



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2026 – 04:28 PM JST

PDB ID : 24HS / pdb_000024hs
Title : Human KRAS G12D (GDP-bound) in complex with macrocyclic peptide inhibitor AP4959
Authors : Yamano, T.; Chiyoda, A.; Fukami, T.A.; Tanada, M.; Irie, M.; Torizawa, T.
Deposited on : 2026-03-04
Resolution : 2.53 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:

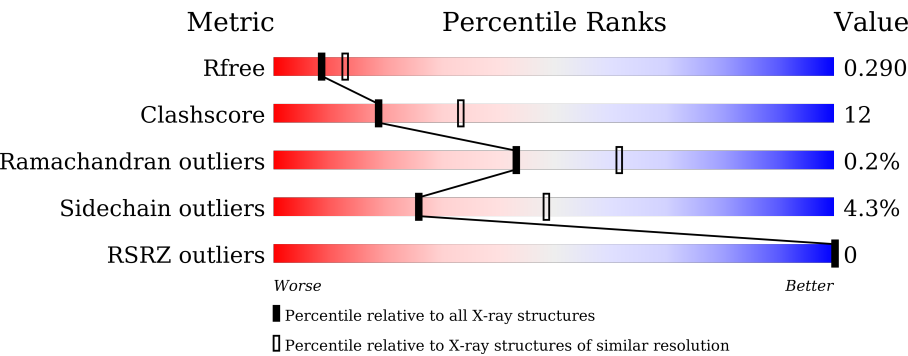
MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
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 i

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

The reported resolution of this entry is 2.53 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.










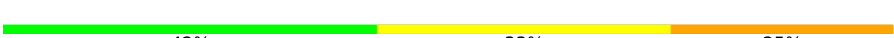


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	179	<div><div>81%15%..</div></div>
1	B	179	<div><div>70%24%.5%</div></div>
1	C	179	<div><div>78%17%..</div></div>
1	D	179	<div><div>73%22%..</div></div>
1	E	179	<div><div>74%22%..</div></div>
1	F	179	<div><div>56%38%.5%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	179	
1	H	179	
2	I	12	
2	J	12	
2	K	12	
2	L	12	
2	M	12	
2	N	12	
2	O	12	
2	P	12	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12116 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 Isoform 2B of GTPase KRas.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	173	Total	C	N	O	S	0	0	0
			1370	855	236	272	7			
1	B	170	Total	C	N	O	S	0	0	0
			1356	847	233	270	6			
1	C	173	Total	C	N	O	S	0	0	0
			1370	855	236	272	7			
1	D	171	Total	C	N	O	S	0	0	0
			1364	852	234	271	7			
1	E	172	Total	C	N	O	S	0	0	0
			1334	833	231	264	6			
1	F	170	Total	C	N	O	S	0	0	0
			1308	818	221	263	6			
1	G	172	Total	C	N	O	S	0	0	0
			1335	837	230	261	7			
1	H	171	Total	C	N	O	S	0	0	0
			1317	825	220	265	7			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P01116
A	-3	SER	-	expression tag	UNP P01116
A	-2	SER	-	expression tag	UNP P01116
A	-1	GLY	-	expression tag	UNP P01116
A	0	GLY	-	expression tag	UNP P01116
A	1	SER	-	expression tag	UNP P01116
A	12	ASP	GLY	engineered mutation	UNP P01116
B	-4	GLY	-	expression tag	UNP P01116
B	-3	SER	-	expression tag	UNP P01116
B	-2	SER	-	expression tag	UNP P01116
B	-1	GLY	-	expression tag	UNP P01116
B	0	GLY	-	expression tag	UNP P01116
B	1	SER	-	expression tag	UNP P01116

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Chain	Residue	Modelled	Actual	Comment	Reference
B	12	ASP	GLY	engineered mutation	UNP P01116
C	-4	GLY	-	expression tag	UNP P01116
C	-3	SER	-	expression tag	UNP P01116
C	-2	SER	-	expression tag	UNP P01116
C	-1	GLY	-	expression tag	UNP P01116
C	0	GLY	-	expression tag	UNP P01116
C	1	SER	-	expression tag	UNP P01116
C	12	ASP	GLY	engineered mutation	UNP P01116
D	-4	GLY	-	expression tag	UNP P01116
D	-3	SER	-	expression tag	UNP P01116
D	-2	SER	-	expression tag	UNP P01116
D	-1	GLY	-	expression tag	UNP P01116
D	0	GLY	-	expression tag	UNP P01116
D	1	SER	-	expression tag	UNP P01116
D	12	ASP	GLY	engineered mutation	UNP P01116
E	-4	GLY	-	expression tag	UNP P01116
E	-3	SER	-	expression tag	UNP P01116
E	-2	SER	-	expression tag	UNP P01116
E	-1	GLY	-	expression tag	UNP P01116
E	0	GLY	-	expression tag	UNP P01116
E	1	SER	-	expression tag	UNP P01116
E	12	ASP	GLY	engineered mutation	UNP P01116
F	-4	GLY	-	expression tag	UNP P01116
F	-3	SER	-	expression tag	UNP P01116
F	-2	SER	-	expression tag	UNP P01116
F	-1	GLY	-	expression tag	UNP P01116
F	0	GLY	-	expression tag	UNP P01116
F	1	SER	-	expression tag	UNP P01116
F	12	ASP	GLY	engineered mutation	UNP P01116
G	-4	GLY	-	expression tag	UNP P01116
G	-3	SER	-	expression tag	UNP P01116
G	-2	SER	-	expression tag	UNP P01116
G	-1	GLY	-	expression tag	UNP P01116
G	0	GLY	-	expression tag	UNP P01116
G	1	SER	-	expression tag	UNP P01116
G	12	ASP	GLY	engineered mutation	UNP P01116
H	-4	GLY	-	expression tag	UNP P01116
H	-3	SER	-	expression tag	UNP P01116
H	-2	SER	-	expression tag	UNP P01116
H	-1	GLY	-	expression tag	UNP P01116
H	0	GLY	-	expression tag	UNP P01116
H	1	SER	-	expression tag	UNP P01116

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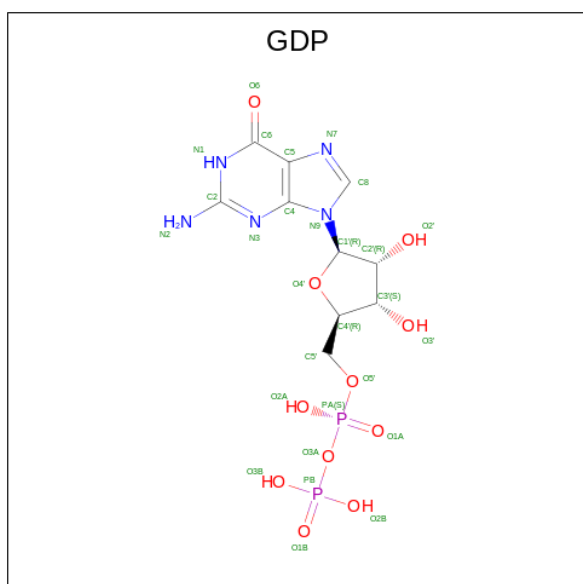
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Chain	Residue	Modelled	Actual	Comment	Reference
H	12	ASP	GLY	engineered mutation	UNP P01116

- Molecule 2 is a protein called AP4959.

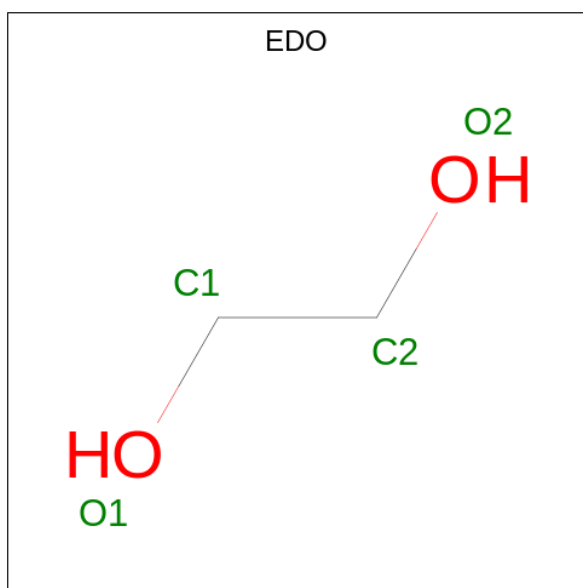
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	12	Total 99	C 71	F 4	N 12	O 12	0	0	0
2	J	12	Total 99	C 71	F 4	N 12	O 12	0	0	0
2	K	12	Total 99	C 71	F 4	N 12	O 12	0	0	0
2	L	12	Total 99	C 71	F 4	N 12	O 12	0	0	0
2	M	12	Total 99	C 71	F 4	N 12	O 12	0	0	0
2	N	12	Total 99	C 71	F 4	N 12	O 12	0	0	0
2	O	12	Total 99	C 71	F 4	N 12	O 12	0	0	0
2	P	12	Total 99	C 71	F 4	N 12	O 12	0	0	0

- Molecule 3 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
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		
3	E	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	F	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	G	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	H	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		
5	G	1	Total	Mg	0	0
			1	1		
5	H	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	72	Total	O	0	0
			72	72		
6	B	57	Total	O	0	0
			57	57		
6	C	41	Total	O	0	0
			41	41		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	32	Total 32	O 32	0	0
6	E	30	Total 30	O 30	0	0
6	F	16	Total 16	O 16	0	0
6	G	22	Total 22	O 22	0	0
6	H	18	Total 18	O 18	0	0
6	I	3	Total 3	O 3	0	0
6	J	1	Total 1	O 1	0	0
6	K	5	Total 5	O 5	0	0
6	L	1	Total 1	O 1	0	0

3 Residue-property plots [i](#)

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

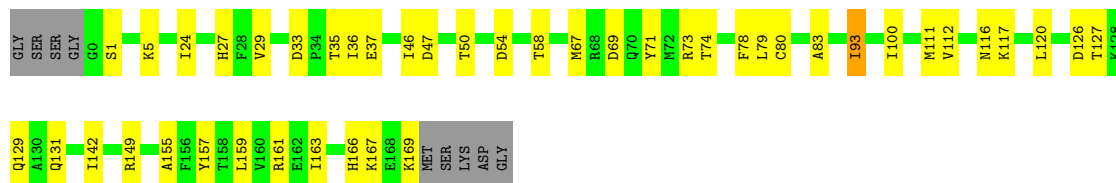
- Molecule 1: Isoform 2B of GTPase KRas

Chain A: 




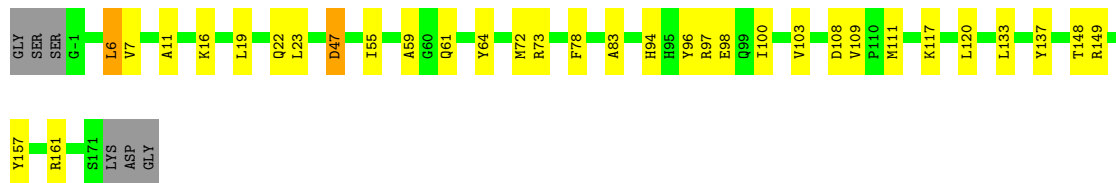
- Molecule 1: Isoform 2B of GTPase KRas

Chain B: 



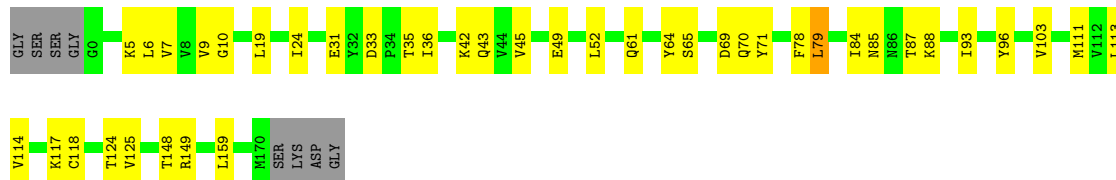
- Molecule 1: Isoform 2B of GTPase KRas

Chain C: 



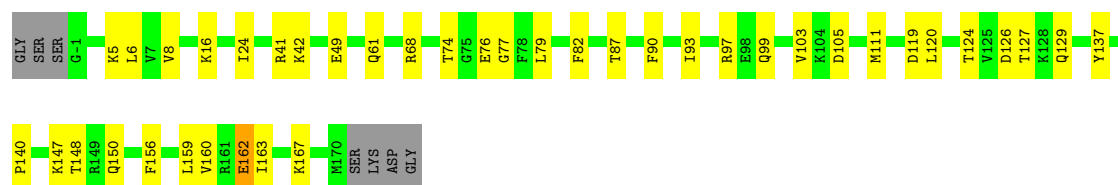
- Molecule 1: Isoform 2B of GTPase KRas

Chain D: 



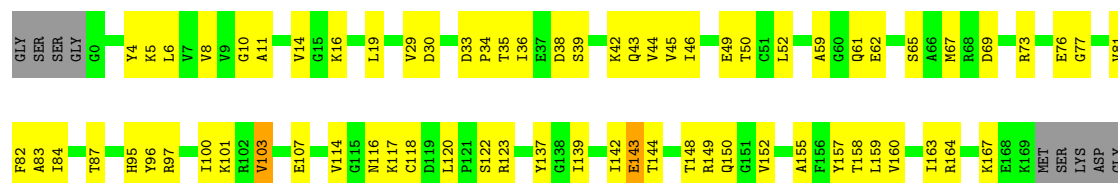
- Molecule 1: Isoform 2B of GTPase KRas

Chain E:  74% 22% . .



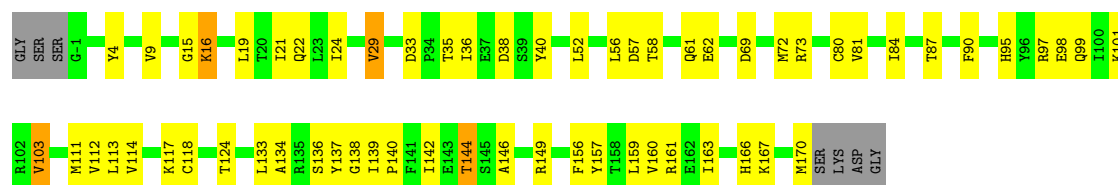
- Molecule 1: Isoform 2B of GTPase KRas

Chain F:  56% 38% . 5%



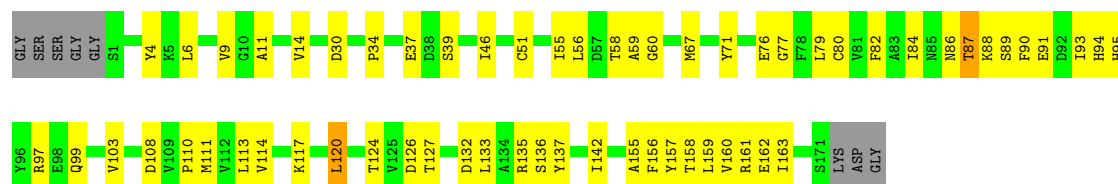
- Molecule 1: Isoform 2B of GTPase KRas

Chain G:  62% 32% . .



- Molecule 1: Isoform 2B of GTPase KRas

Chain H:  61% 33% . .



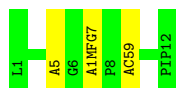
- Molecule 2: AP4959

Chain I:  75% 25%

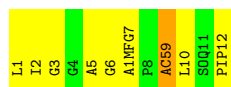
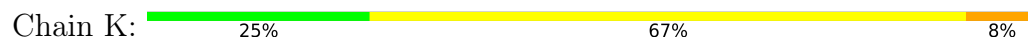


- Molecule 2: AP4959

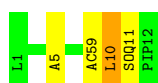
Chain J:  75% 25%



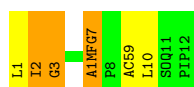
• Molecule 2: AP4959



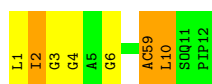
• Molecule 2: AP4959



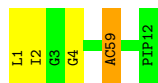
• Molecule 2: AP4959



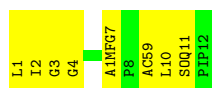
• Molecule 2: AP4959



• Molecule 2: AP4959



• Molecule 2: AP4959



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.25Å 112.81Å 202.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	101.39 – 2.53 101.39 – 2.53	Depositor EDS
% Data completeness (in resolution range)	66.7 (101.39-2.53) 62.2 (101.39-2.53)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.227 , 0.290 0.227 , 0.290	Depositor DCC
R_{free} test set	2883 reflections (3.34%)	wwPDB-VP
Wilson B-factor (Å ²)	17.9	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 16.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.069 for k,h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12116	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: PIP, SAR, A1MFG, MG, EDO, SOQ, AC5, H7V, MLE, GDP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.43	0/1391	0.60	0/1875
1	B	0.46	0/1377	0.61	0/1857
1	C	0.44	0/1391	0.59	0/1875
1	D	0.45	1/1385 (0.1%)	0.60	0/1867
1	E	0.38	0/1355	0.59	0/1834
1	F	0.38	0/1329	0.59	0/1800
1	G	0.35	0/1356	0.57	0/1833
1	H	0.44	1/1338 (0.1%)	0.64	1/1813 (0.1%)
2	I	0.35	0/14	1.20	0/16
2	J	0.38	0/14	1.30	0/16
2	K	0.39	0/14	1.36	0/16
2	L	0.30	0/14	0.88	0/16
2	M	0.28	0/14	1.20	0/16
2	N	0.31	0/14	0.91	0/16
2	O	0.32	0/14	0.86	0/16
2	P	0.26	0/14	1.07	0/16
All	All	0.42	2/11034 (0.0%)	0.61	1/14882 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	114	VAL	C-N	6.01	1.36	1.33
1	H	120	LEU	CG-CD2	5.44	1.70	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	120	LEU	CD1-CG-CD2	5.06	121.93	110.80

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	1370	0	1347	19	0
1	B	1356	0	1333	26	0
1	C	1370	0	1347	20	0
1	D	1364	0	1342	30	0
1	E	1334	0	1280	33	0
1	F	1308	0	1242	44	0
1	G	1335	0	1293	42	0
1	H	1317	0	1248	42	0
2	I	99	0	77	3	0
2	J	99	0	77	0	0
2	K	99	0	77	4	0
2	L	99	0	77	2	0
2	M	99	0	77	7	0
2	N	99	0	77	8	0
2	O	99	0	77	5	0
2	P	99	0	77	7	0
3	A	28	0	12	1	0
3	B	28	0	12	0	0
3	C	28	0	12	1	0
3	D	28	0	12	4	0
3	E	28	0	12	0	0
3	F	28	0	12	1	0
3	G	28	0	12	4	0
3	H	28	0	12	2	0
4	A	12	0	18	1	0
4	B	12	0	18	0	0
4	C	8	0	12	0	0
4	E	4	0	6	0	0
4	F	4	0	6	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	72	0	0	1	0
6	B	57	0	0	0	0
6	C	41	0	0	0	0
6	D	32	0	0	3	0
6	E	30	0	0	2	0
6	F	16	0	0	0	0
6	G	22	0	0	0	0
6	H	18	0	0	0	0
6	I	3	0	0	0	0
6	J	1	0	0	0	0
6	K	5	0	0	0	0
6	L	1	0	0	0	0
All	All	12116	0	11204	273	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 12.

All (273) 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:E:87:THR:HG23	1:E:124:THR:HG22	1.46	0.97
1:H:97:ARG:HD3	1:H:137:TYR:CD1	2.06	0.90
1:H:97:ARG:HD3	1:H:137:TYR:HD1	1.36	0.89
1:D:35:THR:HA	1:D:61:GLN:HE21	1.37	0.88
1:F:45:VAL:HG22	1:F:50:THR:HG22	1.62	0.82
1:F:160:VAL:HA	1:F:163:ILE:HD12	1.63	0.79
1:G:19:LEU:HD23	1:G:146:ALA:HB2	1.65	0.78
1:E:97:ARG:HE	1:E:137:TYR:HD2	1.31	0.77
1:G:113:LEU:HD12	1:G:139:ILE:HG22	1.67	0.77
1:H:142:ILE:HD12	1:H:155:ALA:HA	1.66	0.76
1:H:82:PHE:HB3	1:H:93:ILE:HD11	1.68	0.75
1:C:73:ARG:HH22	1:D:88:LYS:HE2	1.52	0.74
1:F:81:VAL:HG22	1:F:114:VAL:HB	1.72	0.71
1:E:97:ARG:NE	1:E:137:TYR:HD2	1.90	0.69
1:F:101:LYS:HE2	1:F:107:GLU:HA	1.75	0.69
1:E:68:ARG:HH21	2:M:7:A1MFG:CE2	2.06	0.68
1:H:4:TYR:CE2	1:H:160:VAL:HG23	2.29	0.68
4:A:205:EDO:H22	1:B:149:ARG:HH12	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:ASP:HB2	1:E:129:GLN:HB2	1.77	0.66
1:F:142:ILE:HD11	1:F:158:THR:HG21	1.77	0.66
1:G:33:ASP:HB3	1:G:36:ILE:HD12	1.77	0.66
1:F:163:ILE:HG22	1:F:167:LYS:HD3	1.79	0.64
1:H:80:CYS:SG	1:H:111:MET:HE3	2.38	0.63
1:E:82:PHE:HB3	1:E:93:ILE:HD11	1.81	0.63
1:H:90:PHE:O	1:H:93:ILE:HG12	1.98	0.63
1:D:24:ILE:HA	1:D:42:LYS:HE3	1.82	0.62
1:G:142:ILE:HG22	1:G:144:THR:HG22	1.83	0.61
1:A:164:ARG:HD2	6:A:337:HOH:O	2.00	0.61
1:D:5:LYS:HE2	6:D:302:HOH:O	1.99	0.61
1:G:72:MET:HE3	1:G:73:ARG:HG2	1.82	0.61
1:G:156:PHE:O	1:G:160:VAL:HG23	2.01	0.60
1:H:34:PRO:O	1:H:59:ALA:HB1	2.02	0.60
1:G:80:CYS:SG	1:G:111:MET:HE3	2.42	0.59
1:G:113:LEU:HD12	1:G:139:ILE:CG2	2.31	0.59
1:D:148:THR:O	1:D:149:ARG:HB2	2.02	0.59
1:F:149:ARG:O	1:F:152:VAL:HG12	2.03	0.59
1:G:138:GLY:C	1:G:139:ILE:HD12	2.27	0.59
1:C:117:LYS:HB3	1:C:120:LEU:HD12	1.85	0.58
1:H:56:LEU:HB2	1:H:71:TYR:CD2	2.38	0.58
1:B:80:CYS:SG	1:B:111:MET:HE3	2.43	0.58
1:A:165:LYS:HE3	1:A:169:LYS:NZ	2.19	0.58
2:N:1:MLE:HN3	2:N:2:ILE:N	2.18	0.58
1:C:97:ARG:HD2	1:C:111:MET:HE1	1.86	0.58
1:H:46:ILE:HD11	1:H:157:TYR:CE1	2.40	0.57
1:F:97:ARG:O	1:F:101:LYS:HG3	2.05	0.57
1:F:163:ILE:O	1:F:167:LYS:HG3	2.05	0.57
1:A:120:LEU:HD21	3:A:201:GDP:N2	2.20	0.56
1:C:78:PHE:HB2	1:C:111:MET:HG3	1.86	0.56
1:B:83:ALA:HB1	1:B:117:LYS:HD2	1.87	0.56
1:B:5:LYS:HD2	1:B:74:THR:OG1	2.05	0.56
1:H:99:GLN:O	1:H:103:VAL:HG23	2.07	0.55
1:F:8:VAL:HG12	1:F:16:LYS:HG2	1.87	0.55
1:B:142:ILE:HD12	1:B:155:ALA:HA	1.89	0.55
1:B:126:ASP:HB2	1:B:129:GLN:HG3	1.88	0.55
1:E:156:PHE:O	1:E:160:VAL:HG23	2.07	0.54
1:A:64:TYR:CZ	2:I:12:PIP:H52	2.42	0.54
1:G:95:HIS:HA	2:O:4:SAR:HN3	1.89	0.54
1:D:84:ILE:HD13	1:D:118:CYS:HA	1.88	0.54
1:H:110:PRO:O	1:H:111:MET:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5:LYS:C	1:F:6:LEU:HD23	2.33	0.54
1:A:23:LEU:HD22	1:A:156:PHE:CG	2.43	0.54
1:D:117:LYS:HG2	3:D:201:GDP:C6	2.43	0.54
1:D:84:ILE:O	1:D:125:VAL:HG23	2.08	0.53
1:G:21:ILE:HD12	1:G:29:VAL:HG21	1.90	0.53
1:F:157:TYR:HA	1:F:160:VAL:HG22	1.91	0.53
1:E:97:ARG:CD	1:E:137:TYR:CD2	2.92	0.53
1:G:22:GLN:OE1	1:G:149:ARG:HG2	2.09	0.53
1:F:77:GLY:HA3	1:F:159:LEU:HD11	1.91	0.52
1:A:97:ARG:HG3	1:A:111:MET:SD	2.49	0.52
1:E:147:LYS:HG3	1:E:148:THR:HG23	1.92	0.52
1:C:16:LYS:HE3	3:C:201:GDP:O1B	2.10	0.52
1:G:99:GLN:O	1:G:103:VAL:HG22	2.09	0.52
1:F:36:ILE:O	1:F:59:ALA:HB2	2.09	0.52
1:H:97:ARG:HD2	1:H:111:MET:HE1	1.92	0.52
1:E:97:ARG:NE	1:E:137:TYR:CD2	2.77	0.52
1:G:90:PHE:HE1	1:G:133:LEU:HD23	1.75	0.52
1:D:117:LYS:HE2	3:D:201:GDP:C4	2.45	0.52
1:E:97:ARG:HD2	1:E:137:TYR:CE2	2.45	0.52
1:F:117:LYS:O	1:F:120:LEU:HD12	2.10	0.51
1:H:86:ASN:HB3	1:H:89:SER:OG	2.10	0.51
1:B:1:SER:HA	1:B:50:THR:HG23	1.90	0.51
1:A:41:ARG:HA	1:A:53:LEU:O	2.11	0.51
1:H:157:TYR:HA	1:H:160:VAL:HG12	1.92	0.51
2:M:1:MLE:HN3	2:M:2:ILE:HG13	1.91	0.51
1:E:8:VAL:HG12	1:E:16:LYS:HG2	1.93	0.51
1:H:95:HIS:CD2	2:P:4:SAR:HA2	2.46	0.51
1:G:166:HIS:O	1:G:170:MET:HG3	2.11	0.51
1:H:46:ILE:HB	1:H:51:CYS:SG	2.50	0.51
1:E:97:ARG:HD2	1:E:137:TYR:CD2	2.46	0.50
1:E:148:THR:C	1:E:150:GLN:H	2.20	0.50
1:H:97:ARG:HD3	1:H:137:TYR:CE1	2.46	0.50
1:B:27:HIS:HE1	1:E:41:ARG:HH21	1.59	0.50
1:F:84:ILE:HD12	1:F:123:ARG:HB3	1.93	0.50
1:E:24:ILE:HA	1:E:42:LYS:HE2	1.93	0.50
1:G:15:GLY:HA2	3:G:201:GDP:O1A	2.11	0.50
1:G:4:TYR:CD2	1:G:160:VAL:HG13	2.47	0.50
1:F:38:ASP:HA	1:F:67:MET:HE1	1.93	0.50
1:F:95:HIS:HA	2:N:4:SAR:HN3	1.93	0.49
1:D:61:GLN:HA	1:D:61:GLN:OE1	2.13	0.49
1:E:97:ARG:CD	1:E:137:TYR:HD2	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:16:LYS:HE3	1:G:58:THR:O	2.12	0.49
1:G:112:VAL:HG22	1:G:140:PRO:HD2	1.94	0.49
1:F:103:VAL:HG23	2:N:2:ILE:HD12	1.94	0.49
3:H:201:GDP:H8	3:H:201:GDP:H5''	1.78	0.49
1:C:133:LEU:HD11	1:C:137:TYR:CZ	2.48	0.49
1:B:166:HIS:HA	1:B:169:LYS:HE2	1.94	0.49
1:C:7:VAL:HB	1:C:78:PHE:CD2	2.48	0.49
2:K:1:MLE:HN3	2:K:2:ILE:HG13	1.95	0.49
1:B:127:THR:O	1:B:131:GLN:HG3	2.13	0.49
1:H:158:THR:HA	1:H:161:ARG:HG3	1.95	0.48
1:C:6:LEU:HD12	1:C:55:ILE:HG12	1.95	0.48
1:F:19:LEU:HD21	1:F:116:ASN:OD1	2.13	0.48
2:K:2:ILE:HA	2:K:3:SAR:HN1	1.56	0.48
1:F:35:THR:HG22	1:F:61:GLN:CD	2.38	0.48
1:F:42:LYS:O	1:F:52:LEU:HD12	2.14	0.48
1:F:97:ARG:HD3	1:F:101:LYS:HD2	1.95	0.48
1:G:134:ALA:HB1	1:G:139:ILE:O	2.14	0.48
1:A:72:MET:HE3	1:A:73:ARG:HB3	1.96	0.48
1:A:72:MET:HE2	2:I:12:PIP:H42	1.94	0.47
1:C:94:HIS:O	1:C:98:GLU:HG2	2.12	0.47
1:G:62:GLU:HG3	2:O:9:AC5:HG22	1.96	0.47
1:H:97:ARG:CD	1:H:137:TYR:HD1	2.18	0.47
1:E:159:LEU:O	1:E:163:ILE:HG13	2.15	0.47
1:B:79:LEU:HD13	1:B:159:LEU:HD22	1.95	0.47
1:E:5:LYS:HD3	1:E:74:THR:HG22	1.96	0.47
1:F:164:ARG:HA	1:F:167:LYS:NZ	2.29	0.47
1:H:46:ILE:HD12	1:H:160:VAL:HG11	1.97	0.47
1:H:133:LEU:O	1:H:137:TYR:CD2	2.68	0.47
1:E:49:GLU:HB3	6:E:324:HOH:O	2.15	0.47
1:G:159:LEU:O	1:G:163:ILE:HD12	2.14	0.47
1:H:79:LEU:HG	1:H:159:LEU:HD12	1.96	0.47
1:H:133:LEU:O	1:H:137:TYR:HD2	1.98	0.47
1:G:97:ARG:NH1	1:G:137:TYR:HB3	2.30	0.47
1:B:33:ASP:HB3	1:B:36:ILE:HG12	1.97	0.47
1:E:103:VAL:HG21	2:M:10:MLE:CD2	2.45	0.47
1:E:90:PHE:HD1	1:E:93:ILE:HG13	1.79	0.46
1:E:97:ARG:HG2	1:E:111:MET:SD	2.55	0.46
1:A:41:ARG:HG3	1:A:54:ASP:OD2	2.14	0.46
1:F:62:GLU:O	2:N:9:AC5:HG22	2.15	0.46
1:D:10:GLY:HA2	1:D:96:TYR:CE2	2.51	0.46
1:G:69:ASP:O	1:G:72:MET:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:1:MLE:HN3	2:N:2:ILE:H	1.78	0.46
1:C:83:ALA:HB1	1:C:117:LYS:HD2	1.96	0.46
1:G:69:ASP:O	1:G:73:ARG:HG3	2.16	0.46
1:B:47:ASP:CG	1:B:161:ARG:HH11	2.23	0.46
1:G:97:ARG:HE	1:G:101:LYS:NZ	2.13	0.46
1:E:103:VAL:HG21	2:M:10:MLE:HD21	1.97	0.46
1:A:123:ARG:HH22	1:A:143:GLU:CD	2.24	0.46
1:F:43:GLN:HB2	1:F:52:LEU:CD1	2.46	0.46
1:H:4:TYR:CD2	1:H:160:VAL:HG23	2.50	0.46
1:H:37:GLU:HG3	1:H:58:THR:HA	1.97	0.46
2:P:2:ILE:HA	2:P:3:SAR:HN1	1.54	0.46
1:A:84:ILE:HD12	1:A:123:ARG:HG3	1.97	0.46
3:H:201:GDP:H5''	3:H:201:GDP:C8	2.51	0.46
2:K:9:AC5:N	2:K:10:MLE:HN1	2.30	0.46
1:B:69:ASP:O	1:B:73:ARG:HG2	2.16	0.46
1:D:93:ILE:HG21	1:D:113:LEU:HD11	1.97	0.46
1:C:19:LEU:HD23	1:C:19:LEU:HA	1.74	0.46
1:D:43:GLN:HG3	1:D:52:LEU:HD13	1.98	0.46
1:H:6:LEU:HD22	1:H:159:LEU:HD22	1.98	0.46
1:D:71:TYR:HA	6:D:302:HOH:O	2.16	0.45
1:D:111:MET:HE3	1:D:111:MET:HB2	1.87	0.45
1:H:77:GLY:HA3	1:H:159:LEU:HD21	1.97	0.45
1:F:82:PHE:HD1	1:F:83:ALA:O	1.99	0.45
1:C:96:TYR:O	1:C:100:ILE:HG13	2.16	0.45
1:D:117:LYS:HE2	3:D:201:GDP:N9	2.32	0.45
1:F:30:ASP:HA	3:F:201:GDP:O2'	2.15	0.45
1:F:43:GLN:HB2	1:F:52:LEU:HD12	1.98	0.45
1:B:47:ASP:OD2	1:B:161:ARG:HD3	2.17	0.45
1:G:24:ILE:HG13	1:G:40:TYR:HB3	1.97	0.45
1:G:35:THR:HG23	1:G:61:GLN:CD	2.42	0.45
1:G:163:ILE:O	1:G:167:LYS:HG3	2.17	0.45
1:D:117:LYS:HG2	3:D:201:GDP:C5	2.52	0.45
1:F:16:LYS:HE3	1:F:16:LYS:HB2	1.57	0.45
1:B:54:ASP:HB3	1:B:71:TYR:OH	2.17	0.45
1:F:137:TYR:HB2	1:F:139:ILE:HG13	1.98	0.45
1:H:132:ASP:HA	1:H:135:ARG:HB2	1.98	0.45
1:A:142:ILE:HD12	1:A:155:ALA:HA	1.99	0.44
1:C:64:TYR:OH	2:K:12:PIP:H31	2.17	0.44
1:D:7:VAL:HB	1:D:78:PHE:CD2	2.52	0.44
1:E:77:GLY:HA3	1:E:163:ILE:HD11	1.98	0.44
1:F:144:THR:HG21	1:F:155:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:97:ARG:HD2	1:G:137:TYR:CE1	2.52	0.44
1:H:79:LEU:HD22	1:H:114:VAL:CG2	2.47	0.44
1:B:46:ILE:HG12	1:B:157:TYR:CD1	2.52	0.44
1:E:79:LEU:HD12	1:E:159:LEU:HD22	2.00	0.44
1:G:15:GLY:HA2	3:G:201:GDP:PA	2.58	0.44
1:H:11:ALA:O	1:H:14:VAL:HG22	2.17	0.44
1:A:23:LEU:HD22	1:A:156:PHE:CD2	2.52	0.44
1:D:85:ASN:HA	1:D:124:THR:HB	1.99	0.44
1:G:81:VAL:HG22	1:G:114:VAL:HB	2.00	0.44
1:C:72:MET:SD	1:C:103:VAL:HG11	2.58	0.44
1:D:79:LEU:HD13	1:D:159:LEU:HD22	2.00	0.44
1:B:163:ILE:O	1:B:167:LYS:HG3	2.17	0.44
1:A:165:LYS:HE3	1:A:169:LYS:HZ2	1.83	0.43
1:F:69:ASP:O	1:F:73:ARG:HG3	2.18	0.43
1:C:157:TYR:O	1:C:161:ARG:HG3	2.18	0.43
1:D:33:ASP:HB3	1:D:36:ILE:HD12	2.01	0.43
1:D:35:THR:CA	1:D:61:GLN:HE21	2.20	0.43
1:E:99:GLN:OE1	2:M:7:A1MFG:N	2.52	0.43
1:G:98:GLU:HB3	2:O:4:SAR:HN1	2.00	0.43
1:D:45:VAL:HA	1:D:49:GLU:O	2.18	0.43
1:F:10:GLY:N	1:F:16:LYS:HD3	2.33	0.43
1:D:103:VAL:HG11	2:L:10:MLE:CD2	2.48	0.43
1:H:117:LYS:HB3	1:H:120:LEU:CD1	2.49	0.43
1:F:35:THR:HG22	1:F:61:GLN:NE2	2.34	0.43
1:B:120:LEU:HD23	1:B:120:LEU:HA	1.68	0.43
1:H:55:ILE:HD13	1:H:156:PHE:CE2	2.54	0.43
2:L:10:MLE:HN3	2:L:11:SOQ:OD1	2.19	0.43
1:C:73:ARG:NH2	1:D:88:LYS:HE2	2.26	0.42
1:G:4:TYR:CE2	1:G:160:VAL:HG13	2.54	0.42
1:G:117:LYS:HG2	3:G:201:GDP:C6	2.53	0.42
1:A:97:ARG:HD2	1:A:137:TYR:CD2	2.53	0.42
1:F:67:MET:HE3	1:F:67:MET:HB3	1.84	0.42
1:H:99:GLN:NE2	2:P:10:MLE:HD22	2.35	0.42
2:M:1:MLE:HD12	2:O:9:AC5:HG11	2.02	0.42
1:A:9:VAL:HG13	1:A:96:TYR:CD1	2.55	0.42
1:A:56:LEU:HB2	1:A:71:TYR:CD2	2.54	0.42
1:D:64:TYR:CE1	1:D:69:ASP:HB2	2.54	0.42
1:E:119:ASP:OD2	1:E:147:LYS:HD3	2.20	0.42
1:E:120:LEU:HD23	1:E:120:LEU:HA	1.90	0.42
1:B:37:GLU:HG3	1:B:58:THR:HA	2.01	0.42
1:G:84:ILE:HD11	1:G:118:CYS:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:GLU:O	1:B:67:MET:HE1	2.19	0.42
1:G:52:LEU:HD23	1:G:52:LEU:O	2.19	0.42
1:H:67:MET:HE3	1:H:67:MET:HB2	1.81	0.42
1:G:38:ASP:O	1:G:56:LEU:HD12	2.20	0.42
2:P:9:AC5:N	2:P:10:MLE:HN1	2.34	0.42
1:A:145:SER:OG	1:A:148:THR:HG23	2.19	0.42
1:B:116:ASN:O	1:B:117:LYS:HB2	2.20	0.41
1:G:19:LEU:CD2	1:G:146:ALA:HB2	2.43	0.41
1:F:148:THR:C	1:F:150:GLN:H	2.27	0.41
1:B:67:MET:HE2	1:B:67:MET:HB3	1.86	0.41
1:D:19:LEU:HD23	1:D:19:LEU:HA	1.88	0.41
1:E:76:GLU:HB2	1:E:163:ILE:HD13	2.01	0.41
1:F:11:ALA:O	1:F:14:VAL:HG22	2.19	0.41
2:M:2:ILE:HA	2:M:3:SAR:HN1	1.62	0.41
1:F:96:TYR:O	1:F:100:ILE:HG13	2.21	0.41
2:N:2:ILE:HA	2:N:3:SAR:HN1	1.65	0.41
1:H:56:LEU:HB2	1:H:71:TYR:CE2	2.56	0.41
1:H:87:THR:O	1:H:88:LYS:C	2.64	0.41
1:B:78:PHE:HB2	1:B:111:MET:HG2	2.02	0.41
1:H:76:GLU:HB2	1:H:163:ILE:HD13	2.01	0.41
2:I:9:AC5:N	2:I:10:MLE:HN1	2.36	0.41
1:F:44:VAL:HG23	1:F:46:ILE:HG13	2.02	0.41
1:F:118:CYS:SG	1:F:143:GLU:HG2	2.60	0.41
2:P:1:MLE:HD22	2:P:1:MLE:HA	1.87	0.41
1:C:148:THR:O	1:C:149:ARG:HB2	2.21	0.41
1:F:33:ASP:HA	1:F:34:PRO:HD3	1.95	0.41
1:B:93:ILE:HD13	1:B:93:ILE:HA	1.75	0.41
1:C:11:ALA:O	1:C:16:LYS:HE2	2.21	0.41
1:D:70:GLN:HG2	6:D:302:HOH:O	2.21	0.41
1:F:49:GLU:HA	1:F:49:GLU:OE1	2.21	0.41
1:G:117:LYS:HG2	3:G:201:GDP:C5	2.56	0.41
2:O:1:MLE:HN3	2:O:2:ILE:N	2.35	0.41
1:C:22:GLN:O	1:C:23:LEU:C	2.64	0.41
1:E:61:GLN:HB3	6:E:309:HOH:O	2.20	0.41
1:H:162:GLU:H	1:H:162:GLU:HG2	1.68	0.41
1:B:79:LEU:CD1	1:B:159:LEU:HD22	2.50	0.40
1:D:93:ILE:HG21	1:D:113:LEU:CD1	2.51	0.40
1:C:59:ALA:O	1:C:61:GLN:HG2	2.21	0.40
1:H:157:TYR:O	1:H:161:ARG:HG2	2.21	0.40
1:F:4:TYR:HA	1:F:76:GLU:OE2	2.21	0.40
1:G:157:TYR:O	1:G:160:VAL:HB	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:LEU:HD13	1:D:159:LEU:HD23	2.03	0.40
1:E:140:PRO:HD3	1:E:162:GLU:OE1	2.20	0.40
1:G:133:LEU:HA	1:G:133:LEU:HD12	1.76	0.40
1:H:82:PHE:CD2	1:H:113:LEU:HD11	2.56	0.40
1:H:94:HIS:CE1	1:H:95:HIS:CE1	3.09	0.40
2:N:9:AC5:HG12	2:P:1:MLE:HG	2.03	0.40
2:N:9:AC5:N	2:N:10:MLE:HN1	2.36	0.40
1:E:163:ILE:O	1:E:167:LYS:HG3	2.21	0.40
2:P:10:MLE:HN3	2:P:11:SOQ:OD1	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	171/179 (96%)	160 (94%)	10 (6%)	1 (1%)	21	36
1	B	168/179 (94%)	156 (93%)	12 (7%)	0	100	100
1	C	171/179 (96%)	159 (93%)	11 (6%)	1 (1%)	21	36
1	D	169/179 (94%)	156 (92%)	13 (8%)	0	100	100
1	E	170/179 (95%)	164 (96%)	6 (4%)	0	100	100
1	F	168/179 (94%)	156 (93%)	12 (7%)	0	100	100
1	G	170/179 (95%)	160 (94%)	10 (6%)	0	100	100
1	H	169/179 (94%)	158 (94%)	10 (6%)	1 (1%)	21	36
2	I	2/12 (17%)	2 (100%)	0	0	100	100
2	J	2/12 (17%)	2 (100%)	0	0	100	100
2	K	2/12 (17%)	2 (100%)	0	0	100	100
2	L	2/12 (17%)	2 (100%)	0	0	100	100
2	M	2/12 (17%)	2 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	2/12 (17%)	2 (100%)	0	0	100	100
2	O	2/12 (17%)	2 (100%)	0	0	100	100
2	P	2/12 (17%)	2 (100%)	0	0	100	100
All	All	1372/1528 (90%)	1285 (94%)	84 (6%)	3 (0%)	43	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	C	47	ASP
1	H	60	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	151/156 (97%)	149 (99%)	2 (1%)	61	81
1	B	150/156 (96%)	144 (96%)	6 (4%)	28	51
1	C	151/156 (97%)	147 (97%)	4 (3%)	40	66
1	D	151/156 (97%)	146 (97%)	5 (3%)	33	58
1	E	142/156 (91%)	138 (97%)	4 (3%)	38	64
1	F	139/156 (89%)	132 (95%)	7 (5%)	22	42
1	G	142/156 (91%)	132 (93%)	10 (7%)	14	27
1	H	140/156 (90%)	129 (92%)	11 (8%)	11	22
2	I	2/2 (100%)	2 (100%)	0	100	100
2	J	2/2 (100%)	2 (100%)	0	100	100
2	K	2/2 (100%)	2 (100%)	0	100	100
2	L	2/2 (100%)	2 (100%)	0	100	100
2	M	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	N	2/2 (100%)	1 (50%)	1 (50%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	O	2/2 (100%)	2 (100%)	0	100	100
2	P	2/2 (100%)	2 (100%)	0	100	100
All	All	1182/1264 (94%)	1131 (96%)	51 (4%)	26	49

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	150	GLN
1	B	24	ILE
1	B	29	VAL
1	B	35	THR
1	B	93	ILE
1	B	100	ILE
1	B	112	VAL
1	C	6	LEU
1	C	47	ASP
1	C	108	ASP
1	C	109	VAL
1	D	9	VAL
1	D	31	GLU
1	D	65	SER
1	D	79	LEU
1	D	87	THR
1	E	6	LEU
1	E	105	ASP
1	E	127	THR
1	E	162	GLU
1	F	29	VAL
1	F	39	SER
1	F	65	SER
1	F	87	THR
1	F	103	VAL
1	F	122	SER
1	F	143	GLU
1	G	9	VAL
1	G	16	LYS
1	G	29	VAL
1	G	57	ASP
1	G	87	THR
1	G	103	VAL

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Mol	Chain	Res	Type
1	G	124	THR
1	G	136	SER
1	G	144	THR
1	G	161	ARG
1	H	9	VAL
1	H	30	ASP
1	H	39	SER
1	H	84	ILE
1	H	87	THR
1	H	91	GLU
1	H	108	ASP
1	H	124	THR
1	H	126	ASP
1	H	127	THR
1	H	136	SER
2	M	2	ILE
2	N	2	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	86	ASN
1	B	25	GLN
1	B	94	HIS
1	B	131	GLN
1	C	85	ASN
1	D	22	GLN
1	D	61	GLN
1	D	70	GLN
1	E	166	HIS
1	F	22	GLN
1	F	27	HIS
1	F	43	GLN
1	F	61	GLN
1	F	150	GLN
1	G	27	HIS
1	G	43	GLN
1	G	94	HIS
1	H	61	GLN
1	H	94	HIS
1	H	95	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

64 non-standard protein/DNA/RNA residues 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	AC5	P	9	2	6,8,9	0.61	0	5,11,13	1.05	0
2	H7V	P	5	2	11,12,13	0.32	0	11,14,16	0.82	0
2	SAR	L	6	2	4,4,5	0.62	0	1,3,5	1.34	0
2	MLE	L	1	2	7,8,9	0.41	0	6,9,11	0.91	0
2	MLE	O	1	2	7,8,9	0.42	0	6,9,11	0.84	0
2	A1MFG	O	7	2	16,17,18	0.31	0	19,24,26	0.80	0
2	SAR	K	6	2	4,4,5	0.62	0	1,3,5	2.15	1 (100%)
2	SAR	O	4	2	4,4,5	0.70	0	1,3,5	1.55	0
2	AC5	J	9	2	6,8,9	0.53	0	5,11,13	1.61	2 (40%)
2	MLE	I	10	2	7,8,9	0.44	0	6,9,11	0.76	0
2	MLE	M	1	2	7,8,9	0.45	0	6,9,11	0.91	0
2	A1MFG	K	7	2	16,17,18	0.40	0	19,24,26	0.87	1 (5%)
2	H7V	J	5	2	11,12,13	0.30	0	11,14,16	0.96	2 (18%)
2	H7V	O	5	2	11,12,13	0.40	0	11,14,16	0.85	0
2	AC5	O	9	2	6,8,9	0.51	0	5,11,13	1.73	2 (40%)
2	A1MFG	I	7	2	16,17,18	0.34	0	19,24,26	0.73	0
2	AC5	K	9	2	6,8,9	0.43	0	5,11,13	1.52	1 (20%)
2	H7V	K	5	2	11,12,13	0.36	0	11,14,16	1.18	1 (9%)
2	SAR	O	3	2	4,4,5	0.77	0	1,3,5	1.39	0
2	A1MFG	M	7	2	16,17,18	0.37	0	19,24,26	0.90	2 (10%)
2	H7V	L	5	2	11,12,13	0.40	0	11,14,16	0.89	1 (9%)
2	AC5	M	9	2	6,8,9	0.51	0	5,11,13	1.53	2 (40%)
2	MLE	J	1	2	7,8,9	0.52	0	6,9,11	0.89	0
2	SAR	L	3	2	4,4,5	0.78	0	1,3,5	1.70	0
2	SAR	K	3	2	4,4,5	0.76	0	1,3,5	1.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SAR	J	4	2	4,4,5	0.76	0	1,3,5	1.65	0
2	SAR	I	4	2	4,4,5	0.75	0	1,3,5	1.74	0
2	SAR	J	6	2	4,4,5	0.54	0	1,3,5	1.11	0
2	MLE	K	10	2	7,8,9	0.40	0	6,9,11	0.75	0
2	MLE	O	10	2	7,8,9	0.44	0	6,9,11	0.93	0
2	A1MFG	P	7	2	16,17,18	0.40	0	19,24,26	0.75	1 (5%)
2	A1MFG	N	7	2	16,17,18	0.36	0	19,24,26	0.69	0
2	MLE	N	1	2	7,8,9	0.38	0	6,9,11	1.04	0
2	H7V	M	5	2	11,12,13	0.33	0	11,14,16	0.73	0
2	MLE	K	1	2	7,8,9	0.49	0	6,9,11	0.89	0
2	SAR	M	3	2	4,4,5	0.68	0	1,3,5	2.01	1 (100%)
2	SAR	N	4	2	4,4,5	0.74	0	1,3,5	1.83	0
2	AC5	N	9	2	6,8,9	0.46	0	5,11,13	1.73	1 (20%)
2	MLE	L	10	2	7,8,9	0.41	0	6,9,11	0.95	1 (16%)
2	MLE	I	1	2	7,8,9	0.44	0	6,9,11	0.97	0
2	SAR	I	6	2	4,4,5	0.65	0	1,3,5	1.35	0
2	MLE	J	10	2	7,8,9	0.42	0	6,9,11	0.88	0
2	H7V	N	5	2	11,12,13	0.36	0	11,14,16	0.73	0
2	A1MFG	L	7	2	16,17,18	0.53	0	19,24,26	0.89	0
2	AC5	L	9	2	6,8,9	0.52	0	5,11,13	1.84	2 (40%)
2	MLE	M	10	2	7,8,9	0.43	0	6,9,11	0.92	0
2	SAR	M	6	2	4,4,5	0.63	0	1,3,5	1.77	0
2	SAR	P	3	2	4,4,5	0.73	0	1,3,5	1.81	0
2	SAR	N	3	2	4,4,5	0.74	0	1,3,5	1.38	0
2	SAR	L	4	2	4,4,5	0.75	0	1,3,5	1.47	0
2	SAR	K	4	2	4,4,5	0.72	0	1,3,5	1.62	0
2	AC5	I	9	2	6,8,9	0.52	0	5,11,13	1.02	0
2	SAR	J	3	2	4,4,5	0.75	0	1,3,5	1.60	0
2	SAR	P	6	2	4,4,5	0.59	0	1,3,5	1.86	0
2	MLE	P	1	2	7,8,9	0.47	0	6,9,11	0.95	0
2	SAR	N	6	2	4,4,5	0.70	0	1,3,5	2.18	1 (100%)
2	MLE	N	10	2	7,8,9	0.47	0	6,9,11	0.94	1 (16%)
2	SAR	M	4	2	4,4,5	0.78	0	1,3,5	1.70	0
2	A1MFG	J	7	2	16,17,18	0.53	0	19,24,26	1.02	2 (10%)
2	SAR	P	4	2	4,4,5	0.78	0	1,3,5	1.34	0
2	SAR	O	6	2	4,4,5	0.70	0	1,3,5	1.33	0
2	MLE	P	10	2	7,8,9	0.40	0	6,9,11	0.87	0
2	H7V	I	5	2	11,12,13	0.34	0	11,14,16	0.86	0
2	SAR	I	3	2	4,4,5	0.73	0	1,3,5	1.76	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	AC5	P	9	2	-	0/2/12/15	0/1/1/1
2	H7V	P	5	2	-	5/5/16/18	0/1/1/1
2	SAR	L	6	2	-	1/1/2/3	-
2	MLE	L	1	2	-	0/5/8/10	-
2	MLE	O	1	2	-	1/5/8/10	-
2	A1MFG	O	7	2	-	3/12/13/15	0/1/1/1
2	SAR	K	6	2	-	1/1/2/3	-
2	SAR	O	4	2	-	1/1/2/3	-
2	AC5	J	9	2	-	0/2/12/15	0/1/1/1
2	MLE	I	10	2	-	1/5/8/10	-
2	MLE	M	1	2	-	0/5/8/10	-
2	A1MFG	K	7	2	-	3/12/13/15	0/1/1/1
2	H7V	J	5	2	-	2/5/16/18	0/1/1/1
2	H7V	O	5	2	-	2/5/16/18	0/1/1/1
2	AC5	O	9	2	-	0/2/12/15	0/1/1/1
2	A1MFG	I	7	2	-	1/12/13/15	0/1/1/1
2	AC5	K	9	2	-	0/2/12/15	0/1/1/1
2	H7V	K	5	2	-	3/5/16/18	0/1/1/1
2	SAR	O	3	2	-	1/1/2/3	-
2	A1MFG	M	7	2	-	1/12/13/15	0/1/1/1
2	H7V	L	5	2	-	4/5/16/18	0/1/1/1
2	AC5	M	9	2	-	0/2/12/15	0/1/1/1
2	MLE	J	1	2	-	3/5/8/10	-
2	SAR	L	3	2	-	1/1/2/3	-
2	SAR	K	3	2	-	1/1/2/3	-
2	SAR	J	4	2	-	1/1/2/3	-
2	SAR	I	4	2	-	1/1/2/3	-
2	SAR	J	6	2	-	1/1/2/3	-
2	MLE	K	10	2	-	0/5/8/10	-
2	MLE	O	10	2	-	0/5/8/10	-
2	A1MFG	P	7	2	-	3/12/13/15	0/1/1/1
2	A1MFG	N	7	2	-	3/12/13/15	0/1/1/1
2	MLE	N	1	2	-	1/5/8/10	-
2	H7V	M	5	2	-	4/5/16/18	0/1/1/1
2	MLE	K	1	2	-	0/5/8/10	-
2	SAR	M	3	2	-	1/1/2/3	-
2	SAR	N	4	2	-	1/1/2/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AC5	N	9	2	-	0/2/12/15	0/1/1/1
2	MLE	L	10	2	-	0/5/8/10	-
2	MLE	I	1	2	-	0/5/8/10	-
2	SAR	I	6	2	-	1/1/2/3	-
2	MLE	J	10	2	-	0/5/8/10	-
2	H7V	N	5	2	-	1/5/16/18	0/1/1/1
2	A1MFG	L	7	2	-	3/12/13/15	0/1/1/1
2	AC5	L	9	2	-	0/2/12/15	0/1/1/1
2	MLE	M	10	2	-	0/5/8/10	-
2	SAR	M	6	2	-	1/1/2/3	-
2	SAR	P	3	2	-	1/1/2/3	-
2	SAR	N	3	2	-	1/1/2/3	-
2	SAR	L	4	2	-	1/1/2/3	-
2	SAR	K	4	2	-	1/1/2/3	-
2	AC5	I	9	2	-	0/2/12/15	0/1/1/1
2	SAR	J	3	2	-	1/1/2/3	-
2	SAR	P	6	2	-	1/1/2/3	-
2	MLE	P	1	2	-	2/5/8/10	-
2	SAR	N	6	2	-	1/1/2/3	-
2	MLE	N	10	2	-	3/5/8/10	-
2	SAR	M	4	2	-	1/1/2/3	-
2	A1MFG	J	7	2	-	2/12/13/15	0/1/1/1
2	SAR	P	4	2	-	1/1/2/3	-
2	SAR	O	6	2	-	1/1/2/3	-
2	MLE	P	10	2	-	1/5/8/10	-
2	H7V	I	5	2	-	4/5/16/18	0/1/1/1
2	SAR	I	3	2	-	1/1/2/3	-

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	9	AC5	CB2-CG2-CG1	-3.08	97.51	105.79
2	O	9	AC5	CB2-CG2-CG1	-2.92	97.96	105.79
2	L	9	AC5	CB1-CG1-CG2	-2.55	98.94	105.79
2	J	9	AC5	CG1-CB1-CA	-2.35	99.66	104.03
2	J	7	A1MFG	CB-CG-CD	-2.33	105.07	113.18
2	L	9	AC5	CB2-CG2-CG1	-2.23	99.81	105.79
2	J	9	AC5	CB1-CG1-CG2	-2.21	99.87	105.79
2	M	9	AC5	CB1-CG1-CG2	-2.21	99.87	105.79
2	O	9	AC5	CB1-CG1-CG2	-2.19	99.92	105.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	6	SAR	O-C-CA	-2.18	119.11	125.42
2	M	7	A1MFG	CZ2-CH-CT	2.16	122.44	118.12
2	K	6	SAR	O-C-CA	-2.15	119.19	125.42
2	K	9	AC5	CB1-CG1-CG2	-2.15	100.03	105.79
2	M	9	AC5	CG1-CB1-CA	-2.11	100.10	104.03
2	M	7	A1MFG	CB-CG-CD	-2.11	105.85	113.18
2	L	10	MLE	O-C-CA	-2.09	119.31	124.78
2	N	10	MLE	O-C-CA	-2.08	119.32	124.78
2	P	7	A1MFG	CZ2-CH-CT	2.08	122.27	118.12
2	K	5	H7V	O-C-CA	-2.07	119.36	124.78
2	J	5	H7V	C07-N-CA	2.07	120.07	113.64
2	J	7	A1MFG	CZ2-CH-CT	2.04	122.20	118.12
2	L	5	H7V	C07-N-CA	2.04	119.98	113.64
2	K	7	A1MFG	CZ2-CH-CT	2.02	122.15	118.12
2	M	3	SAR	O-C-CA	-2.01	119.60	125.42
2	J	5	H7V	O-C-CA	-2.01	119.51	124.78

There are no chirality outliers.

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	1	MLE	C-CA-CB-CG
2	N	1	MLE	O-C-CA-CB
2	O	1	MLE	O-C-CA-CB
2	I	3	SAR	C-CA-N-CN
2	J	3	SAR	C-CA-N-CN
2	K	3	SAR	C-CA-N-CN
2	L	3	SAR	C-CA-N-CN
2	M	3	SAR	C-CA-N-CN
2	N	3	SAR	C-CA-N-CN
2	P	3	SAR	C-CA-N-CN
2	I	4	SAR	C-CA-N-CN
2	J	4	SAR	C-CA-N-CN
2	K	4	SAR	C-CA-N-CN
2	L	4	SAR	C-CA-N-CN
2	M	4	SAR	C-CA-N-CN
2	N	4	SAR	C-CA-N-CN
2	O	4	SAR	C-CA-N-CN
2	P	4	SAR	C-CA-N-CN
2	I	5	H7V	C06-C01-CB-CA
2	J	5	H7V	C06-C01-CB-CA
2	K	5	H7V	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
2	K	5	H7V	C06-C01-CB-CA
2	L	5	H7V	O-C-CA-CB
2	L	5	H7V	C-CA-CB-C01
2	M	5	H7V	O-C-CA-CB
2	M	5	H7V	C06-C01-CB-CA
2	P	5	H7V	O-C-CA-CB
2	P	5	H7V	C06-C01-CB-CA
2	I	6	SAR	C-CA-N-CN
2	J	6	SAR	C-CA-N-CN
2	K	6	SAR	C-CA-N-CN
2	L	6	SAR	C-CA-N-CN
2	M	6	SAR	C-CA-N-CN
2	N	6	SAR	C-CA-N-CN
2	O	6	SAR	C-CA-N-CN
2	P	6	SAR	C-CA-N-CN
2	K	7	A1MFG	CZ1-CH-CT-FT3
2	L	7	A1MFG	CZ1-CH-CT-FT1
2	L	7	A1MFG	CZ1-CH-CT-FT2
2	L	7	A1MFG	CZ1-CH-CT-FT3
2	N	7	A1MFG	CZ1-CH-CT-FT1
2	N	7	A1MFG	CZ1-CH-CT-FT2
2	N	7	A1MFG	CZ1-CH-CT-FT3
2	O	7	A1MFG	CZ1-CH-CT-FT1
2	O	7	A1MFG	CZ1-CH-CT-FT3
2	J	1	MLE	N-CA-CB-CG
2	L	5	H7V	N-CA-CB-C01
2	O	7	A1MFG	CZ1-CH-CT-FT2
2	I	5	H7V	C02-C01-CB-CA
2	K	5	H7V	C02-C01-CB-CA
2	P	5	H7V	C02-C01-CB-CA
2	K	7	A1MFG	CZ1-CH-CT-FT2
2	P	1	MLE	C-CA-CB-CG
2	I	5	H7V	C-CA-CB-C01
2	M	5	H7V	C-CA-CB-C01
2	N	5	H7V	C-CA-CB-C01
2	O	5	H7V	C-CA-CB-C01
2	P	5	H7V	C-CA-CB-C01
2	N	10	MLE	CA-CB-CG-CD2
2	J	7	A1MFG	CZ1-CH-CT-FT2
2	K	7	A1MFG	CZ1-CH-CT-FT1
2	P	7	A1MFG	CZ1-CH-CT-FT2
2	J	5	H7V	C02-C01-CB-CA

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Mol	Chain	Res	Type	Atoms
2	P	1	MLE	CA-CB-CG-CD2
2	M	5	H7V	N-CA-CB-C01
2	J	7	A1MFG	CZ1-CH-CT-FT1
2	M	7	A1MFG	CZ1-CH-CT-FT1
2	N	10	MLE	N-CA-CB-CG
2	J	1	MLE	CA-CB-CG-CD1
2	I	10	MLE	N-CA-CB-CG
2	N	10	MLE	CA-CB-CG-CD1
2	P	7	A1MFG	CZ1-CH-CT-FT1
2	P	7	A1MFG	CZ1-CH-CT-FT3
2	P	5	H7V	N-CA-CB-C01
2	P	10	MLE	CA-CB-CG-CD1
2	O	3	SAR	C-CA-N-CN
2	L	5	H7V	C06-C01-CB-CA
2	O	5	H7V	N-CA-CB-C01
2	I	7	A1MFG	CZ1-CH-CT-FT3
2	I	5	H7V	N-CA-CB-C01

There are no ring outliers.

24 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	9	AC5	1	0
2	O	1	MLE	1	0
2	O	4	SAR	2	0
2	I	10	MLE	1	0
2	M	1	MLE	2	0
2	O	9	AC5	2	0
2	K	9	AC5	1	0
2	M	7	A1MFG	2	0
2	K	3	SAR	1	0
2	K	10	MLE	1	0
2	N	1	MLE	2	0
2	K	1	MLE	1	0
2	M	3	SAR	1	0
2	N	4	SAR	1	0
2	N	9	AC5	3	0
2	L	10	MLE	2	0
2	M	10	MLE	2	0
2	P	3	SAR	1	0
2	N	3	SAR	1	0
2	I	9	AC5	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	1	MLE	2	0
2	N	10	MLE	1	0
2	P	4	SAR	1	0
2	P	10	MLE	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 8 are monoatomic - leaving 18 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
4	EDO	C	202	-	3,3,3	0.29	0	2,2,2	0.08	0
3	GDP	A	201	5	28,30,30	1.27	4 (14%)	44,47,47	1.67	6 (13%)
3	GDP	C	201	5	28,30,30	1.26	3 (10%)	44,47,47	1.67	6 (13%)
4	EDO	A	203	-	3,3,3	0.29	0	2,2,2	0.11	0
3	GDP	H	201	5	28,30,30	1.23	2 (7%)	44,47,47	2.14	11 (25%)
4	EDO	A	202	-	3,3,3	0.37	0	2,2,2	0.28	0
4	EDO	C	203	-	3,3,3	0.25	0	2,2,2	0.38	0
3	GDP	E	201	5	28,30,30	1.20	3 (10%)	44,47,47	1.76	7 (15%)
4	EDO	A	205	-	3,3,3	0.25	0	2,2,2	0.24	0
4	EDO	F	202	-	3,3,3	0.34	0	2,2,2	0.11	0
3	GDP	F	201	5	28,30,30	1.18	4 (14%)	44,47,47	1.58	7 (15%)
3	GDP	D	201	5	28,30,30	1.19	2 (7%)	44,47,47	1.76	7 (15%)
4	EDO	E	202	-	3,3,3	0.29	0	2,2,2	0.43	0
4	EDO	B	203	-	3,3,3	0.33	0	2,2,2	0.05	0
4	EDO	B	205	-	3,3,3	0.28	0	2,2,2	0.19	0
3	GDP	G	201	5	28,30,30	1.20	4 (14%)	44,47,47	1.81	10 (22%)
4	EDO	B	202	-	3,3,3	0.31	0	2,2,2	0.31	0
3	GDP	B	201	5	28,30,30	1.25	2 (7%)	44,47,47	1.79	7 (15%)

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
4	EDO	C	202	-	-	1/1/1/1	-
3	GDP	A	201	5	-	2/16/32/32	0/3/3/3
3	GDP	C	201	5	-	2/16/32/32	0/3/3/3
4	EDO	A	203	-	-	1/1/1/1	-
3	GDP	H	201	5	-	4/16/32/32	0/3/3/3
4	EDO	A	202	-	-	1/1/1/1	-
4	EDO	C	203	-	-	1/1/1/1	-
3	GDP	E	201	5	-	0/16/32/32	0/3/3/3
4	EDO	A	205	-	-	1/1/1/1	-
4	EDO	F	202	-	-	1/1/1/1	-
3	GDP	F	201	5	-	2/16/32/32	0/3/3/3
3	GDP	D	201	5	-	1/16/32/32	0/3/3/3
4	EDO	E	202	-	-	0/1/1/1	-
4	EDO	B	203	-	-	0/1/1/1	-
4	EDO	B	205	-	-	0/1/1/1	-
3	GDP	G	201	5	-	0/16/32/32	0/3/3/3
4	EDO	B	202	-	-	1/1/1/1	-
3	GDP	B	201	5	-	0/16/32/32	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	201	GDP	C5-C4	3.32	1.48	1.38
3	H	201	GDP	C5-C4	3.32	1.48	1.38
3	F	201	GDP	C5-C4	3.27	1.47	1.38
3	C	201	GDP	C5-C4	3.25	1.47	1.38
3	D	201	GDP	C5-C4	3.25	1.47	1.38
3	E	201	GDP	C5-C4	3.17	1.47	1.38
3	A	201	GDP	C6-N1	-3.10	1.33	1.38
3	G	201	GDP	C5-C4	2.94	1.46	1.38
3	A	201	GDP	C5-C4	2.81	1.46	1.38
3	E	201	GDP	C6-N1	-2.78	1.33	1.38
3	B	201	GDP	C6-N1	-2.73	1.33	1.38
3	D	201	GDP	C6-N1	-2.65	1.33	1.38
3	C	201	GDP	C6-N1	-2.62	1.34	1.38
3	G	201	GDP	C6-N1	-2.58	1.34	1.38
3	G	201	GDP	C4-N9	-2.49	1.31	1.38
3	H	201	GDP	C5-N7	-2.35	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	201	GDP	C5-N7	-2.34	1.34	1.39
3	F	201	GDP	C6-N1	-2.32	1.34	1.38
3	F	201	GDP	C5-N7	-2.30	1.34	1.39
3	A	201	GDP	C5-N7	-2.26	1.34	1.39
3	E	201	GDP	C5-N7	-2.26	1.34	1.39
3	A	201	GDP	C4-N9	-2.21	1.32	1.38
3	F	201	GDP	C4-N9	-2.18	1.32	1.38
3	G	201	GDP	C5-N7	-2.15	1.34	1.39

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	201	GDP	C5-C4-N3	-6.58	117.79	128.46
3	E	201	GDP	C5-C4-N3	-5.92	118.86	128.46
3	D	201	GDP	C5-C4-N3	-5.91	118.88	128.46
3	B	201	GDP	C5-C4-N3	-5.82	119.01	128.46
3	C	201	GDP	C5-C4-N3	-5.47	119.58	128.46
3	A	201	GDP	C5-C4-N3	-5.41	119.69	128.46
3	F	201	GDP	C5-C4-N3	-5.13	120.14	128.46
3	G	201	GDP	C5-C4-N3	-5.10	120.19	128.46
3	H	201	GDP	C2-N3-C4	5.02	121.24	112.30
3	H	201	GDP	N9-C4-N3	4.90	135.78	125.94
3	B	201	GDP	C2-N3-C4	4.88	120.99	112.30
3	H	201	GDP	C5'-C4'-C3'	-4.87	96.92	115.18
3	D	201	GDP	C2-N3-C4	4.71	120.70	112.30
3	A	201	GDP	C2-N3-C4	4.63	120.55	112.30
3	B	201	GDP	PA-O3A-PB	-4.60	117.05	132.83
3	G	201	GDP	C2-N3-C4	4.56	120.42	112.30
3	E	201	GDP	C2-N3-C4	4.46	120.24	112.30
3	H	201	GDP	PA-O3A-PB	-4.32	117.98	132.83
3	E	201	GDP	N9-C4-N3	4.32	134.62	125.94
3	C	201	GDP	N9-C4-N3	4.31	134.58	125.94
3	D	201	GDP	N9-C4-N3	4.22	134.42	125.94
3	B	201	GDP	N9-C4-N3	4.16	134.29	125.94
3	F	201	GDP	C2-N3-C4	4.15	119.69	112.30
3	C	201	GDP	C2-N3-C4	4.02	119.47	112.30
3	E	201	GDP	PA-O3A-PB	-3.82	119.70	132.83
3	F	201	GDP	N9-C4-N3	3.78	133.53	125.94
3	G	201	GDP	PA-O3A-PB	-3.63	120.38	132.83
3	G	201	GDP	C6-C5-N7	3.60	136.95	130.25
3	A	201	GDP	N9-C4-N3	3.54	133.05	125.94
3	D	201	GDP	PA-O3A-PB	-3.47	120.93	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	201	GDP	N9-C4-N3	3.46	132.89	125.94
3	C	201	GDP	PA-O3A-PB	-3.37	121.27	132.83
3	E	201	GDP	C6-C5-N7	3.31	136.41	130.25
3	A	201	GDP	C6-C5-N7	3.26	136.32	130.25
3	A	201	GDP	PA-O3A-PB	-3.21	121.81	132.83
3	B	201	GDP	C6-C5-N7	3.16	136.12	130.25
3	F	201	GDP	C6-C5-N7	3.05	135.93	130.25
3	D	201	GDP	C6-C5-N7	3.05	135.91	130.25
3	E	201	GDP	C4-C5-N7	-2.96	106.03	110.72
3	H	201	GDP	O6-C6-C5	-2.96	118.74	126.60
3	H	201	GDP	O3'-C3'-C4'	-2.95	102.51	111.05
3	C	201	GDP	C6-C5-N7	2.89	135.63	130.25
3	G	201	GDP	C4-C5-N7	-2.48	106.79	110.72
3	H	201	GDP	PA-O5'-C5'	-2.48	107.14	121.68
3	B	201	GDP	C4-C5-N7	-2.47	106.82	110.72
3	F	201	GDP	PA-O3A-PB	-2.43	124.48	132.83
3	G	201	GDP	O3'-C3'-C4'	-2.43	104.04	111.05
3	C	201	GDP	C4-C5-N7	-2.42	106.89	110.72
3	A	201	GDP	C4-C5-N7	-2.35	107.00	110.72
3	G	201	GDP	C2'-C3'-C4'	2.30	107.10	102.64
3	F	201	GDP	C4-C5-N7	-2.28	107.11	110.72
3	G	201	GDP	O6-C6-C5	-2.24	120.65	126.60
3	F	201	GDP	O6-C6-C5	-2.24	120.66	126.60
3	H	201	GDP	O2'-C2'-C3'	-2.23	104.60	111.82
3	D	201	GDP	C4-C5-N7	-2.20	107.23	110.72
3	B	201	GDP	O4'-C1'-N9	-2.18	103.39	108.36
3	G	201	GDP	O2B-PB-O3A	2.13	111.77	104.64
3	H	201	GDP	C6-C5-N7	2.12	134.19	130.25
3	E	201	GDP	C8-N7-C5	2.09	108.02	104.24
3	D	201	GDP	C5-C6-N1	2.05	118.39	113.19
3	H	201	GDP	C2-N1-C6	-2.00	121.44	125.10

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	GDP	PA-O3A-PB-O3B
3	C	201	GDP	PA-O3A-PB-O3B
3	F	201	GDP	PA-O3A-PB-O3B
3	H	201	GDP	PA-O3A-PB-O3B
3	H	201	GDP	C5'-O5'-PA-O1A
4	A	205	EDO	O1-C1-C2-O2

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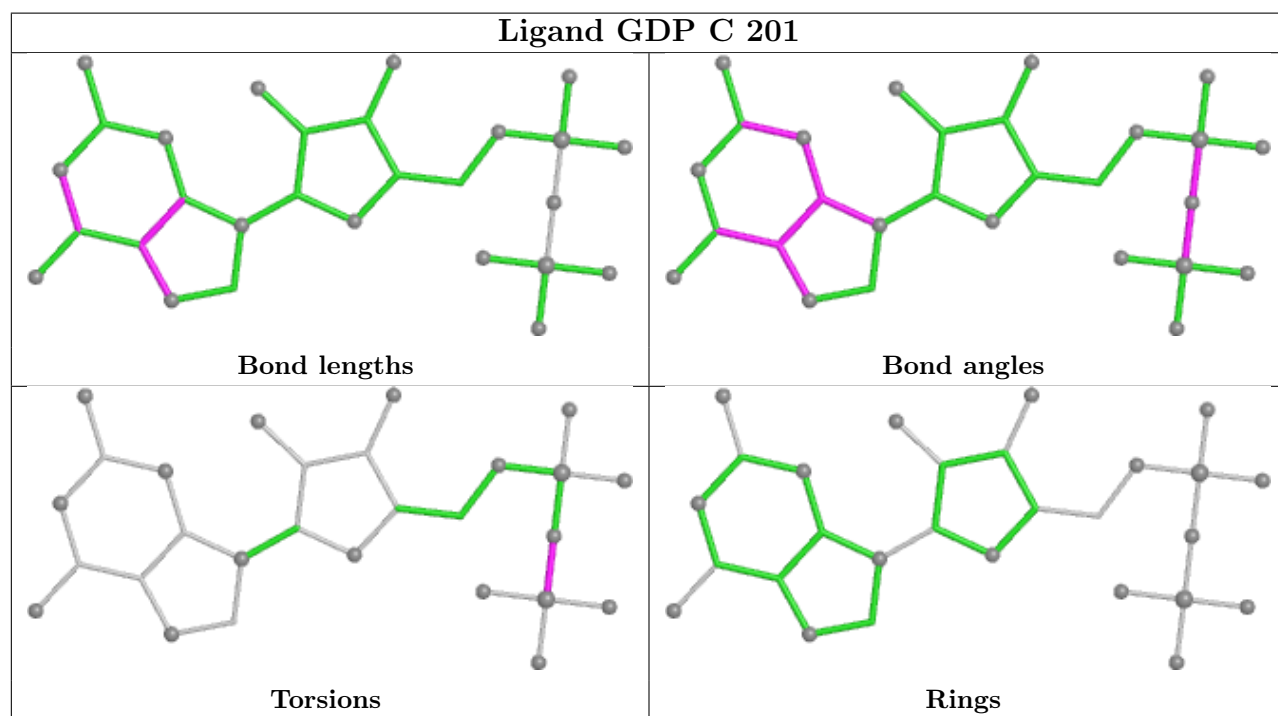
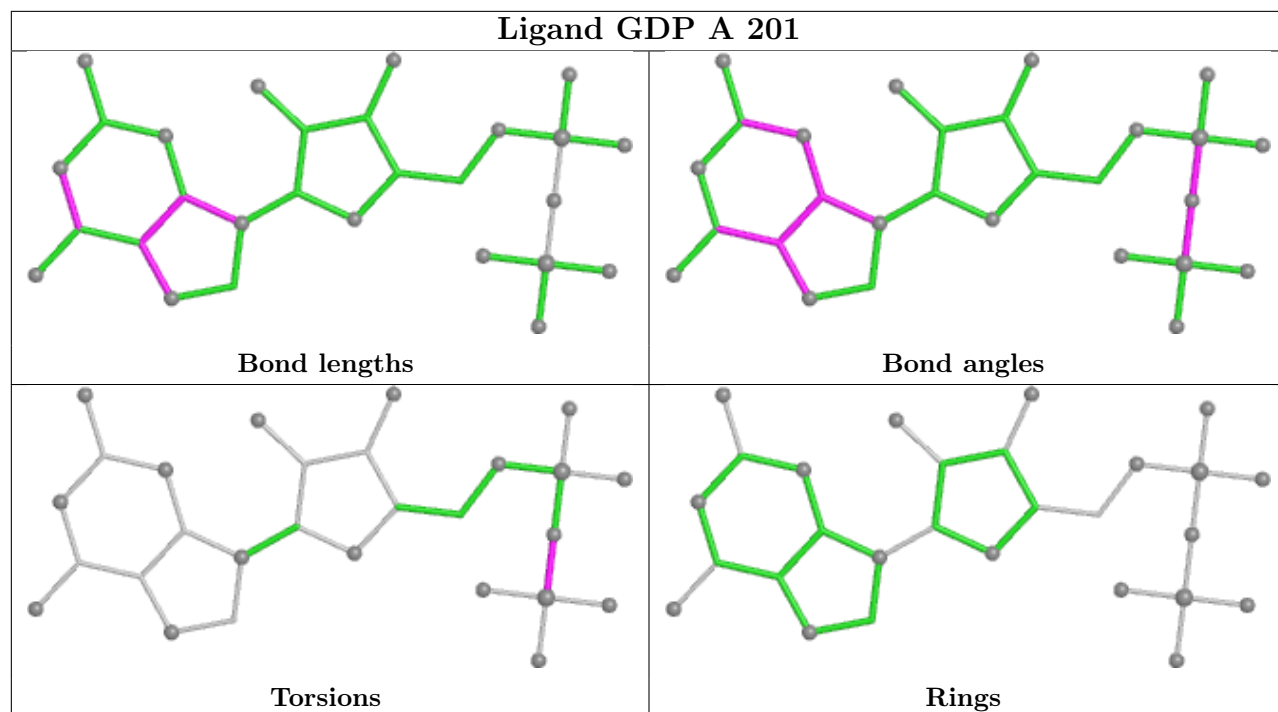
Mol	Chain	Res	Type	Atoms
4	A	202	EDO	O1-C1-C2-O2
4	B	202	EDO	O1-C1-C2-O2
4	C	203	EDO	O1-C1-C2-O2
4	F	202	EDO	O1-C1-C2-O2
4	C	202	EDO	O1-C1-C2-O2
3	A	201	GDP	PA-O3A-PB-O1B
3	F	201	GDP	PA-O3A-PB-O1B
3	H	201	GDP	PA-O3A-PB-O1B
4	A	203	EDO	O1-C1-C2-O2
3	H	201	GDP	C5'-O5'-PA-O3A
3	D	201	GDP	C5'-O5'-PA-O1A
3	C	201	GDP	PA-O3A-PB-O1B

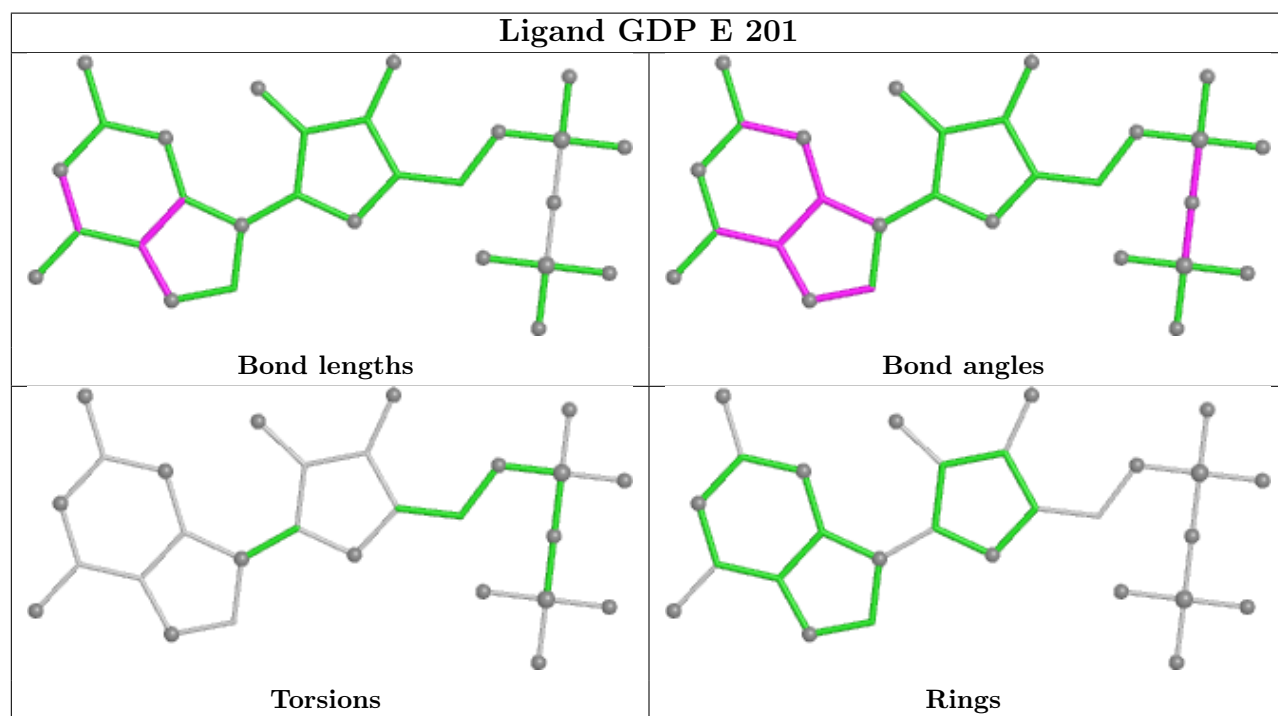
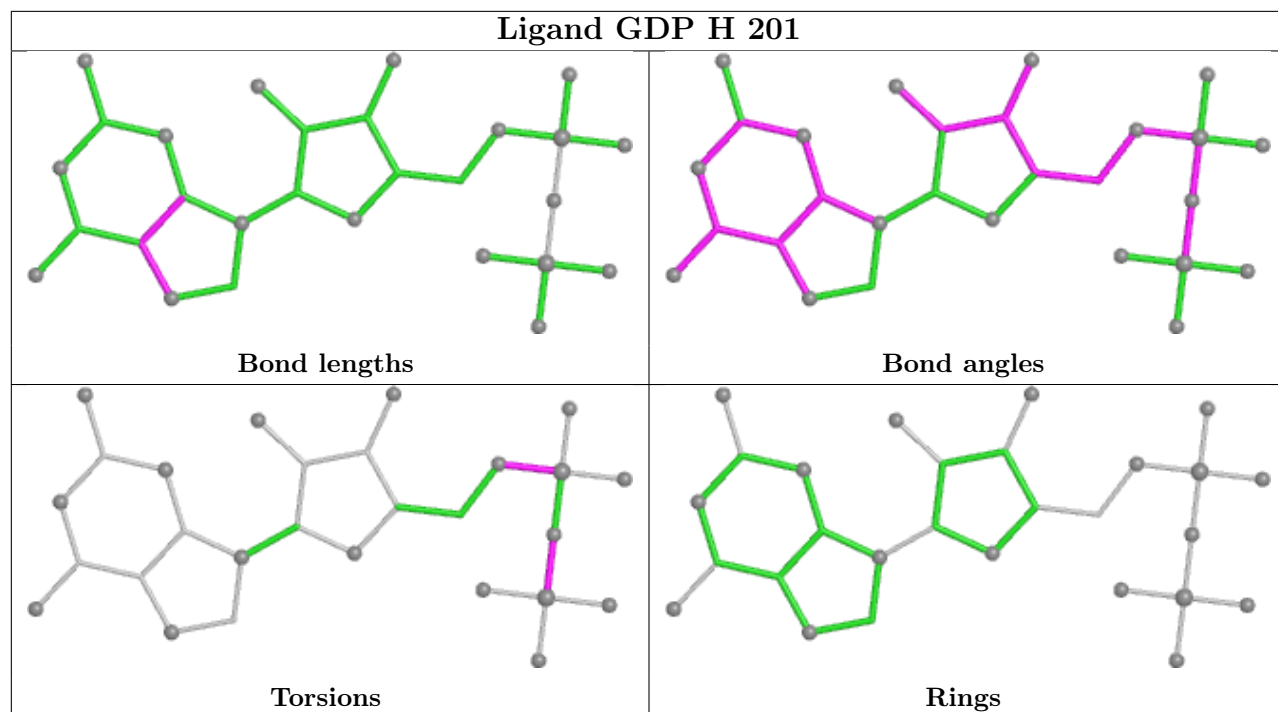
There are no ring outliers.

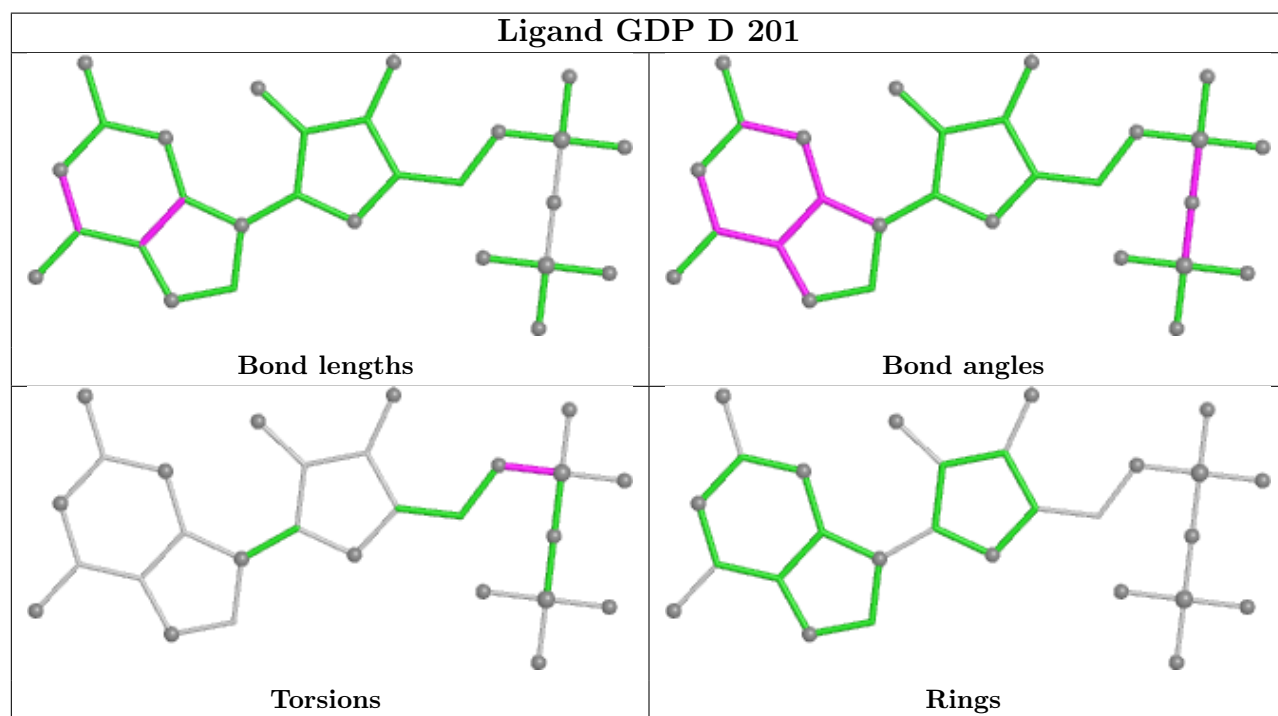
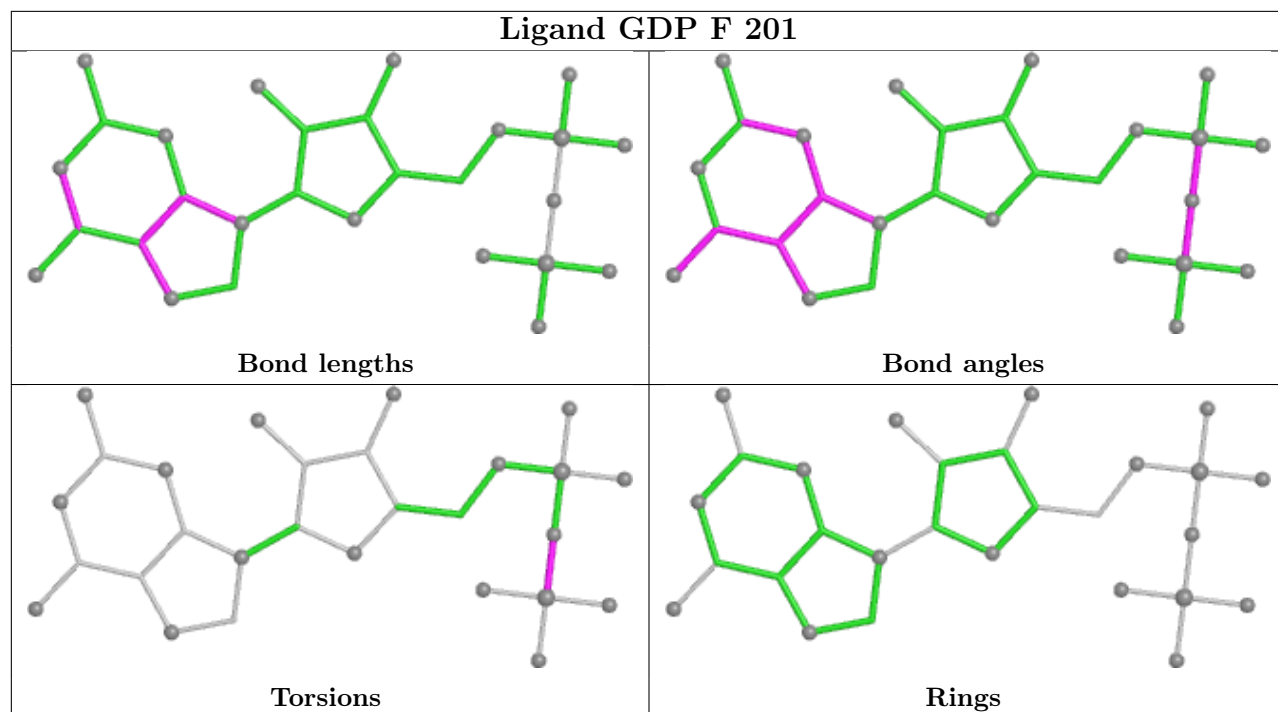
7 monomers are involved in 14 short contacts:

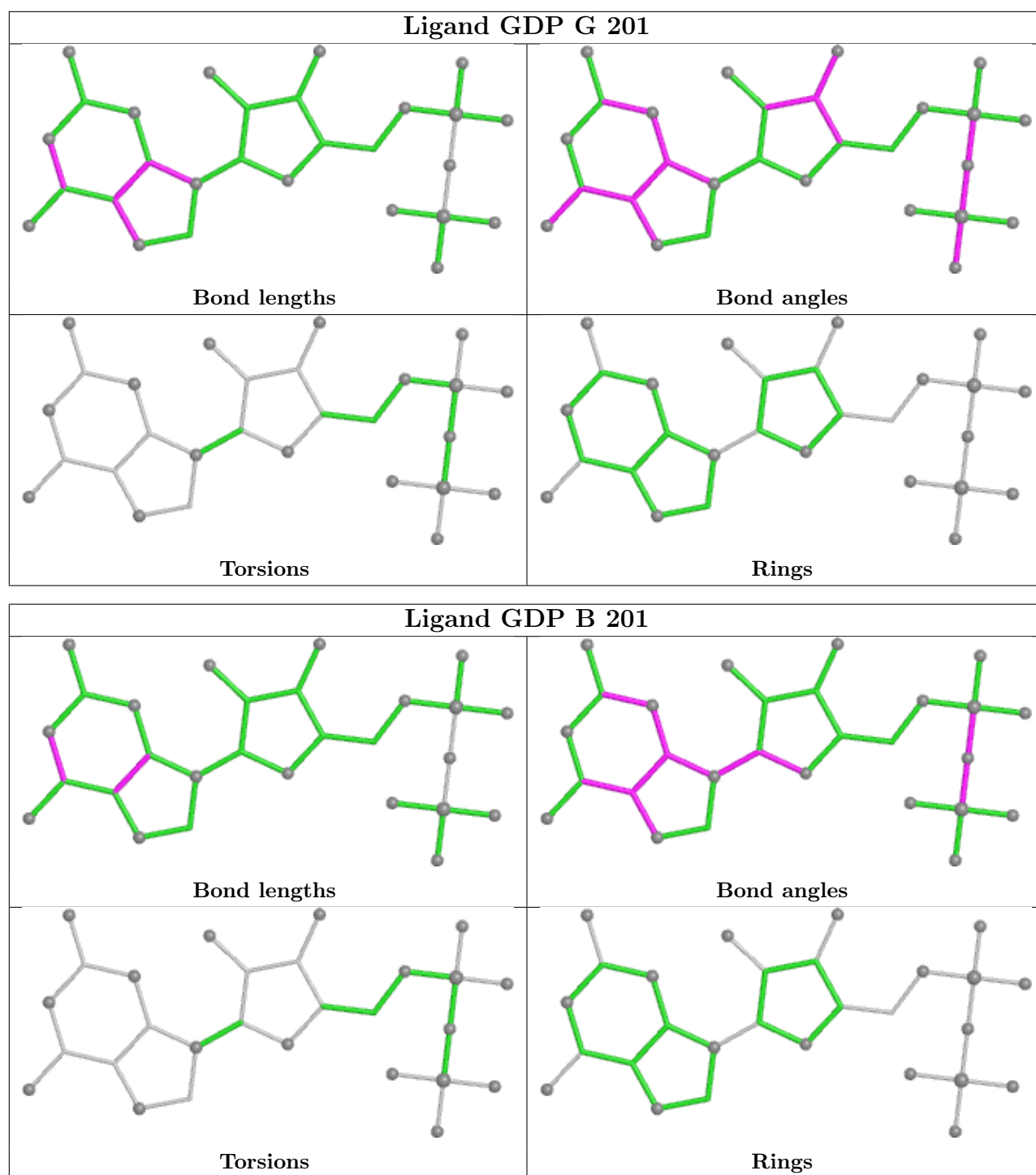
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	201	GDP	1	0
3	C	201	GDP	1	0
3	H	201	GDP	2	0
4	A	205	EDO	1	0
3	F	201	GDP	1	0
3	D	201	GDP	4	0
3	G	201	GDP	4	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	173/179 (96%)	-1.72	0 100 100	4, 11, 26, 36	0
1	B	170/179 (94%)	-1.73	0 100 100	4, 11, 23, 48	0
1	C	173/179 (96%)	-1.64	0 100 100	4, 16, 38, 52	0
1	D	171/179 (95%)	-1.64	0 100 100	7, 18, 34, 49	0
1	E	172/179 (96%)	-1.50	0 100 100	10, 27, 51, 57	0
1	F	170/179 (94%)	-1.35	0 100 100	15, 37, 63, 69	0
1	G	172/179 (96%)	-1.43	0 100 100	14, 34, 54, 67	0
1	H	171/179 (95%)	-1.35	0 100 100	19, 38, 51, 56	0
2	I	2/12 (16%)	-1.77	0 100 100	8, 8, 8, 9	0
2	J	2/12 (16%)	-1.76	0 100 100	6, 6, 6, 7	0
2	K	2/12 (16%)	-1.70	0 100 100	7, 7, 7, 13	0
2	L	2/12 (16%)	-1.54	0 100 100	17, 17, 17, 18	0
2	M	2/12 (16%)	-1.69	0 100 100	21, 21, 21, 28	0
2	N	2/12 (16%)	-1.37	0 100 100	26, 26, 26, 40	0
2	O	2/12 (16%)	-1.62	0 100 100	26, 26, 26, 32	0
2	P	2/12 (16%)	-1.68	0 100 100	27, 27, 27, 30	0
All	All	1388/1528 (90%)	-1.55	0 100 100	4, 23, 51, 69	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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(\AA^2)	Q<0.9
2	MLE	N	1	9/10	0.98	0.05	29,35,39,43	0
2	MLE	O	1	9/10	0.98	0.04	18,23,30,33	0
2	MLE	L	1	9/10	0.99	0.04	11,13,15,16	0
2	MLE	M	1	9/10	0.99	0.04	23,25,27,31	0
2	MLE	P	1	9/10	0.99	0.05	31,33,35,35	0
2	SAR	L	3	5/6	0.99	0.03	17,19,21,25	0
2	SAR	N	3	5/6	0.99	0.03	30,33,39,43	0
2	SAR	O	3	5/6	0.99	0.03	28,30,32,34	0
2	SAR	M	4	5/6	0.99	0.03	30,32,33,34	0
2	SAR	N	4	5/6	0.99	0.04	32,34,38,43	0
2	SAR	O	4	5/6	0.99	0.04	29,29,35,35	0
2	SAR	P	4	5/6	0.99	0.03	32,34,38,39	0
2	H7V	J	5	12/13	0.99	0.03	8,10,14,14	0
2	H7V	K	5	12/13	0.99	0.03	7,11,16,17	0
2	H7V	L	5	12/13	0.99	0.03	11,15,22,28	0
2	H7V	N	5	12/13	0.99	0.05	24,30,37,39	0
2	H7V	O	5	12/13	0.99	0.03	22,25,34,43	0
2	H7V	P	5	12/13	0.99	0.03	25,33,41,43	0
2	SAR	M	6	5/6	0.99	0.04	27,28,34,36	0
2	SAR	N	6	5/6	0.99	0.03	27,30,33,34	0
2	SAR	P	6	5/6	0.99	0.03	32,35,54,55	0
2	A1MFG	L	7	17/18	0.99	0.03	8,11,15,17	0
2	A1MFG	M	7	17/18	0.99	0.03	16,23,33,37	0
2	A1MFG	N	7	17/18	0.99	0.05	26,31,42,49	0
2	A1MFG	O	7	17/18	0.99	0.04	22,28,44,58	0
2	A1MFG	P	7	17/18	0.99	0.04	27,36,45,45	0
2	AC5	L	9	8/9	0.99	0.04	10,15,18,18	0
2	AC5	M	9	8/9	0.99	0.03	18,23,26,30	0
2	AC5	N	9	8/9	0.99	0.04	32,38,41,46	0
2	AC5	O	9	8/9	0.99	0.03	23,28,30,34	0
2	AC5	P	9	8/9	0.99	0.04	30,40,40,42	0
2	MLE	K	10	9/10	0.99	0.03	9,11,15,17	0
2	MLE	L	10	9/10	0.99	0.03	8,12,13,14	0
2	MLE	P	10	9/10	0.99	0.04	39,40,41,44	0
2	SAR	K	6	5/6	1.00	0.02	12,13,14,17	0
2	SAR	L	6	5/6	1.00	0.02	12,13,13,14	0
2	SAR	K	4	5/6	1.00	0.03	16,17,19,23	0
2	SAR	L	4	5/6	1.00	0.03	9,10,21,28	0
2	SAR	O	6	5/6	1.00	0.03	27,28,32,33	0
2	SAR	I	3	5/6	1.00	0.02	6,8,10,11	0
2	A1MFG	I	7	17/18	1.00	0.02	2,8,14,64	0
2	A1MFG	J	7	17/18	1.00	0.03	4,8,16,26	0
2	A1MFG	K	7	17/18	1.00	0.03	4,9,13,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SAR	J	3	5/6	1.00	0.02	6,7,10,11	0
2	SAR	K	3	5/6	1.00	0.02	13,14,21,22	0
2	MLE	K	1	9/10	1.00	0.02	4,10,14,16	0
2	H7V	I	5	12/13	1.00	0.02	7,10,13,14	0
2	SAR	M	3	5/6	1.00	0.03	22,25,27,30	0
2	AC5	I	9	8/9	1.00	0.02	6,8,9,10	0
2	AC5	J	9	8/9	1.00	0.02	4,6,7,10	0
2	AC5	K	9	8/9	1.00	0.02	5,8,11,12	0
2	MLE	I	1	9/10	1.00	0.02	8,9,10,16	0
2	MLE	J	1	9/10	1.00	0.03	4,5,6,8	0
2	H7V	M	5	12/13	1.00	0.03	19,24,34,42	0
2	SAR	P	3	5/6	1.00	0.03	28,29,34,38	0
2	SAR	I	4	5/6	1.00	0.01	7,9,12,12	0
2	MLE	I	10	9/10	1.00	0.03	1,7,13,13	0
2	MLE	J	10	9/10	1.00	0.02	6,8,9,10	0
2	SAR	J	4	5/6	1.00	0.04	7,10,11,16	0
2	SAR	I	6	5/6	1.00	0.02	6,8,8,9	0
2	MLE	M	10	9/10	1.00	0.03	22,23,26,30	0
2	MLE	N	10	9/10	1.00	0.03	26,30,36,42	0
2	MLE	O	10	9/10	1.00	0.03	17,24,29,30	0
2	SAR	J	6	5/6	1.00	0.02	4,5,6,8	0

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(\AA^2)	Q<0.9
4	EDO	E	202	4/4	0.98	0.04	18,22,27,28	0
4	EDO	F	202	4/4	0.98	0.04	26,26,30,31	0
4	EDO	A	202	4/4	0.99	0.03	17,20,21,23	0
4	EDO	A	205	4/4	0.99	0.05	12,12,12,16	0
4	EDO	B	203	4/4	0.99	0.04	18,20,20,23	0
4	EDO	B	205	4/4	0.99	0.04	31,33,34,37	0
4	EDO	C	202	4/4	0.99	0.03	12,12,12,14	0

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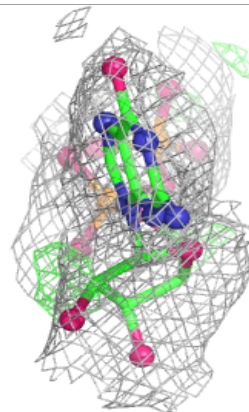
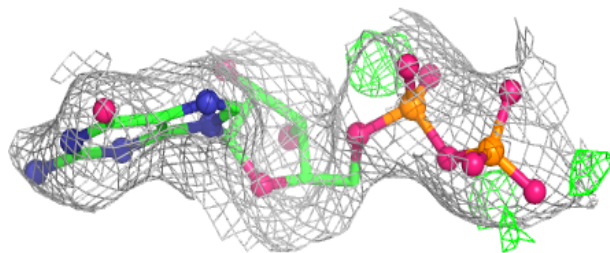
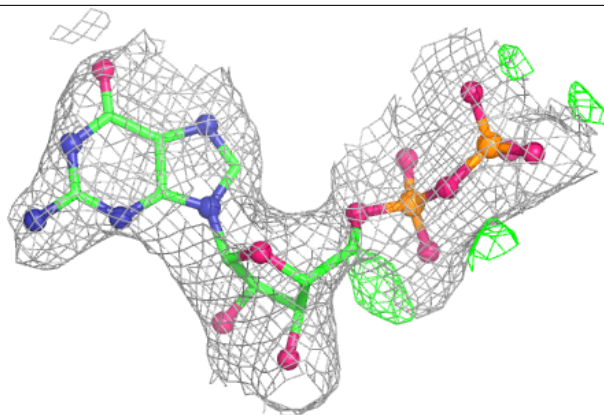
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	C	203	4/4	0.99	0.04	28,31,38,42	0
3	GDP	G	201	28/28	0.99	0.03	21,36,43,46	0
3	GDP	H	201	28/28	0.99	0.03	23,31,38,47	0
5	MG	A	204	1/1	0.99	0.01	10,10,10,10	0
5	MG	H	202	1/1	0.99	0.02	32,32,32,32	0
3	GDP	E	201	28/28	1.00	0.02	13,21,24,30	0
3	GDP	F	201	28/28	1.00	0.02	14,29,35,43	0
3	GDP	A	201	28/28	1.00	0.01	6,8,14,16	0
3	GDP	B	201	28/28	1.00	0.02	1,6,11,20	0
3	GDP	C	201	28/28	1.00	0.02	4,6,10,12	0
4	EDO	A	203	4/4	1.00	0.03	18,18,19,29	0
3	GDP	D	201	28/28	1.00	0.02	10,24,30,36	0
5	MG	B	204	1/1	1.00	0.01	5,5,5,5	0
5	MG	C	204	1/1	1.00	0.02	13,13,13,13	0
5	MG	D	202	1/1	1.00	0.01	21,21,21,21	0
5	MG	E	203	1/1	1.00	0.01	16,16,16,16	0
5	MG	F	203	1/1	1.00	0.02	21,21,21,21	0
5	MG	G	202	1/1	1.00	0.01	23,23,23,23	0
4	EDO	B	202	4/4	1.00	0.04	30,30,30,36	0

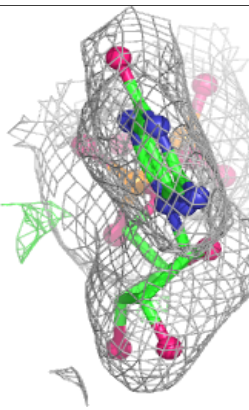
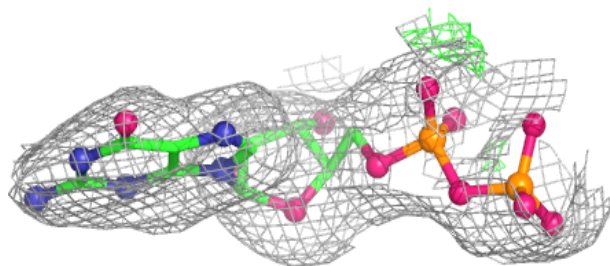
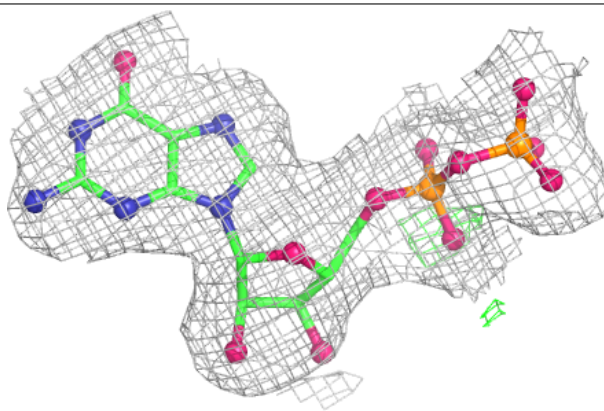
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP G 201:

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

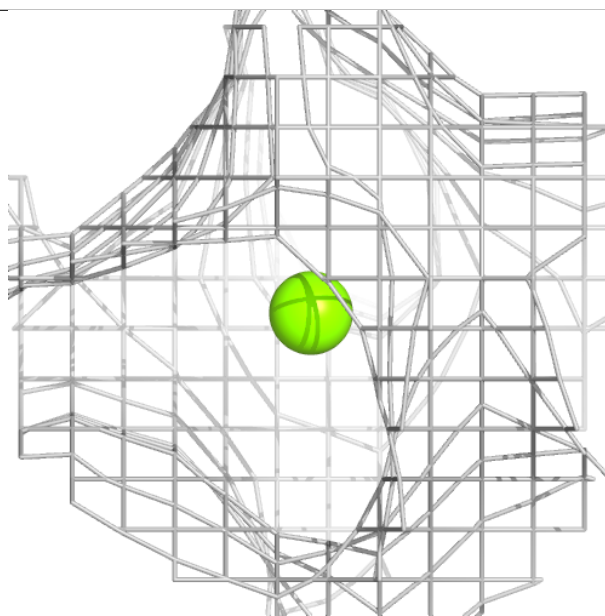
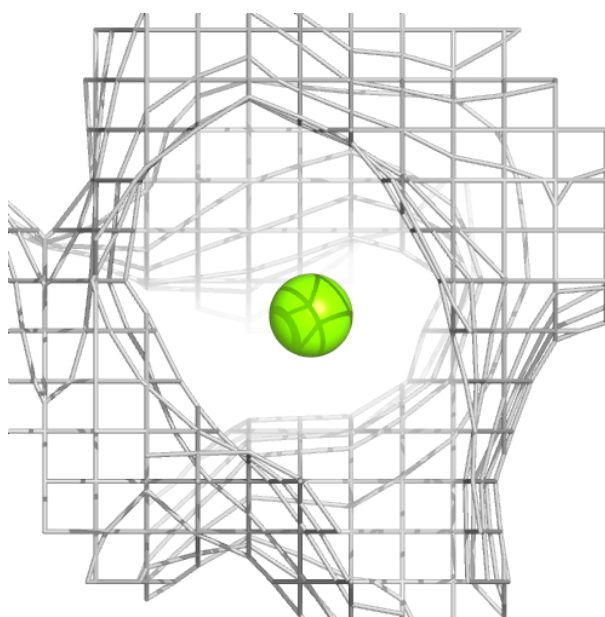
**Electron density around GDP H 201:**

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



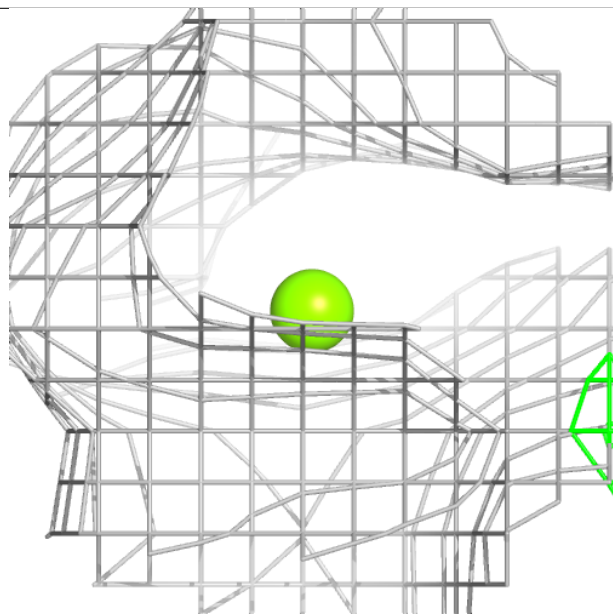
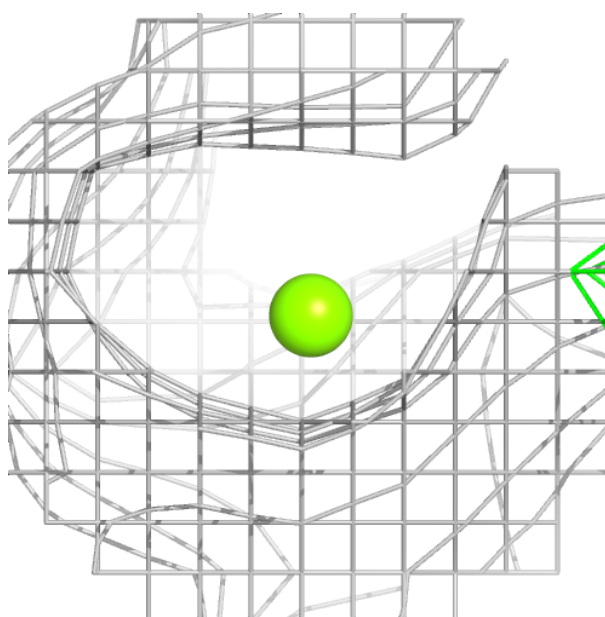
Electron density around MG A 204:

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and green (positive)



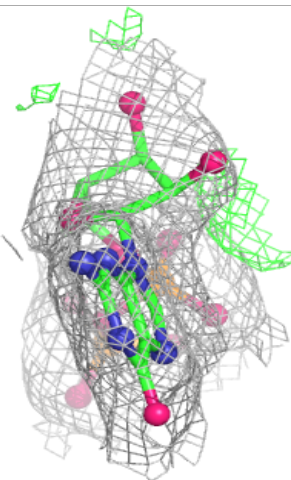
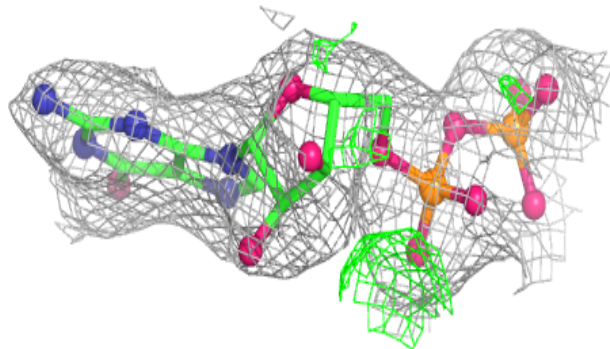
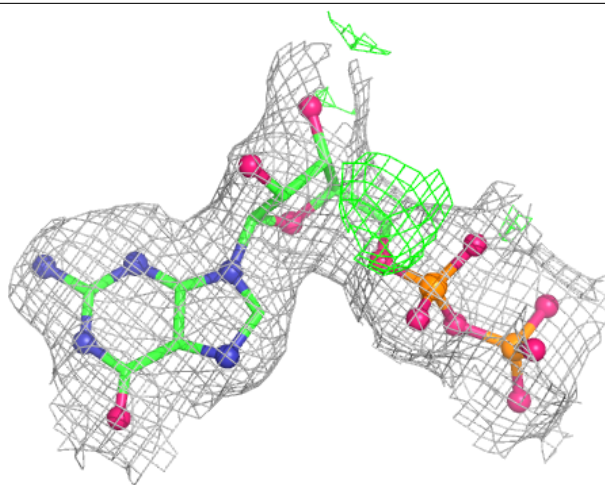
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and green (positive)



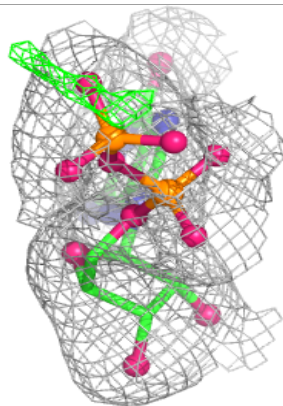
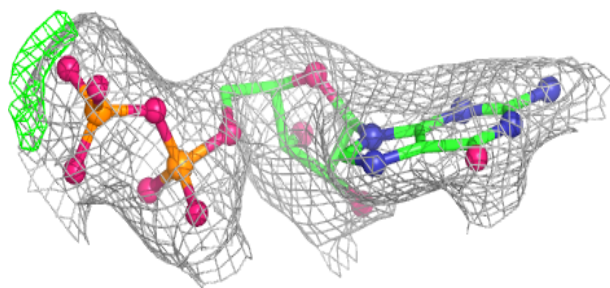
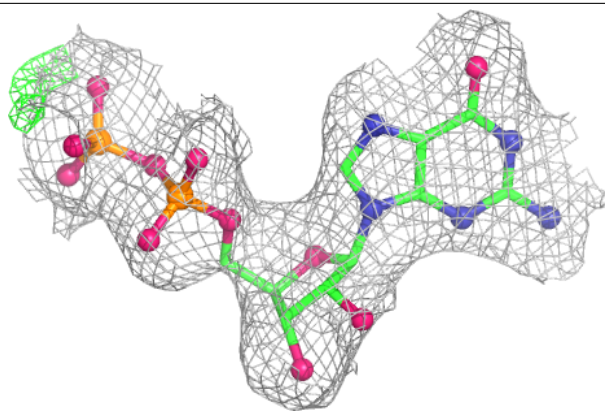
Electron density around GDP E 201:

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and green (positive)

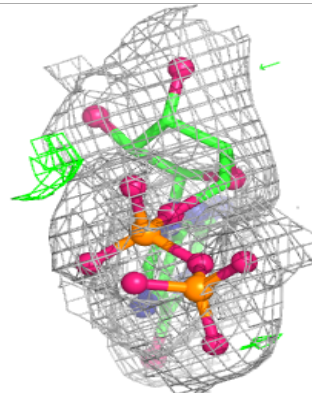
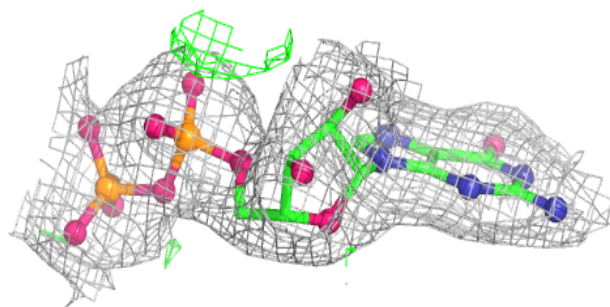
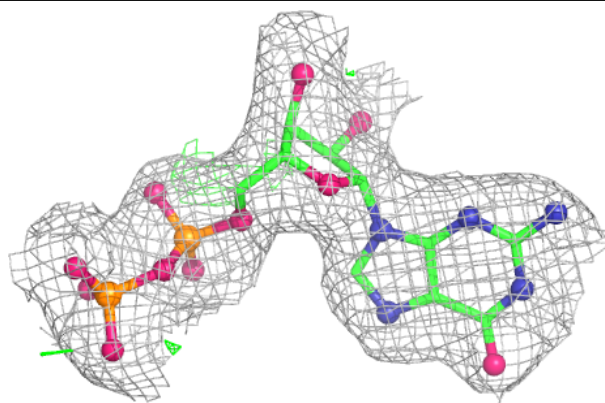


Electron density around GDP F 201:

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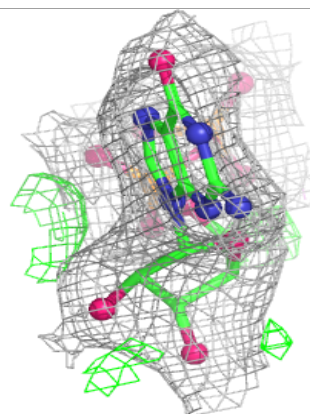
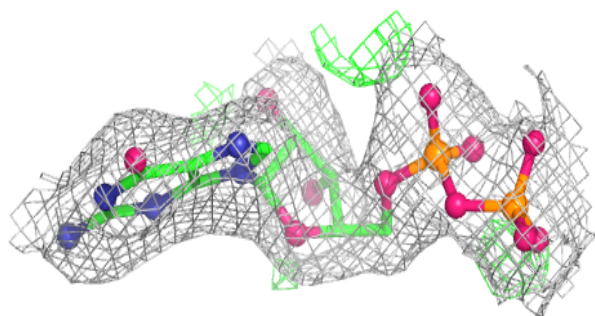
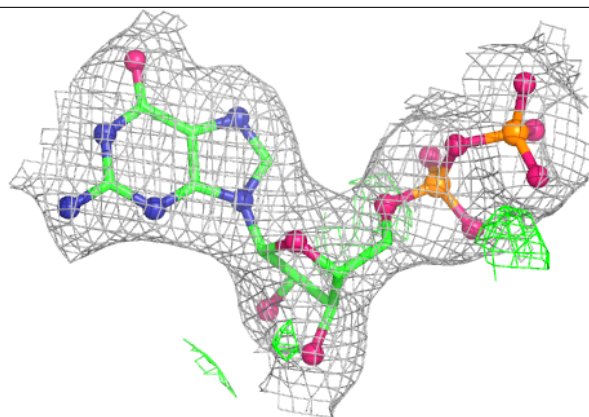
**Electron density around GDP A 201:**

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and green (positive)

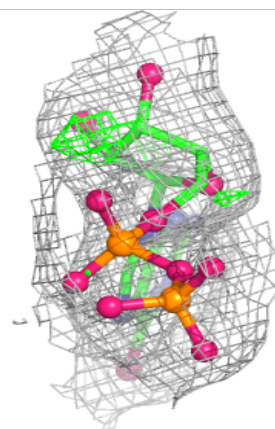
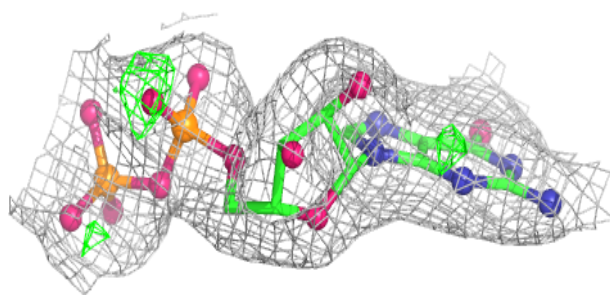
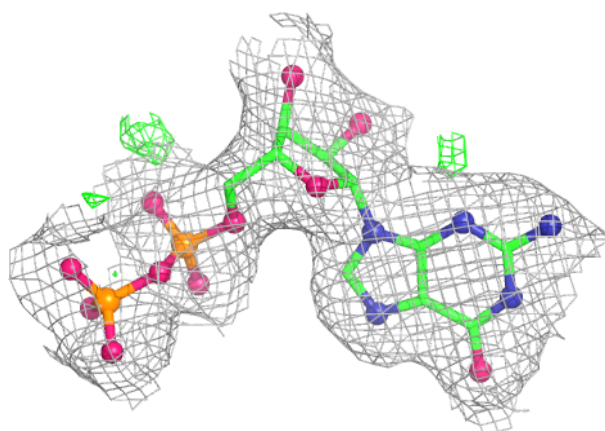


Electron density around GDP B 201:

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and green (positive)

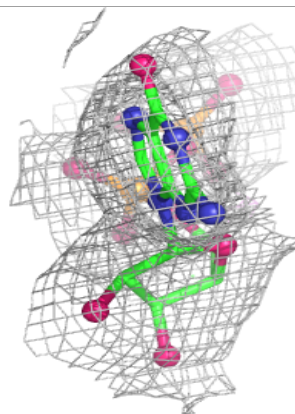
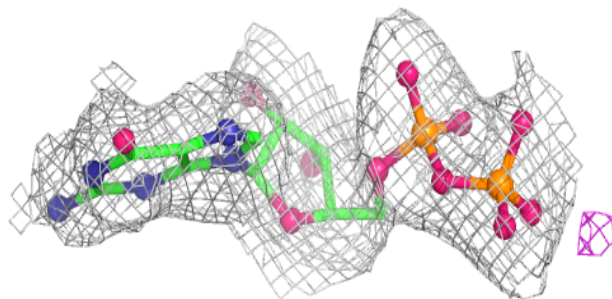
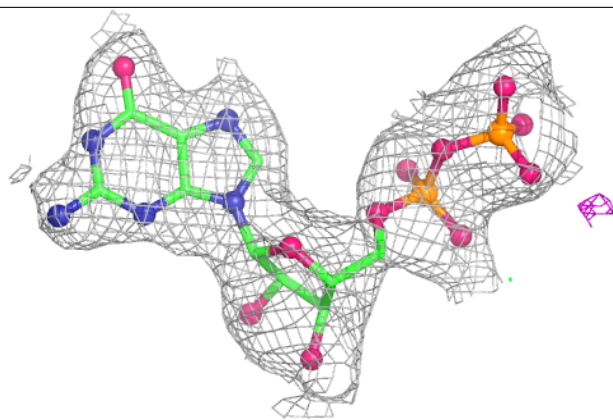
**Electron density around GDP C 201:**

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and green (positive)



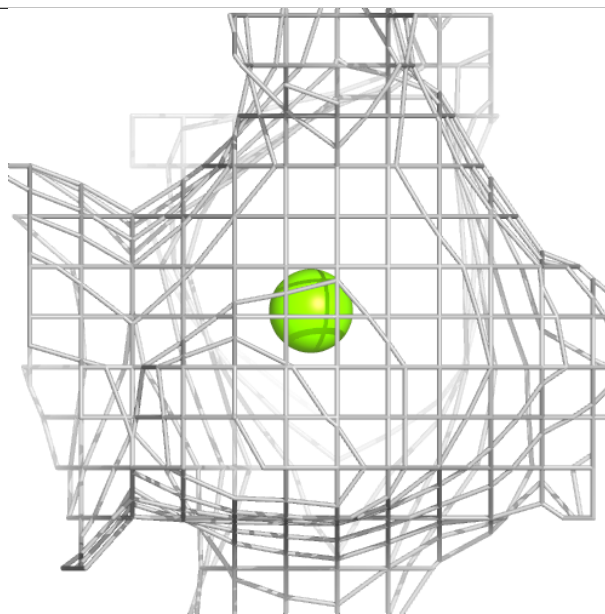
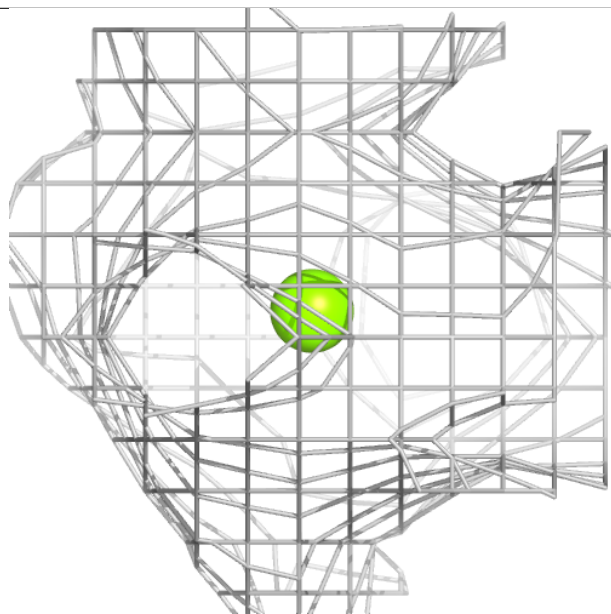
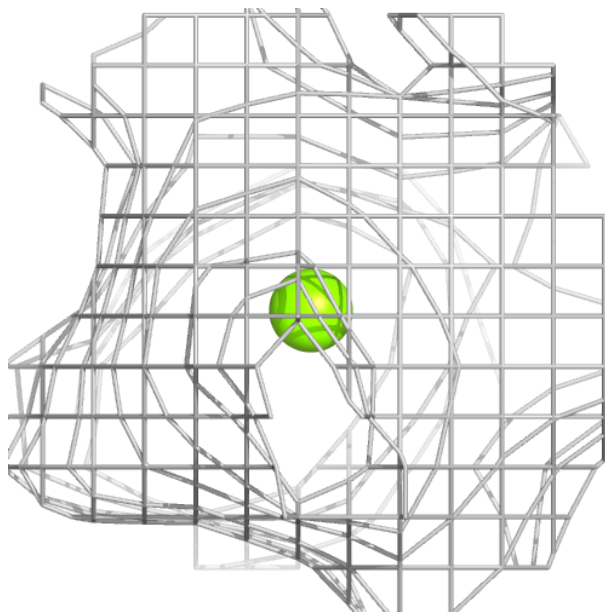
Electron density around GDP D 201:

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and green (positive)



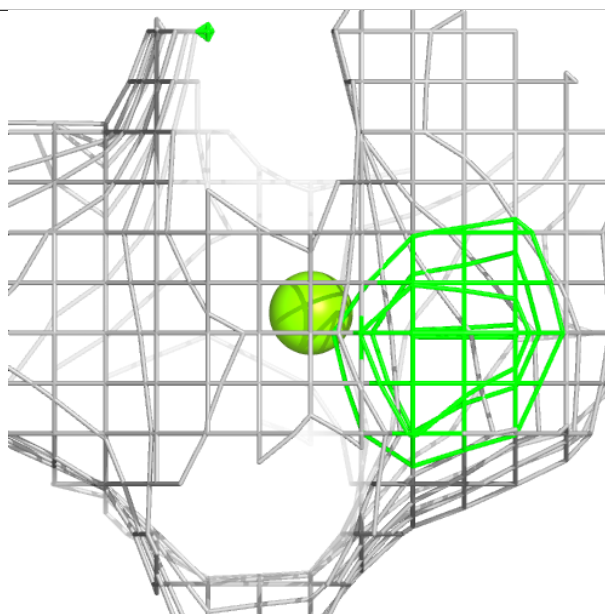
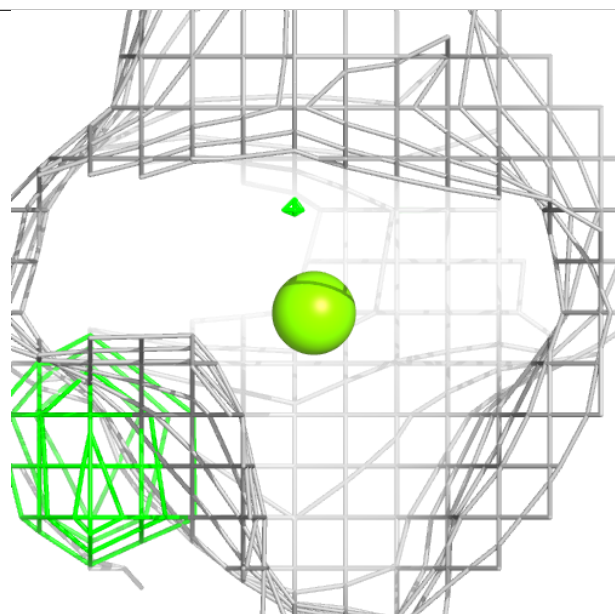
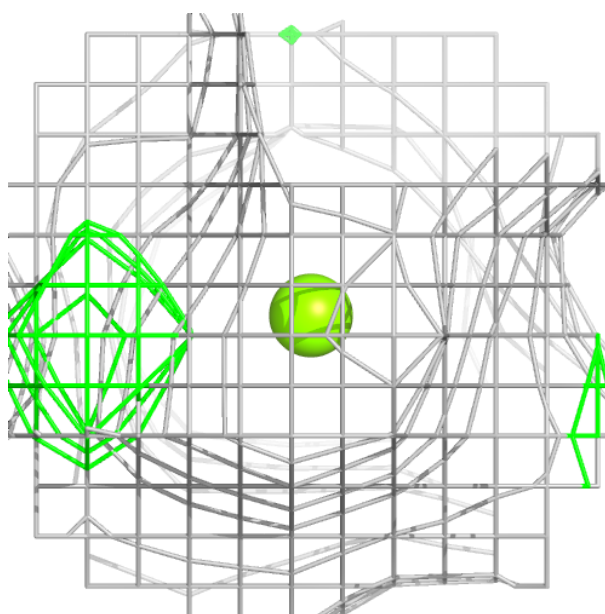
Electron density around MG B 204:

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



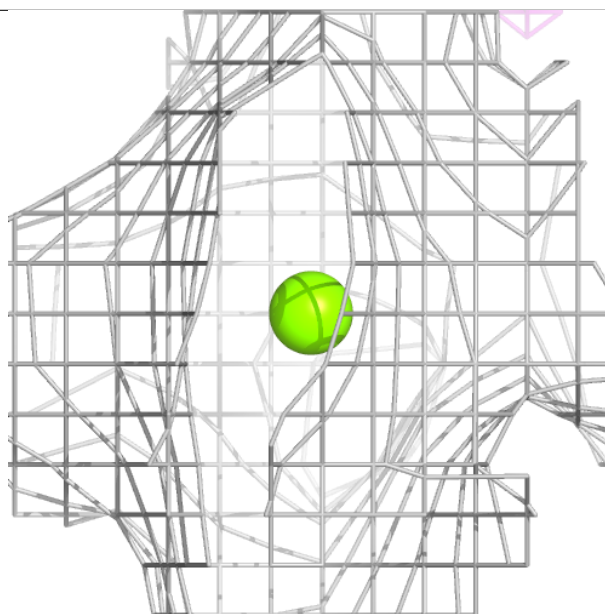
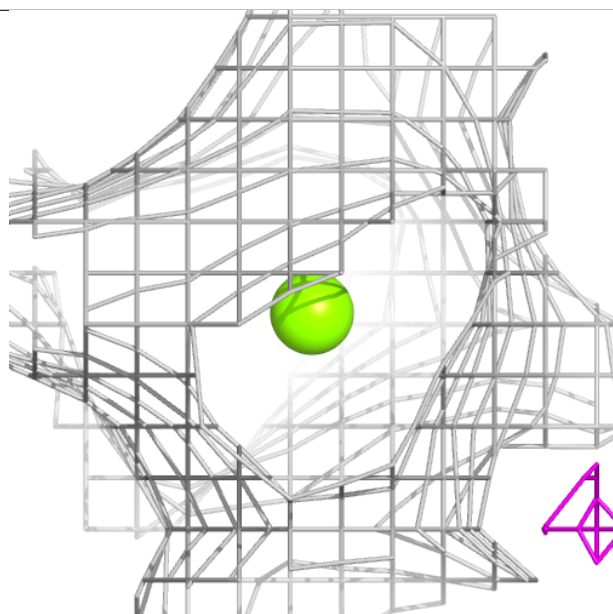
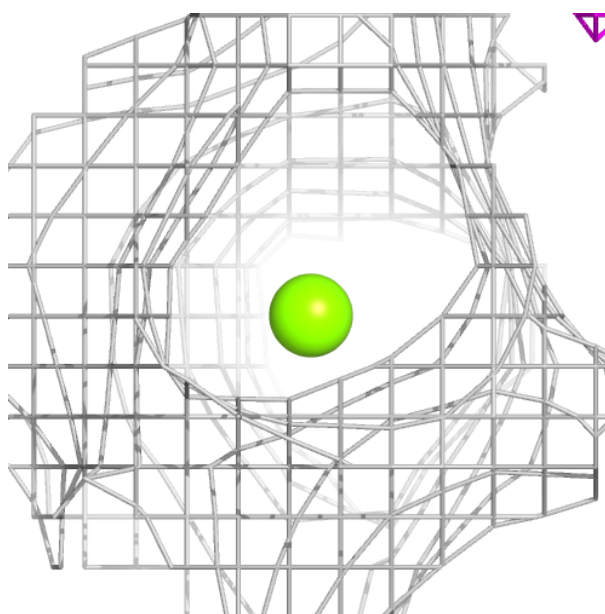
Electron density around MG C 204:

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



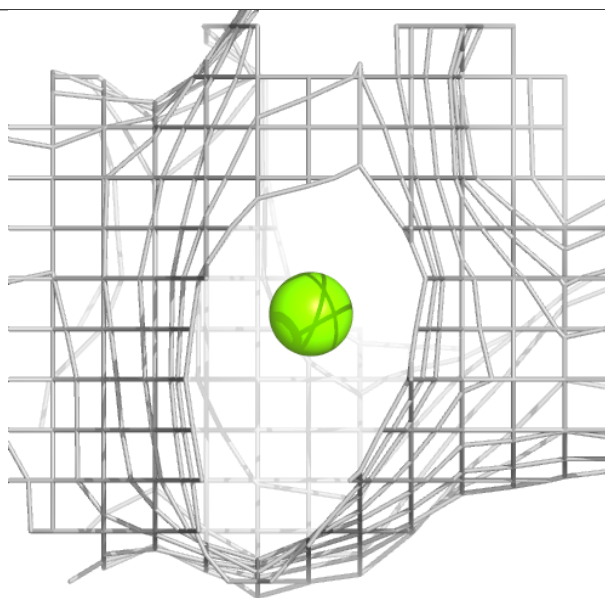
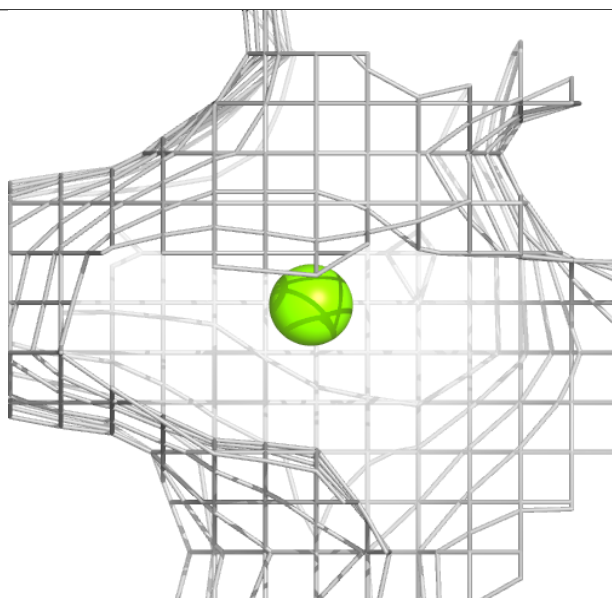
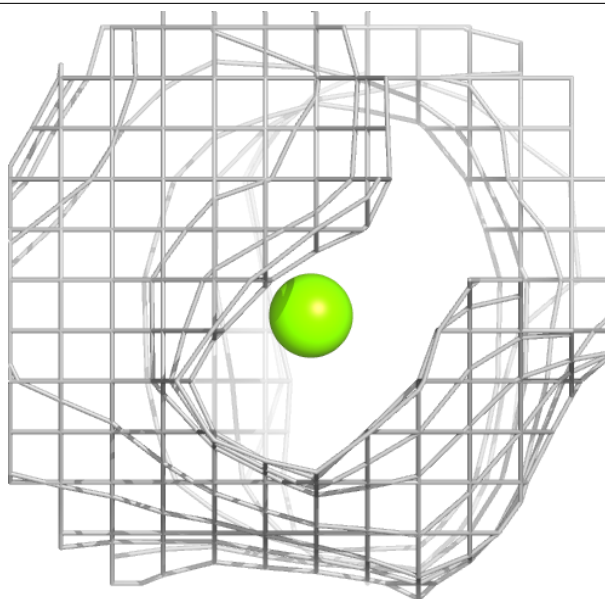
Electron density around MG D 202:

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



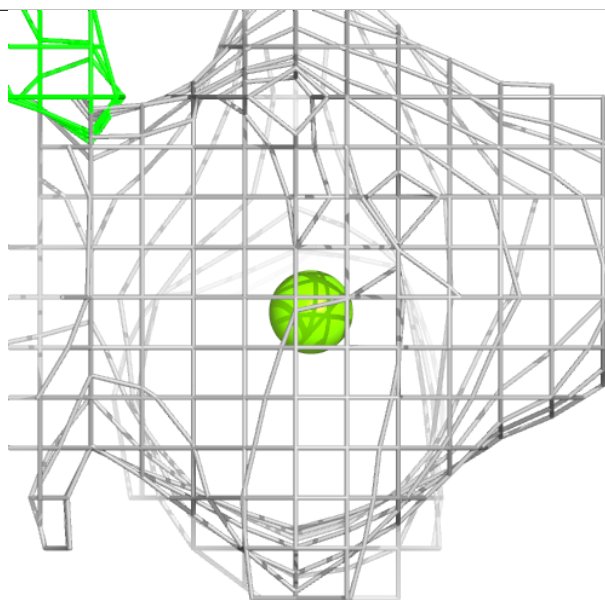
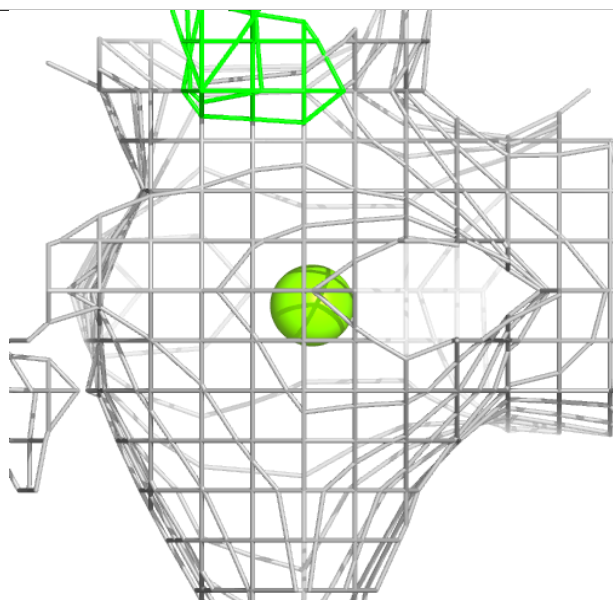
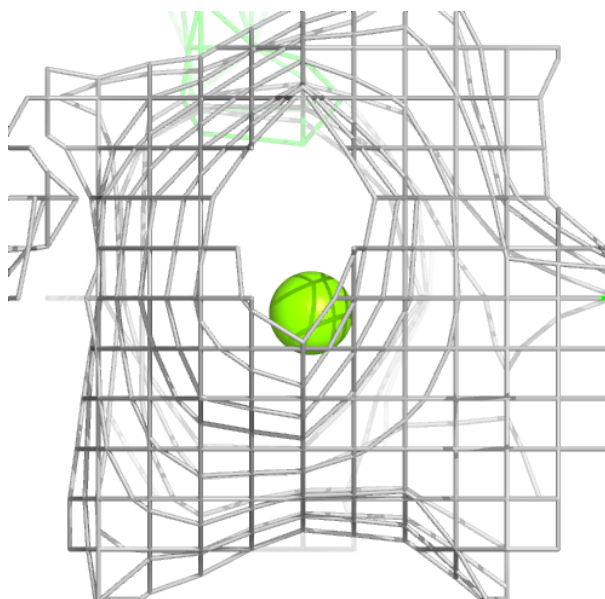
Electron density around MG E 203:

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



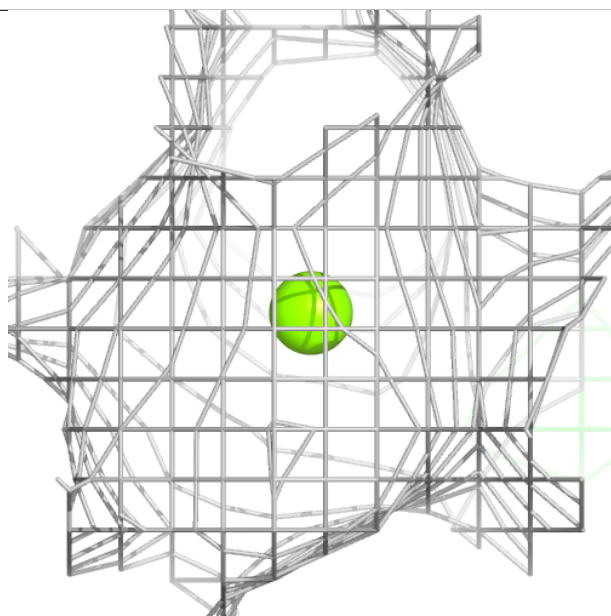
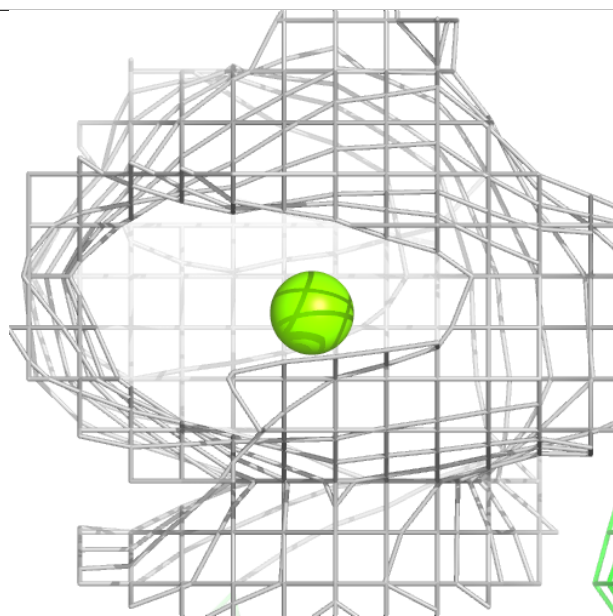
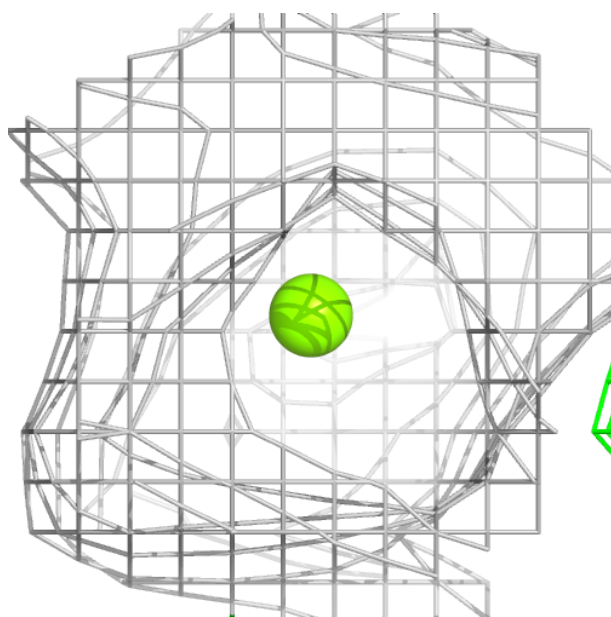
Electron density around MG F 203:

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



Electron density around MG G 202:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.