1:B:267:ASP:C	1:B:267:ASP:OD1	2.56	0.48
1:D:146:LEU:CD1	1:D:151:VAL:HG13	2.42	0.48
1:C:169:TRP:CZ3	1:C:339:VAL:HG13	2.49	0.48
1:C:304:LYS:O	1:C:307:SER:HB3	2.13	0.48
1:D:304:LYS:O	1:D:307:SER:HB3	2.13	0.48
1:C:180:LEU:HD22	1:C:287:PHE:HB2	1.95	0.47
1:C:124:ILE:CG2	1:C:125:LYS:N	2.77	0.47
1:D:224:LYS:HA	1:D:234:LEU:HD12	1.95	0.47
1:B:266:LYS:HE2	7:B:49:HOH:O	2.15	0.47
1:D:234:LEU:HD23	1:D:234:LEU:C	2.40	0.47
1:A:309:VAL:HG23	1:A:310:PRO:HD2	1.95	0.47
1:B:247:LYS:HZ3	1:B:282:SER:HB3	1.78	0.47
1:C:124:ILE:HG22	1:C:125:LYS:N	2.29	0.47
1:D:346:GLN:O	2:H:8:GLN:HB2	2.15	0.47
1:B:147:THR:N	1:B:150:ASN:HD21	2.12	0.47
1:C:217:ILE:CD1	2:H:9:ALA:HB2	2.45	0.47
1:D:125:LYS:HG2	1:D:330:ASN:ND2	2.30	0.47
1:B:221:GLU:O	1:B:225:THR:CG2	2.62	0.46
1:B:234:LEU:HD23	1:B:234:LEU:C	2.41	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:7:ASP:C	2:G:9:ALA:N	2.73	0.46
1:C:309:VAL:HG23	1:C:310:PRO:HD2	1.96	0.46
1:B:180:LEU:HG	1:B:192:LEU:HD13	1.98	0.46
1:B:309:VAL:HG23	1:B:310:PRO:HD2	1.98	0.46
1:A:173:ILE:HG23	1:A:178:ILE:HD11	1.98	0.46
1:B:173:ILE:HG23	1:B:178:ILE:HD11	1.97	0.46
1:A:214:THR:HB	2:F:6:TYR:CE2	2.48	0.46
1:B:205:LYS:HE3	7:B:27:HOH:O	2.15	0.46
1:A:180:LEU:HG	1:A:192:LEU:HD13	1.98	0.46
1:B:124:ILE:HG22	1:B:125:LYS:N	2.30	0.46
1:D:173:ILE:HG23	1:D:178:ILE:HD11	1.97	0.46
1:A:180:LEU:HD22	1:A:287:PHE:HB2	1.97	0.46
1:A:200:MET:O	1:A:204:HIS:HA	2.16	0.46
1:B:124:ILE:CG2	1:B:125:LYS:N	2.79	0.46
1:A:147:THR:HB	1:A:149:GLU:H	1.81	0.45
1:A:182:GLY:N	1:A:188:LYS:HD3	2.31	0.45
1:C:188:LYS:HE2	7:C:373:HOH:O	2.16	0.45
1:C:317:THR:HA	1:C:343:THR:OG1	2.16	0.45
1:C:295:LYS:HG2	6:D:6:SO4:O1	2.16	0.45
2:F:7:ASP:C	2:F:9:ALA:N	2.73	0.45
1:B:125:LYS:HG2	1:B:330:ASN:ND2	2.31	0.45
1:A:359:GLY:HA3	6:A:7:SO4:O1	2.17	0.45
1:B:346:GLN:O	2:F:8:GLN:HB2	2.17	0.45
1:A:165:SER:OG	1:A:168:LYS:HE3	2.15	0.45
1:A:221:GLU:O	1:A:225:THR:HG23	2.16	0.45
1:D:147:THR:N	1:D:150:ASN:HD21	2.14	0.45
1:A:221:GLU:O	1:A:225:THR:CG2	2.64	0.45
1:A:247:LYS:NZ	1:A:282:SER:HB3	2.32	0.45
1:B:267:ASP:OD1	1:B:268:PRO:N	2.50	0.45
1:B:348:VAL:HA	1:B:349:PRO:HA	1.68	0.45
1:C:348:VAL:HA	1:C:349:PRO:HA	1.69	0.45
1:B:200:MET:HE1	1:B:230:LEU:O	2.18	0.44
1:C:177:TYR:CD1	1:C:256:VAL:HB	2.52	0.44
1:D:221:GLU:O	1:D:225:THR:CG2	2.64	0.44
1:D:267:ASP:C	1:D:267:ASP:OD1	2.60	0.44
1:A:146:LEU:CD1	1:A:151:VAL:HG13	2.45	0.44
1:B:208:ALA:O	1:B:256:VAL:HA	2.17	0.44
1:B:264:ASN:HB2	6:B:1:SO4:O1	2.18	0.44
1:C:234:LEU:HD23	1:C:234:LEU:C	2.42	0.44
1:D:200:MET:HG2	1:D:201:LEU:HD23	1.98	0.44
2:E:7:ASP:C	2:E:9:ALA:N	2.75	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ASN:N	6:A:3:SO4:O3	2.49	0.44
1:D:180:LEU:HD23	1:D:180:LEU:N	2.32	0.44
3:D:4:GDP:O3B	5:D:368:AF3:F2	2.26	0.44
1:A:182:GLY:O	1:A:265:PHE:HE1	2.01	0.44
1:A:180:LEU:HD23	1:A:180:LEU:N	2.33	0.44
1:A:348:VAL:HA	1:A:349:PRO:HA	1.69	0.44
1:C:188:LYS:N	3:C:3:GDP:O1B	2.48	0.44
1:C:346:GLN:O	2:G:8:GLN:HB2	2.17	0.44
1:A:131:ASN:O	1:A:135:LYS:HG3	2.18	0.43
1:D:124:ILE:HG22	1:D:125:LYS:N	2.33	0.43
1:D:163:LEU:HD21	1:D:329:PHE:CD2	2.52	0.43
1:D:247:LYS:HZ3	1:D:282:SER:HB3	1.82	0.43
1:A:124:ILE:HG22	1:A:125:LYS:N	2.33	0.43
1:D:309:VAL:HG23	1:D:310:PRO:HD2	2.00	0.43
1:D:124:ILE:CG2	1:D:125:LYS:N	2.81	0.43
1:A:272:ASP:O	1:A:273:GLU:C	2.61	0.43
1:A:282:SER:CB	6:A:13:SO4:O2	2.67	0.43
1:B:165:SER:OG	1:B:168:LYS:HE3	2.18	0.43
1:C:125:LYS:HG2	1:C:330:ASN:ND2	2.34	0.43
1:C:200:MET:O	1:C:204:HIS:HA	2.19	0.43
1:C:267:ASP:OD1	1:C:267:ASP:C	2.61	0.43
1:A:118:LEU:HD23	1:A:118:LEU:HA	1.83	0.43
1:A:234:LEU:HD23	1:A:234:LEU:C	2.42	0.43
1:D:267:ASP:OD1	1:D:268:PRO:CD	2.66	0.43
1:C:140:SER:HB2	1:C:146:LEU:HD23	2.01	0.43
1:B:214:THR:O	1:B:214:THR:HG22	2.19	0.43
1:C:119:LEU:HB3	1:C:129:LYS:CG	2.49	0.43
1:C:173:ILE:HG23	1:C:178:ILE:HD11	2.00	0.43
1:D:230:LEU:CD1	2:H:12:LEU:HD11	2.47	0.43
1:C:366:ARG:HD3	1:C:366:ARG:N	2.34	0.42
1:D:247:LYS:NZ	1:D:282:SER:HB3	2.34	0.42
1:D:344:ASN:C	1:D:344:ASN:HD22	2.28	0.42
2:G:18:LYS:HB2	2:G:18:LYS:HE3	1.84	0.42
1:A:124:ILE:CG2	1:A:125:LYS:N	2.82	0.42
1:A:217:ILE:O	1:B:222:GLN:HG3	2.20	0.42
1:A:267:ASP:HA	1:A:268:PRO:HD3	1.86	0.42
1:C:247:LYS:NZ	1:C:282:SER:HB3	2.34	0.42
1:D:200:MET:HE1	1:D:230:LEU:O	2.19	0.42
1:D:348:VAL:HA	1:D:349:PRO:HA	1.67	0.42
2:H:7:ASP:C	2:H:9:ALA:N	2.76	0.42
1:A:358:LEU:N	6:A:10:SO4:O2	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:366:ARG:N	1:D:366:ARG:HD3	2.35	0.42
2:H:18:LYS:HE3	2:H:18:LYS:HB2	1.86	0.42
1:B:247:LYS:NZ	1:B:282:SER:HB3	2.35	0.42
1:C:223:LEU:HD12	1:C:223:LEU:HA	1.86	0.42
1:A:163:LEU:HD21	1:A:329:PHE:CD2	2.53	0.42
1:C:180:LEU:HG	1:C:192:LEU:HD13	2.01	0.42
1:D:267:ASP:HA	1:D:268:PRO:HD3	1.88	0.42
1:A:126:GLU:O	1:A:127:SER:C	2.62	0.42
1:D:131:ASN:O	1:D:135:LYS:HG3	2.20	0.42
1:A:140:SER:HB2	1:A:146:LEU:HD23	2.02	0.42
1:B:316:PHE:CZ	1:B:328:VAL:HG13	2.55	0.42
1:A:267:ASP:OD1	1:A:267:ASP:C	2.63	0.42
1:A:267:ASP:OD1	1:A:268:PRO:CD	2.67	0.42
1:C:118:LEU:HD23	1:C:118:LEU:HA	1.80	0.42
1:D:165:SER:OG	1:D:168:LYS:HE3	2.20	0.42
1:A:341:PHE:CD1	1:A:352:ILE:HD11	2.55	0.41
1:B:213:ASP:HA	1:B:261:ALA:HB2	2.00	0.41
1:B:230:LEU:CD1	2:F:12:LEU:HD11	2.50	0.41
1:B:264:ASN:CB	6:B:1:SO4:O1	2.68	0.41
1:C:182:GLY:N	1:C:188:LYS:HD3	2.35	0.41
1:D:140:SER:HB2	1:D:146:LEU:HD23	2.02	0.41
1:A:200:MET:HE3	1:A:207:ILE:HG12	2.02	0.41
1:D:217:ILE:CD1	2:G:9:ALA:HB2	2.49	0.41
1:B:216:ARG:O	1:B:216:ARG:HG3	2.15	0.41
1:B:267:ASP:OD1	1:B:268:PRO:CD	2.68	0.41
1:A:177:TYR:CD1	1:A:256:VAL:HB	2.56	0.41
1:A:217:ILE:CD1	2:F:9:ALA:HB2	2.45	0.41
1:B:131:ASN:O	1:B:135:LYS:HG3	2.21	0.41
1:A:214:THR:HG21	1:A:238:TYR:HE2	1.80	0.41
1:C:192:LEU:HD11	1:C:257:PHE:HB3	2.02	0.41
1:C:214:THR:HB	2:H:6:TYR:CE2	2.51	0.41
1:D:272:ASP:O	1:D:273:GLU:C	2.64	0.41
1:A:223:LEU:HD12	1:A:223:LEU:HA	1.86	0.41
1:D:208:ALA:O	1:D:256:VAL:HA	2.21	0.41
1:B:126:GLU:O	1:B:127:SER:C	2.63	0.40
1:B:267:ASP:HA	1:B:268:PRO:HD3	1.90	0.40
1:B:344:ASN:C	1:B:344:ASN:HD22	2.29	0.40
1:C:176:LYS:NZ	1:C:251:SER:HA	2.36	0.40
1:C:128:THR:HG23	1:C:162:MET:HE1	2.03	0.40
1:C:165:SER:OG	1:C:168:LYS:HE3	2.20	0.40
1:C:110:GLU:CB	1:C:111:PRO:CD	2.93	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:PRO:O	1:C:114:LYS:HB3	2.22	0.40
1:C:263:ARG:HA	6:C:4:SO4:O4	2.21	0.40
1:D:267:ASP:OD1	1:D:268:PRO:N	2.54	0.40
1:D:221:GLU:O	1:D:222:GLN:C	2.65	0.40
1:B:140:SER:HB2	1:B:146:LEU:HD23	2.04	0.40
1:C:214:THR:O	1:C:214:THR:HG22	2.20	0.40

There are no symmetry-related clashes.

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	256/296 (86%)	238 (93%)	17 (7%)	1 (0%)	30	57
1	B	256/296 (86%)	238 (93%)	17 (7%)	1 (0%)	30	57
1	C	256/296 (86%)	235 (92%)	20 (8%)	1 (0%)	30	57
1	D	256/296 (86%)	237 (93%)	18 (7%)	1 (0%)	30	57
2	E	14/23 (61%)	12 (86%)	1 (7%)	1 (7%)	1	4
2	F	14/23 (61%)	12 (86%)	2 (14%)	0	100	100
2	G	14/23 (61%)	12 (86%)	1 (7%)	1 (7%)	1	4
2	H	14/23 (61%)	12 (86%)	2 (14%)	0	100	100
All	All	1080/1276 (85%)	996 (92%)	78 (7%)	6 (1%)	21	48

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	GLU
1	B	110	GLU
1	C	110	GLU
1	D	110	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	7	ASP
2	G	7	ASP

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	228/262 (87%)	197 (86%)	31 (14%)	3	13
1	B	228/262 (87%)	197 (86%)	31 (14%)	3	13
1	C	228/262 (87%)	197 (86%)	31 (14%)	3	13
1	D	228/262 (87%)	198 (87%)	30 (13%)	4	14
2	E	13/20 (65%)	11 (85%)	2 (15%)	2	10
2	F	13/20 (65%)	11 (85%)	2 (15%)	2	10
2	G	13/20 (65%)	11 (85%)	2 (15%)	2	10
2	H	13/20 (65%)	11 (85%)	2 (15%)	2	10
All	All	964/1128 (86%)	833 (86%)	131 (14%)	3	13

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	GLU
1	A	127	SER
1	A	130	THR
1	A	131	ASN
1	A	141	VAL
1	A	147	THR
1	A	150	ASN
1	A	151	VAL
1	A	152	VAL
1	A	180	LEU
1	A	183	SER
1	A	184	THR
1	A	195	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	199	SER
1	A	212	THR
1	A	216	ARG
1	A	225	THR
1	A	230	LEU
1	A	234	LEU
1	A	275	LYS
1	A	282	SER
1	A	286	SER
1	A	307	SER
1	A	309	VAL
1	A	323	THR
1	A	339	VAL
1	A	344	ASN
1	A	350	GLU
1	A	355	VAL
1	A	358	LEU
1	A	364	LEU
1	B	116	GLU
1	B	127	SER
1	B	131	ASN
1	B	140	SER
1	B	141	VAL
1	B	147	THR
1	B	150	ASN
1	B	151	VAL
1	B	152	VAL
1	B	180	LEU
1	B	183	SER
1	B	184	THR
1	B	195	LEU
1	B	199	SER
1	B	212	THR
1	B	216	ARG
1	B	225	THR
1	B	230	LEU
1	B	234	LEU
1	B	275	LYS
1	B	282	SER
1	B	286	SER
1	B	307	SER
1	B	309	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	323	THR
1	B	339	VAL
1	B	344	ASN
1	B	350	GLU
1	B	355	VAL
1	B	358	LEU
1	B	364	LEU
1	C	116	GLU
1	C	127	SER
1	C	131	ASN
1	C	140	SER
1	C	141	VAL
1	C	147	THR
1	C	150	ASN
1	C	151	VAL
1	C	152	VAL
1	C	180	LEU
1	C	183	SER
1	C	184	THR
1	C	195	LEU
1	C	199	SER
1	C	212	THR
1	C	216	ARG
1	C	225	THR
1	C	230	LEU
1	C	234	LEU
1	C	275	LYS
1	C	282	SER
1	C	286	SER
1	C	307	SER
1	C	309	VAL
1	C	323	THR
1	C	339	VAL
1	C	344	ASN
1	C	350	GLU
1	C	355	VAL
1	C	358	LEU
1	C	364	LEU
1	D	116	GLU
1	D	127	SER
1	D	131	ASN
1	D	140	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	141	VAL
1	D	147	THR
1	D	150	ASN
1	D	151	VAL
1	D	152	VAL
1	D	180	LEU
1	D	183	SER
1	D	184	THR
1	D	195	LEU
1	D	199	SER
1	D	212	THR
1	D	216	ARG
1	D	225	THR
1	D	230	LEU
1	D	234	LEU
1	D	275	LYS
1	D	282	SER
1	D	286	SER
1	D	309	VAL
1	D	323	THR
1	D	339	VAL
1	D	344	ASN
1	D	350	GLU
1	D	355	VAL
1	D	358	LEU
1	D	364	LEU
2	E	19	ARG
2	E	21	ARG
2	F	19	ARG
2	F	21	ARG
2	G	19	ARG
2	G	21	ARG
2	H	19	ARG
2	H	21	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
1	A	174	HIS
1	A	231	GLN
1	A	245	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	269	GLN
1	A	330	ASN
1	B	131	ASN
1	B	150	ASN
1	B	174	HIS
1	B	231	GLN
1	B	244	GLN
1	B	344	ASN
1	B	353	GLN
1	C	150	ASN
1	C	174	HIS
1	C	231	GLN
1	C	330	ASN
1	D	131	ASN
1	D	150	ASN
1	D	231	GLN
1	D	245	GLN
1	D	269	GLN
1	D	330	ASN
1	D	344	ASN
1	D	353	GLN

5.3.3 RNA [i](#)

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 27 ligands modelled in this entry, 4 are monoatomic - leaving 23 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
6	SO4	C	4	-	4,4,4	0.20	0	6,6,6	0.21	0
6	SO4	B	8	-	4,4,4	0.27	0	6,6,6	0.30	0
6	SO4	C	11	-	4,4,4	0.25	0	6,6,6	0.40	0
6	SO4	A	5	-	4,4,4	0.27	0	6,6,6	0.20	0
6	SO4	D	12	-	4,4,4	0.23	0	6,6,6	0.25	0
5	AF3	B	368	3,7	0,3,3	-	-	-	-	-
6	SO4	A	10	-	4,4,4	0.26	0	6,6,6	0.21	0
5	AF3	D	368	3,7	0,3,3	-	-	-	-	-
3	GDP	B	2	5,4	29,30,30	1.14	3 (10%)	45,47,47	1.86	10 (22%)
6	SO4	C	9	-	4,4,4	0.29	0	6,6,6	0.27	0
6	SO4	C	15	-	4,4,4	0.22	0	6,6,6	0.28	0
3	GDP	A	1	5,4	29,30,30	1.44	4 (13%)	45,47,47	1.85	6 (13%)
3	GDP	C	3	5,4	29,30,30	1.38	4 (13%)	45,47,47	1.94	9 (20%)
5	AF3	C	368	3,7	0,3,3	-	-	-	-	-
6	SO4	D	6	-	4,4,4	0.21	0	6,6,6	0.20	0
6	SO4	D	2	-	4,4,4	0.25	0	6,6,6	0.28	0
5	AF3	A	368	3	0,3,3	-	-	-	-	-
6	SO4	B	1	-	4,4,4	0.15	0	6,6,6	0.42	0
6	SO4	A	13	-	4,4,4	0.26	0	6,6,6	0.31	0
6	SO4	B	14	-	4,4,4	0.23	0	6,6,6	0.24	0
6	SO4	A	3	-	4,4,4	0.27	0	6,6,6	0.24	0
6	SO4	A	7	-	4,4,4	0.28	0	6,6,6	0.19	0
3	GDP	D	4	5,4	29,30,30	1.21	4 (13%)	45,47,47	1.81	10 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GDP	A	1	5,4	-	2/16/32/32	0/3/3/3
3	GDP	D	4	5,4	-	3/16/32/32	0/3/3/3
3	GDP	C	3	5,4	-	1/16/32/32	0/3/3/3
3	GDP	B	2	5,4	-	1/16/32/32	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	GDP	PA-O3A	4.30	1.64	1.59
3	C	3	GDP	PA-O3A	3.98	1.63	1.59
3	B	2	GDP	C5-C4	2.92	1.46	1.38
3	C	3	GDP	C5-C4	2.90	1.46	1.38
3	A	1	GDP	C5-N7	-2.83	1.33	1.39
3	A	1	GDP	C6-N1	-2.79	1.33	1.38
3	D	4	GDP	C5-C4	2.77	1.46	1.38
3	A	1	GDP	C5-C4	2.77	1.46	1.38
3	C	3	GDP	C6-N1	-2.72	1.33	1.38
3	D	4	GDP	C6-N1	-2.71	1.33	1.38
3	D	4	GDP	PA-O3A	2.41	1.62	1.59
3	C	3	GDP	C5-N7	-2.33	1.34	1.39
3	D	4	GDP	C5-N7	-2.32	1.34	1.39
3	B	2	GDP	C6-N1	-2.31	1.34	1.38
3	B	2	GDP	C5-N7	-2.09	1.34	1.39

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	GDP	C5-C4-N3	-6.72	117.69	128.39
3	A	1	GDP	C5-C4-N3	-6.65	117.81	128.39
3	D	4	GDP	C5-C4-N3	-6.20	118.52	128.39
3	B	2	GDP	C5-C4-N3	-6.05	118.76	128.39
3	C	3	GDP	C2-N3-C4	5.63	122.00	112.30
3	B	2	GDP	C2-N3-C4	5.41	121.63	112.30
3	A	1	GDP	C2-N3-C4	5.39	121.58	112.30
3	C	3	GDP	N9-C4-N3	4.97	135.89	125.95
3	D	4	GDP	C2-N3-C4	4.95	120.83	112.30
3	A	1	GDP	N9-C4-N3	4.83	135.61	125.95
3	D	4	GDP	N9-C4-N3	4.77	135.50	125.95
3	B	2	GDP	N9-C4-N3	4.28	134.51	125.95
3	B	2	GDP	C6-C5-N7	3.41	136.49	130.29
3	C	3	GDP	O2B-PB-O3A	3.16	115.23	104.64
3	B	2	GDP	O2A-PA-O3A	3.09	115.63	107.27
3	D	4	GDP	C6-C5-N7	3.03	135.80	130.29
3	A	1	GDP	C6-C5-N7	2.89	135.56	130.29
3	C	3	GDP	C6-C5-N7	2.64	135.09	130.29
3	A	1	GDP	C4-C5-N7	-2.54	106.64	110.67
3	B	2	GDP	C4-C5-N7	-2.50	106.71	110.67
3	D	4	GDP	C4-C5-N7	-2.49	106.73	110.67
3	C	3	GDP	O6-C6-C5	-2.37	120.26	126.53
3	D	4	GDP	O2B-PB-O3A	2.33	112.46	104.64
3	D	4	GDP	O6-C6-C5	-2.32	120.40	126.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	GDP	O4'-C1'-C2'	-2.24	101.83	106.62
3	C	3	GDP	O3'-C3'-C2'	-2.22	104.69	111.82
3	C	3	GDP	C4-C5-N7	-2.20	107.18	110.67
3	B	2	GDP	O6-C6-C5	-2.18	120.78	126.53
3	B	2	GDP	O3'-C3'-C2'	-2.18	104.84	111.82
3	A	1	GDP	O4'-C1'-N9	2.15	113.23	108.36
3	D	4	GDP	C8-N7-C5	2.10	108.01	104.26
3	B	2	GDP	O2B-PB-O3A	2.09	111.63	104.64
3	B	2	GDP	C5-C6-N1	2.08	118.54	113.25
3	D	4	GDP	O4'-C1'-C2'	-2.07	102.18	106.62
3	D	4	GDP	C5-C6-N1	2.06	118.49	113.25

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	4	GDP	PA-O3A-PB-O2B
3	A	1	GDP	PA-O3A-PB-O3B
3	B	2	GDP	PA-O3A-PB-O1B
3	A	1	GDP	PA-O3A-PB-O2B
3	C	3	GDP	PA-O3A-PB-O3B
3	D	4	GDP	PA-O3A-PB-O3B
3	D	4	GDP	PA-O3A-PB-O1B

There are no ring outliers.

15 monomers are involved in 27 short contacts:

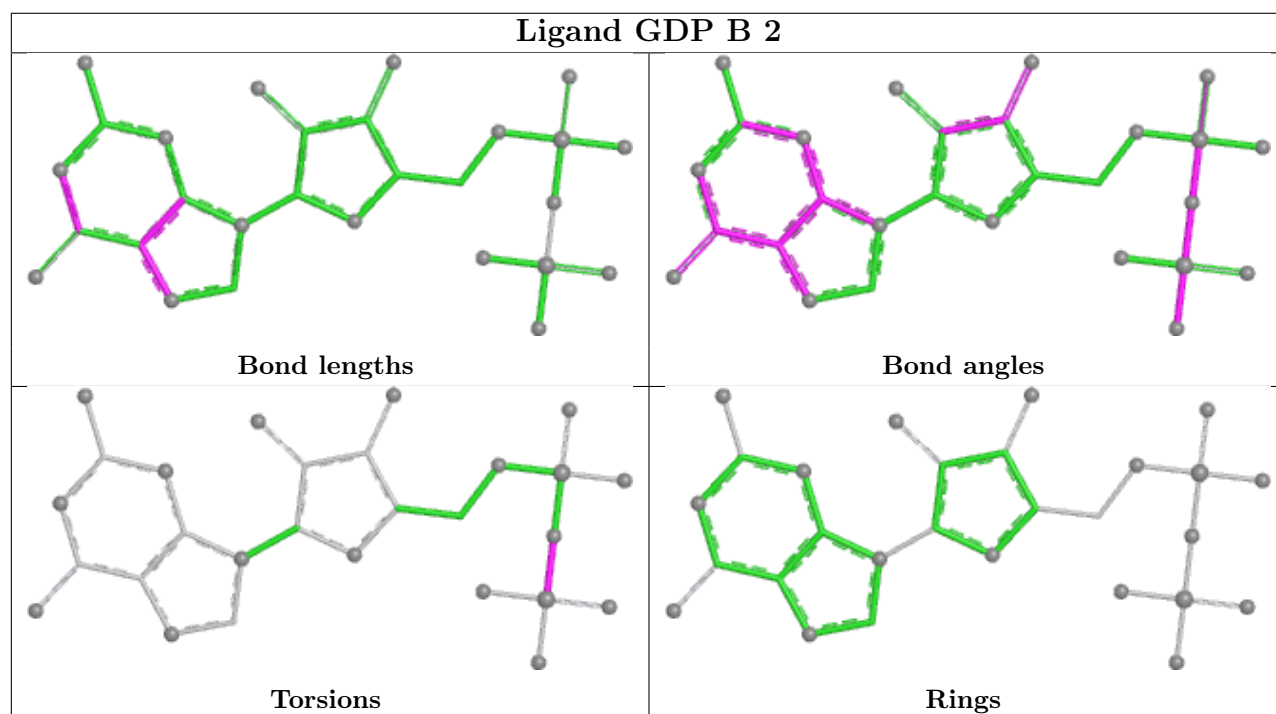
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	4	SO4	2	0
6	B	8	SO4	2	0
6	A	5	SO4	2	0
6	A	10	SO4	3	0
5	D	368	AF3	1	0
6	C	9	SO4	2	0
3	C	3	GDP	1	0
6	D	6	SO4	2	0
6	D	2	SO4	1	0
6	B	1	SO4	4	0
6	A	13	SO4	2	0
6	B	14	SO4	2	0
6	A	3	SO4	1	0

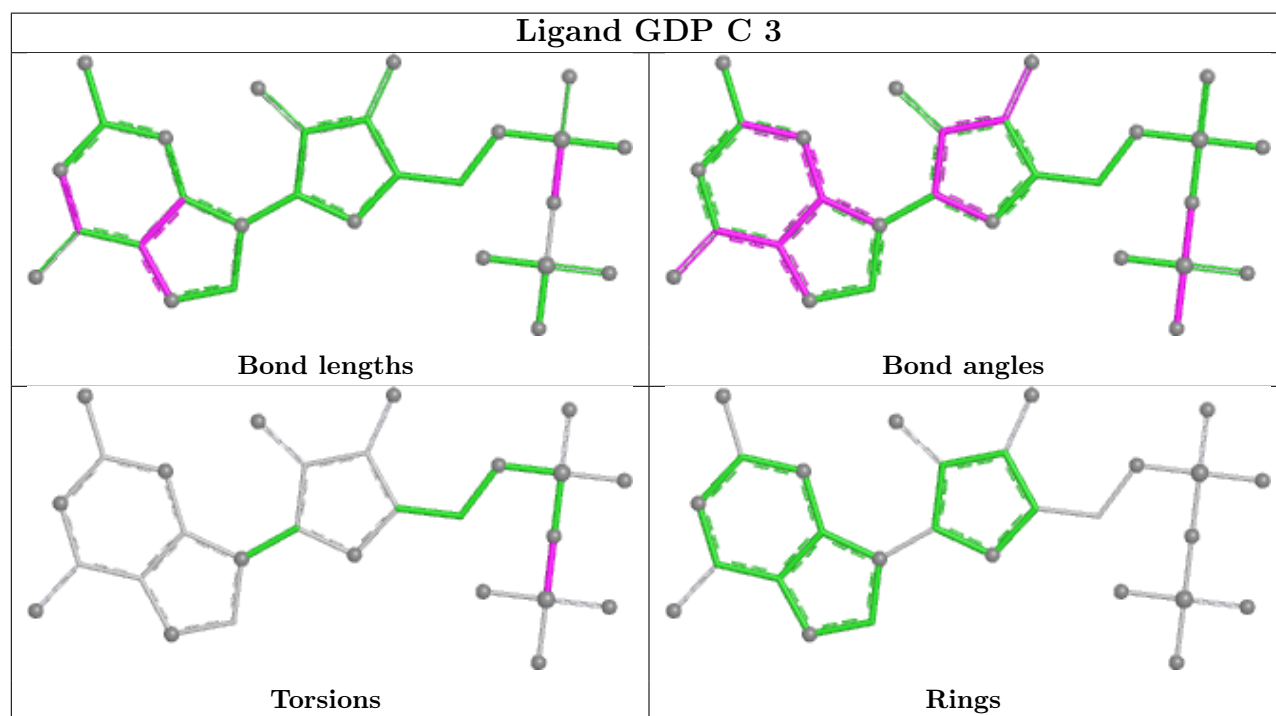
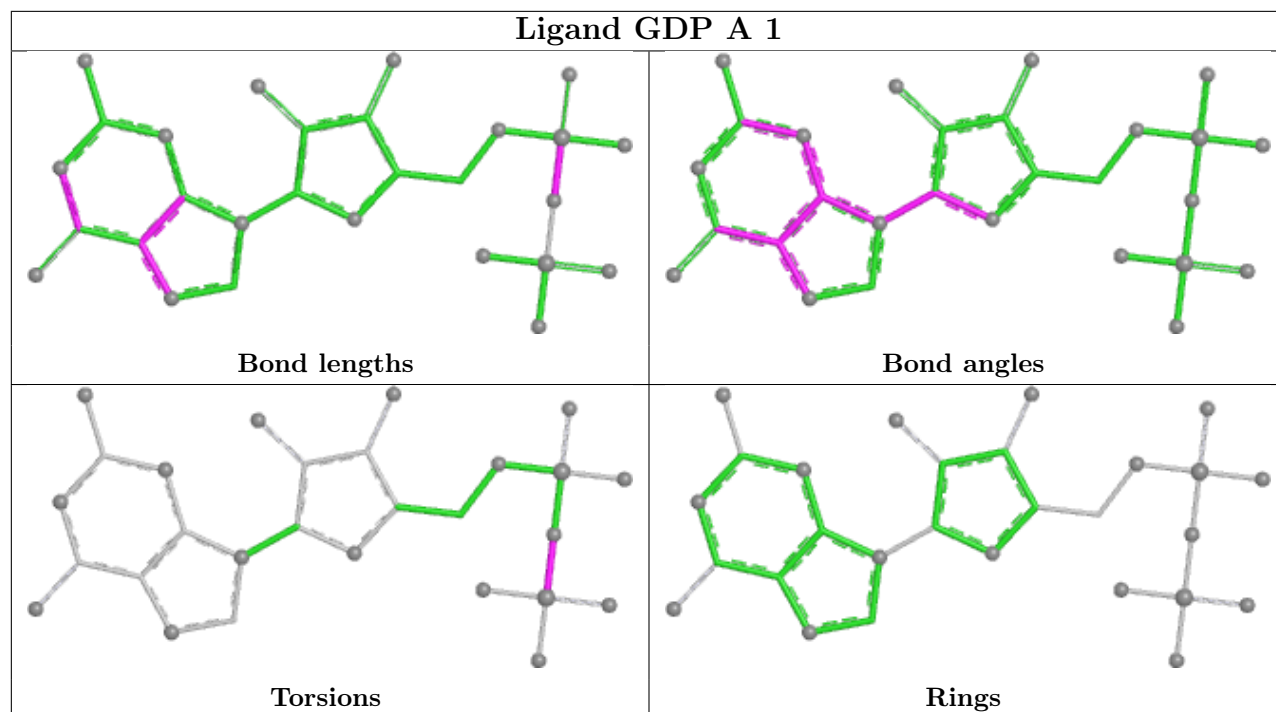
Continued on next page...

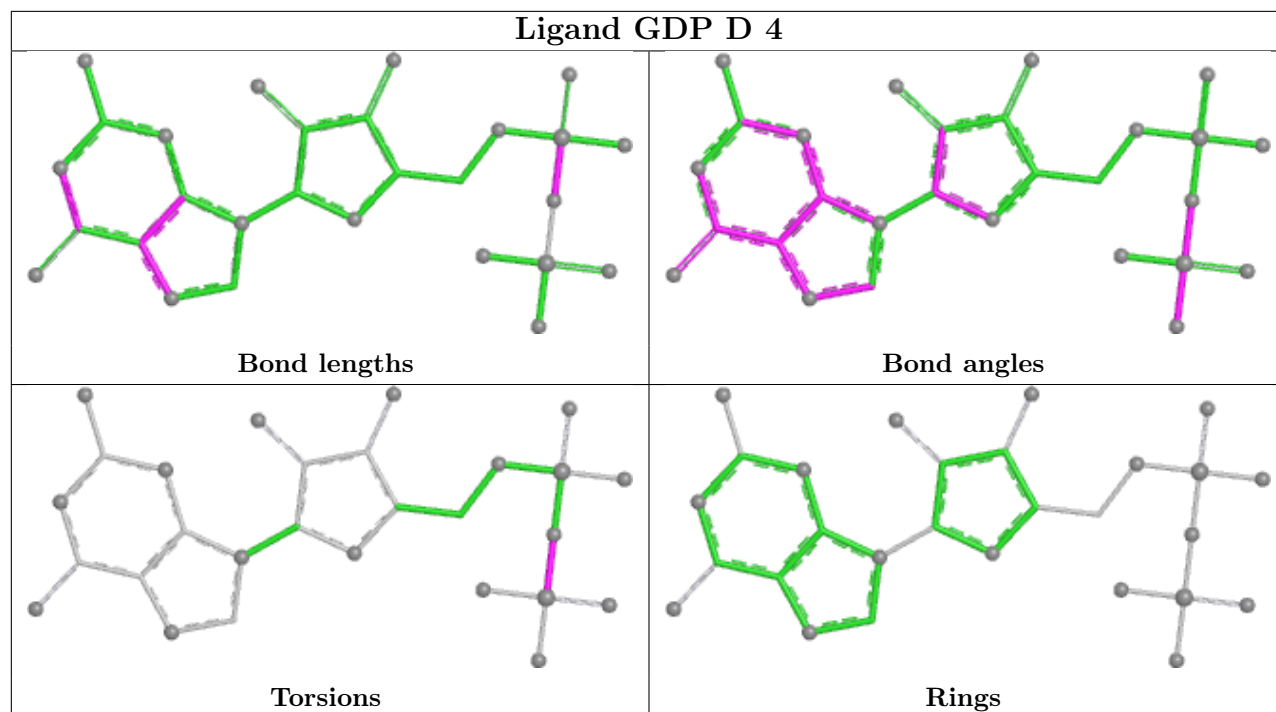
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	7	SO4	1	0
3	D	4	GDP	2	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	258/296 (87%)	-0.23	8 (3%)	51	29	7, 22, 74, 103	0
1	B	258/296 (87%)	-0.25	5 (1%)	66	43	7, 22, 76, 99	0
1	C	258/296 (87%)	-0.23	7 (2%)	56	33	7, 22, 74, 97	0
1	D	258/296 (87%)	-0.22	9 (3%)	47	26	8, 22, 75, 101	0
2	E	16/23 (69%)	0.10	2 (12%)	8	4	12, 20, 90, 98	0
2	F	16/23 (69%)	0.10	2 (12%)	8	4	13, 21, 90, 103	0
2	G	16/23 (69%)	-0.07	3 (18%)	3	2	13, 21, 93, 100	0
2	H	16/23 (69%)	0.07	2 (12%)	8	4	13, 21, 90, 104	0
All	All	1096/1276 (85%)	-0.21	38 (3%)	47	26	7, 22, 78, 104	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	145	GLY	4.8
1	A	143	ALA	4.7
1	A	145	GLY	4.3
1	B	143	ALA	4.2
2	E	6	TYR	4.2
1	C	109	PRO	4.0
1	C	144	GLY	4.0
1	A	144	GLY	3.9
1	D	144	GLY	3.8
1	A	109	PRO	3.6
1	B	109	PRO	3.5
1	A	146	LEU	3.4
1	D	111	PRO	3.2
2	H	21	ARG	3.1
1	A	149	GLU	3.1
2	F	6	TYR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	276	GLU	2.9
1	B	144	GLY	2.9
1	B	142	GLU	2.8
1	C	110	GLU	2.8
2	H	6	TYR	2.8
2	F	21	ARG	2.8
2	G	6	TYR	2.6
1	D	139	PHE	2.5
1	D	109	PRO	2.4
1	C	174	HIS	2.3
1	D	147	THR	2.3
1	D	112	LEU	2.3
1	D	143	ALA	2.3
2	G	21	ARG	2.2
1	A	142	GLU	2.2
1	C	148	GLU	2.2
1	A	110	GLU	2.1
1	C	140	SER	2.1
1	D	141	VAL	2.1
2	E	21	ARG	2.0
2	G	20	GLU	2.0
1	C	113	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	SO4	C	15	5/5	0.83	0.12	42,68,92,109	0

Continued on next page...

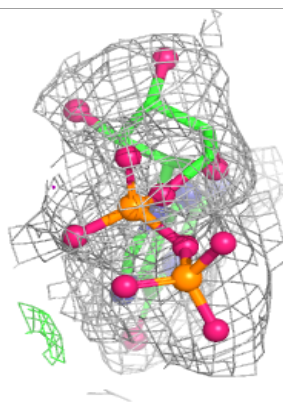
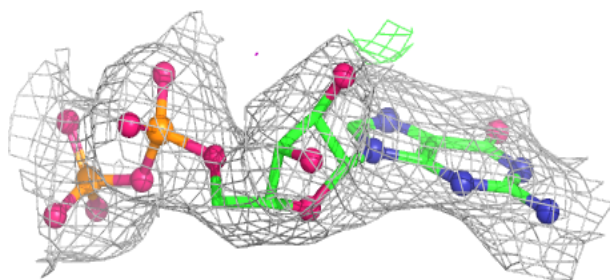
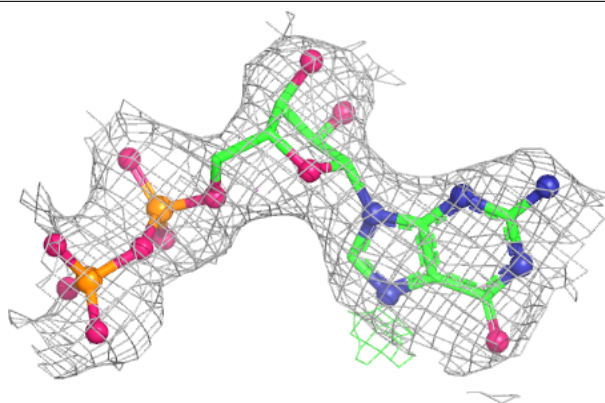
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	D	12	5/5	0.87	0.15	30,46,99,107	0
6	SO4	B	14	5/5	0.88	0.14	66,72,79,79	0
6	SO4	B	8	5/5	0.91	0.18	35,38,56,61	0
6	SO4	A	13	5/5	0.91	0.10	47,60,92,107	0
6	SO4	C	11	5/5	0.93	0.09	31,35,79,97	0
4	MG	C	367	1/1	0.94	0.08	23,23,23,23	0
6	SO4	D	6	5/5	0.94	0.23	23,44,54,55	0
6	SO4	A	10	5/5	0.94	0.25	25,45,65,97	0
6	SO4	A	7	5/5	0.95	0.10	37,46,51,61	0
6	SO4	C	9	5/5	0.95	0.23	11,28,51,75	0
6	SO4	A	5	5/5	0.96	0.19	28,36,46,54	0
4	MG	A	367	1/1	0.97	0.09	14,14,14,14	0
5	AF3	B	368	4/4	0.98	0.05	7,19,24,31	0
5	AF3	C	368	4/4	0.98	0.07	15,16,27,41	0
4	MG	D	367	1/1	0.98	0.08	4,4,4,4	0
5	AF3	A	368	4/4	0.98	0.06	10,15,18,34	0
6	SO4	C	4	5/5	0.98	0.13	17,19,40,46	0
4	MG	B	367	1/1	0.99	0.05	10,10,10,10	0
5	AF3	D	368	4/4	0.99	0.05	13,15,23,31	0
6	SO4	A	3	5/5	0.99	0.09	14,15,31,53	0
3	GDP	B	2	28/28	0.99	0.05	6,12,19,20	0
3	GDP	C	3	28/28	0.99	0.05	6,12,18,21	0
3	GDP	D	4	28/28	0.99	0.05	5,13,17,19	0
6	SO4	D	2	5/5	0.99	0.09	21,25,35,50	0
3	GDP	A	1	28/28	0.99	0.04	6,10,15,19	0
6	SO4	B	1	5/5	0.99	0.10	13,24,30,33	0

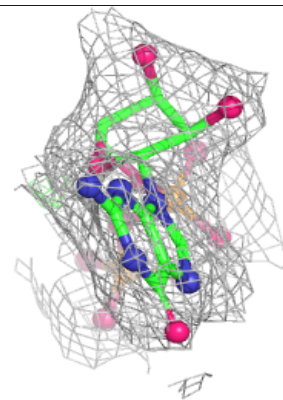
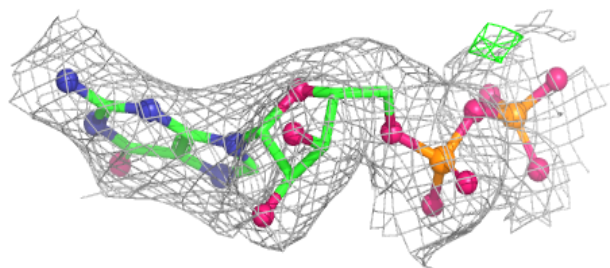
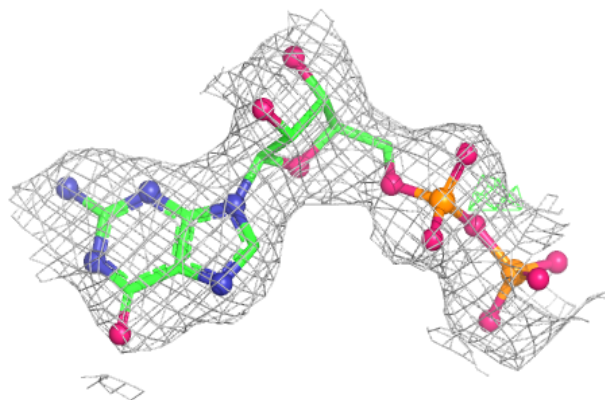
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP B 2:

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

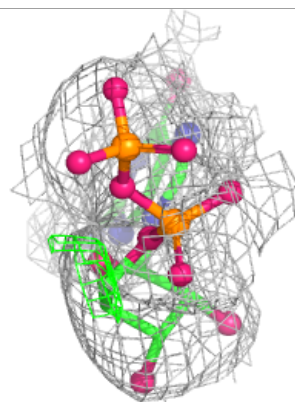
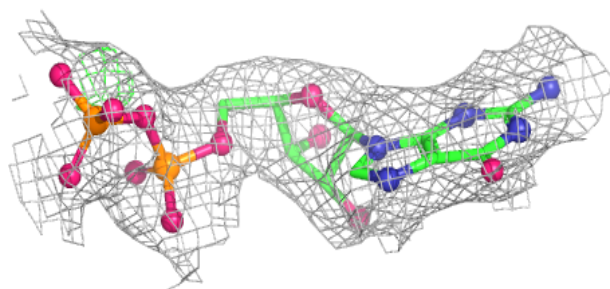
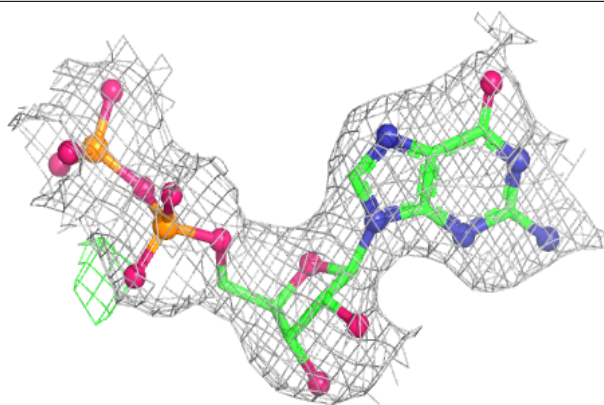
**Electron density around GDP C 3:**

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

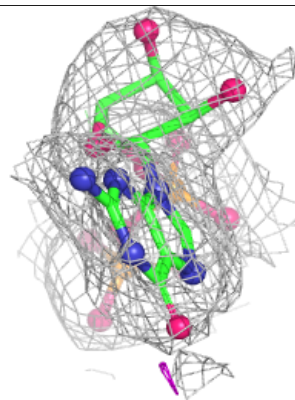
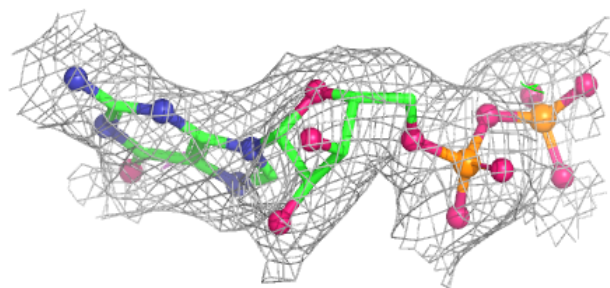
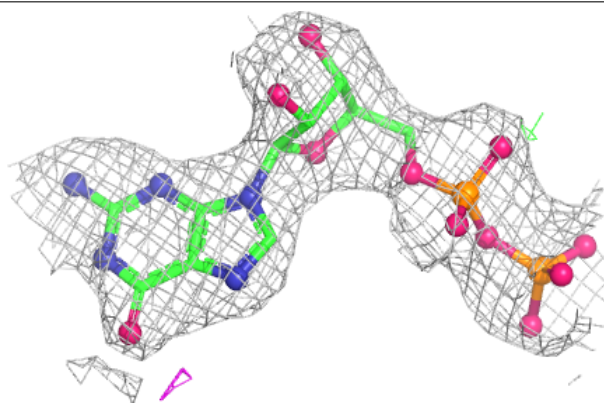


Electron density around GDP D 4:

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

**Electron density around GDP A 1:**

$2mF_o-DF_c$ (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.