W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Nov 28, 2023 – 11:04 pm GMT

PDB ID	:	8QW7
Title	:	Crystal Structure of compound 4 in complex with KRAS G12V C118S GDP and pVHL:ElonginC:ElonginB
Authors	:	Zollman, D.; Farnaby, W.; Ciulli, A.
Deposited on	:	2023-10-18
Resolution	:	2.36 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

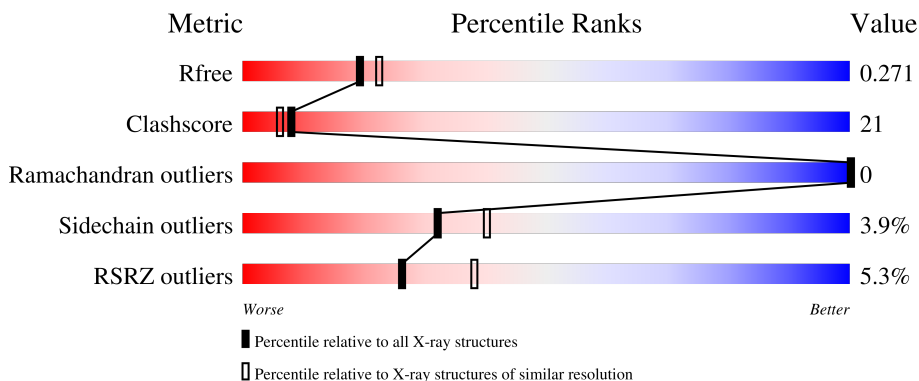|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.36 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.
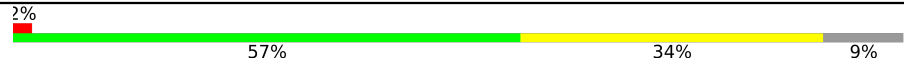
Metric	Percentile Ranks	Value
Rfree		0.271
Clashscore		21
Ramachandran outliers		0
Sidechain outliers		3.9%
RSRZ outliers		5.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 <=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	D	104	12% / 50% 46% · ·
1	H	104	3% / 58% 37% 5% ·
2	C	97	2% / 56% 30% · 12%
2	G	97	2% / 51% 37% · 11%
3	B	162	% / 59% 30% · 9%

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Mol	Chain	Length	Quality of chain
3	F	162	2% 57% 34% 9%
4	A	170	8% 72% 25%
4	E	170	9% 58% 27% 15%

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 7770 atoms, of which 120 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 Elongin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	102	Total 751	C 471	N 128	O 148	S 4	0	0	0
1	H	103	Total 798	C 507	N 136	O 151	S 4	0	0	0

- Molecule 2 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	85	Total 650	C 423	N 103	O 119	S 5	0	0	0
2	G	86	Total 682	C 441	N 107	O 128	S 6	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	16	MET	-	initiating methionine	UNP Q15369
G	16	MET	-	initiating methionine	UNP Q15369

- Molecule 3 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	148	Total 1187	C 755	N 218	O 212	S 2	0	0	0
3	F	148	Total 1192	C 756	N 219	O 215	S 2	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	52	GLY	-	expression tag	UNP P40337
B	53	SER	-	expression tag	UNP P40337

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Chain	Residue	Modelled	Actual	Comment	Reference
F	52	GLY	-	expression tag	UNP P40337
F	53	SER	-	expression tag	UNP P40337

- Molecule 4 is a protein called GTPase KRas.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	166	Total	C	N	O	S	0	0	0
			1191	747	206	233	5			
4	E	144	Total	C	N	O	S	0	0	0
			978	600	172	201	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P01116
A	12	VAL	GLY	engineered mutation	UNP P01116
A	118	SER	CYS	engineered mutation	UNP P01116
E	0	GLY	-	expression tag	UNP P01116
E	12	VAL	GLY	engineered mutation	UNP P01116
E	118	SER	CYS	engineered mutation	UNP P01116

- Molecule 5 is (2S,4R)-1-[(2R)-2-[3-[4-[(3S)-4-[4-[5-[(4S)-2-azanyl-3-cyano-4-methyl-6,7-dihydro-5H-1-benzothiophen-4-yl]-1,2,4-oxadiazol-3-yl]pyrimidin-2-yl]-3-methyl-1,4-diazepan-1-yl]butoxy]-1,2-oxazol-5-yl]-3-methyl-butanoyl]-N-[[4-(4-methyl-1,3-thiazol-5-yl)phenyl]methyl]-4-oxidanyl-pyrrolidine-2-carboxamide (three-letter code: X53) (formula: $C_{50}H_{60}N_{12}O_6S_2$) (labeled as "Ligand of Interest" by depositor).
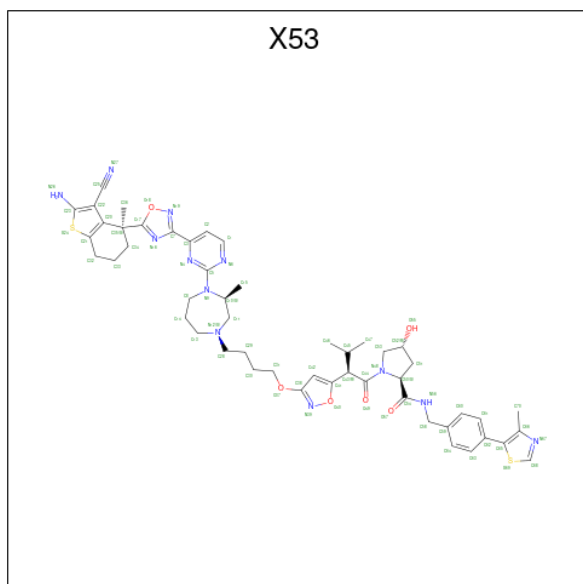
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	H	N	O	S	0	0
			130	50	60	12	6	2		
5	F	1	Total	C	H	N	O	S	0	0
			130	50	60	12	6	2		

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).
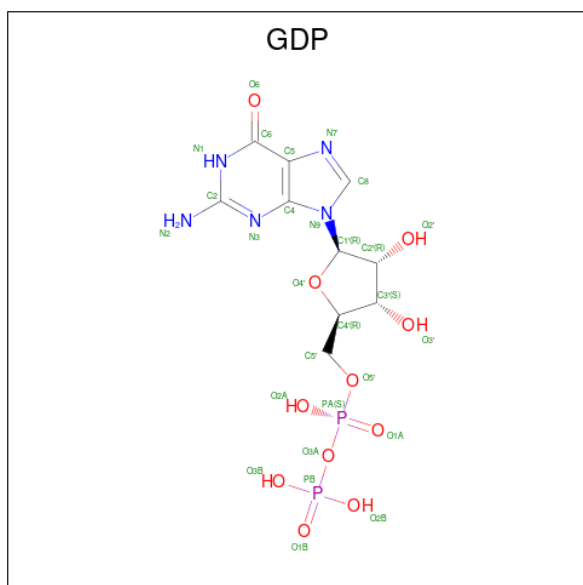
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
6	E	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		
7	E	1	Total	Mg	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	2	Total	O	0	0
			2	2		

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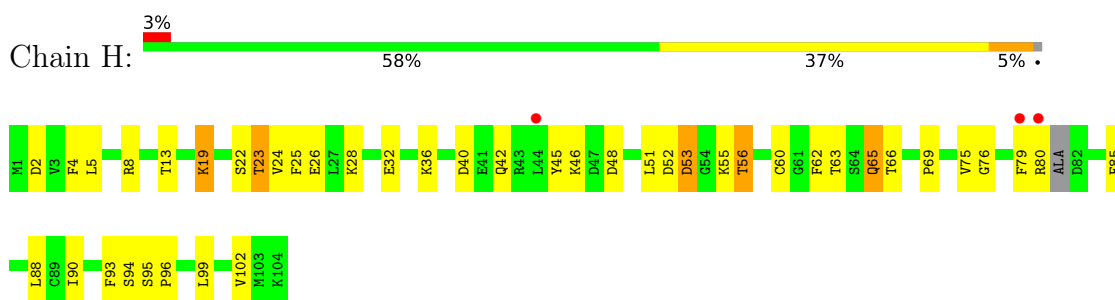| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	8	Total 8	O 8	0	0
8	H	2	Total 2	O 2	0	0
8	G	2	Total 2	O 2	0	0
8	F	5	Total 5	O 5	0	0
8	A	2	Total 2	O 2	0	0
8	E	2	Total 2	O 2	0	0

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.
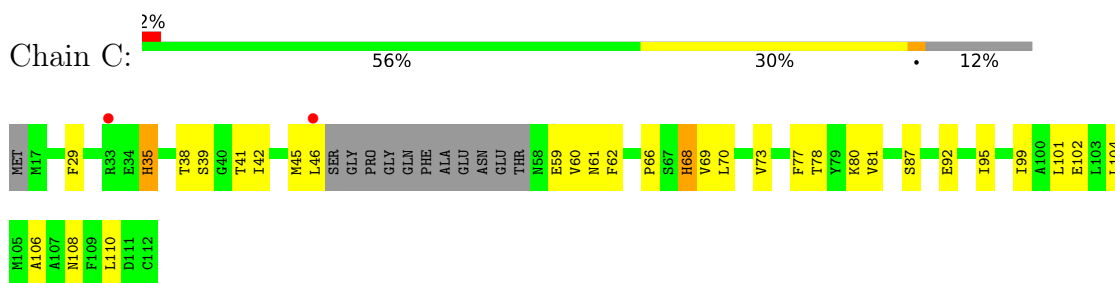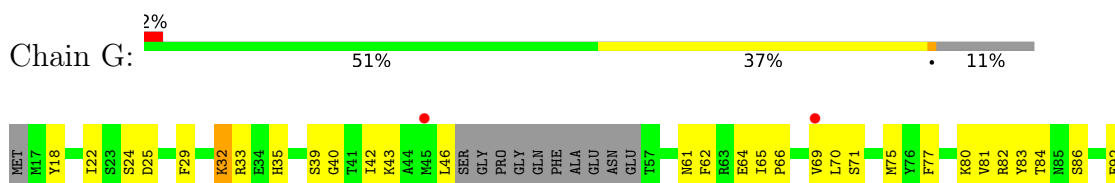
- Molecule 1: Elongin-B
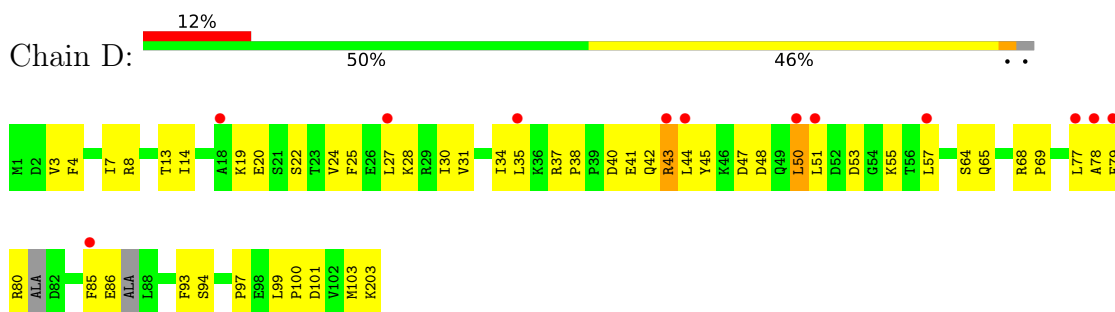
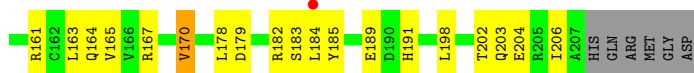- Molecule 1: Elongin-B

- Molecule 2: Elongin-C

- Molecule 2: Elongin-C

I95 E98 L103 L104 M105 A106 A107 N108 F109 L110 D111 C112

• Molecule 3: von Hippel-Lindau disease tumor suppressor

Chain B:

59% 30% • 9%

GLY SER MET GLU ALA GLY ARG PRO R60 P61 V66 N67 S68 R69 E70 Q73 F76 R82 N90 E94 P99 T100 L101 P102 T105 R108 I109 H110 S111 Y112 R113 G114 H115 H125 D126 L129 Q132 T133 E134 L135 S139 L140 N141 Q145 P154

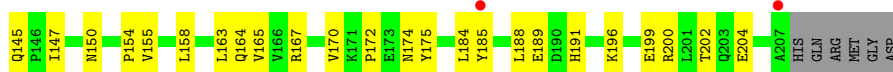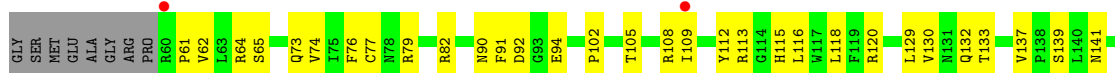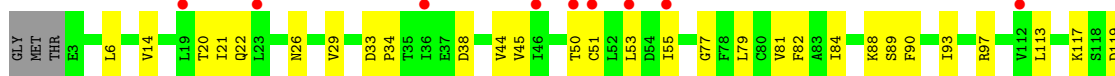R161 C162 L163 Q164 V165 V166 R167 V170 L178 D179 R182 S183 L184 Y185 E189 D190 H191 L198 T202 Q203 E204 R205 I206 A207 HIS GLN ARG MET GLY ASP

• Molecule 3: von Hippel-Lindau disease tumor suppressor

Chain F:

57% 34% 9%

GLY SER MET GLU ALA GLY ARG PRO R60 P61 V62 L63 R64 S65 Q73 V74 I75 F76 C77 N78 R79 R82 N90 F91 D92 G93 E94 P102 T105 R108 I109 Y112 R113 G114 H115 L116 W117 L118 F119 R120 L129 V130 N131 Q132 T133 V137 P138 S139 L140 N141

Q145 P146 I147 N150 P154 V155 L158 L163 Q164 V165 V166 R167 V170 K171 P172 E173 N174 Y175 L184 Y185 L188 E189 D190 H191 K196 E199 R200 L201 T202 Q203 E204 A207 HIS GLN ARG MET GLY ASP

• Molecule 4: GTPase KRas

Chain A:

8% 72% 25% • •

GLY MET THR E3 L6 V14 L19 T20 I21 Q22 L23 N26 V29 D33 P34 T35 I36 E37 D38 V44 V45 I46 T50 C51 L52 L53 D54 I55 G77 F78 L79 C80 V81 F82 A83 I84 K88 S89 F90 I93 R97 V112 L113 K117 S118 D119

V125 D126 T127 A134 Y137 G138 I139 P140 F141 I142 S145 A146 V152 A155 Y157 T158 L159 V160 R161 E162 I163 E168 LYS

• Molecule 4: GTPase KRas

Chain E:

9% 58% 27% 15%
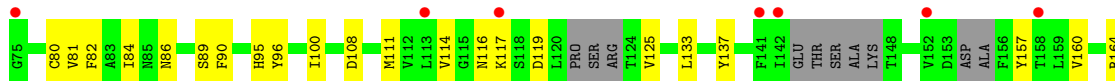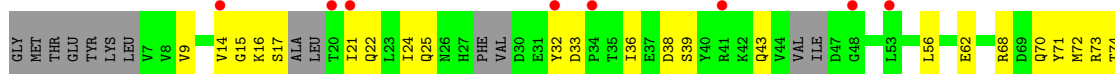
GLY MET THR GLU TYR LYS LEU V7 V8 V9 V14 G15 K16 S17 ALA LEU T20 I21 Q22 L23 I24 Q25 N26 H27 PHE VAL D30 E31 Y32 D33 P34 T35 I36 E37 D38 S39 V40 R41 K42 Q43 V44 VAL ILE D47 G48 L53 L56 E62 R68 D69 Q70 Y71 M72 R73 T74

G75 C80 V81 F82 A83 I84 N85 N86 S89 F90 H95 Y96 I100 D108 M111 V112 L113 V114 G115 N116 K117 S118 D119 L120 PRO SER ARG T124 V125 L133 Y137 F141 I142 GLU THR SER ALA LYS T148 V152 D153 ASP ALA F156 Y157 T158 L159 V160 R164

K165 H166 LYS GLU LYS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.52Å 125.93Å 81.06Å 90.00° 111.61° 90.00°	Depositor
Resolution (Å)	67.42 – 2.36 67.42 – 2.36	Depositor EDS
% Data completeness (in resolution range)	55.6 (67.42-2.36) 55.6 (67.42-2.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.246 , 0.273 0.244 , 0.271	Depositor DCC
R_{free} test set	2011 reflections (6.52%)	wwPDB-VP
Wilson B-factor (Å^2)	58.3	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 44.5	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7770	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: X53, MG, 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	D	0.62	0/763	0.79	0/1034
1	H	0.74	0/813	0.84	0/1098
2	C	0.70	0/664	0.79	0/901
2	G	0.81	0/696	0.77	0/940
3	B	0.86	0/1218	0.87	0/1667
3	F	0.80	0/1223	0.85	0/1673
4	A	0.64	0/1208	0.74	0/1644
4	E	0.66	0/986	0.77	0/1339
All	All	0.74	0/7571	0.81	0/10296

There are no bond length outliers.

There are no bond angle outliers.

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	D	751	0	704	50	0
1	H	798	0	790	37	0
2	C	650	0	629	31	0
2	G	682	0	679	36	0
3	B	1187	0	1170	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1192	0	1171	52	0
4	A	1191	0	1070	37	0
4	E	978	0	780	43	0
5	B	70	60	0	5	0
5	F	70	60	0	5	0
6	A	28	0	12	4	0
6	E	28	0	12	5	0
7	A	1	0	0	0	0
7	E	1	0	0	0	0
8	A	2	0	0	0	0
8	B	8	0	0	1	0
8	C	2	0	0	0	0
8	E	2	0	0	0	0
8	F	5	0	0	0	0
8	G	2	0	0	0	0
8	H	2	0	0	0	0
All	All	7650	120	7017	313	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 21.

The worst 5 of 313 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)
4:E:80:CYS:SG	4:E:111:MET:HE3	1.72	1.29
4:E:80:CYS:SG	4:E:111:MET:CE	2.23	1.26
3:B:102:PRO:O	3:B:105:THR:HG22	1.51	1.11
4:E:80:CYS:SG	4:E:111:MET:HE1	1.99	1.03
6:A:201:GDP:H5'	6:A:201:GDP:H8	1.22	1.02

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	D	96/104 (92%)	85 (88%)	11 (12%)	0	100	100
1	H	99/104 (95%)	91 (92%)	8 (8%)	0	100	100
2	C	81/97 (84%)	76 (94%)	5 (6%)	0	100	100
2	G	82/97 (84%)	77 (94%)	5 (6%)	0	100	100
3	B	146/162 (90%)	140 (96%)	6 (4%)	0	100	100
3	F	146/162 (90%)	140 (96%)	6 (4%)	0	100	100
4	A	164/170 (96%)	152 (93%)	12 (7%)	0	100	100
4	E	130/170 (76%)	121 (93%)	9 (7%)	0	100	100
All	All	944/1066 (89%)	882 (93%)	62 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	D	77/92 (84%)	74 (96%)	3 (4%)	32	40
1	H	86/92 (94%)	79 (92%)	7 (8%)	11	11
2	C	69/86 (80%)	66 (96%)	3 (4%)	29	35
2	G	77/86 (90%)	76 (99%)	1 (1%)	69	80
3	B	132/148 (89%)	125 (95%)	7 (5%)	22	26
3	F	133/148 (90%)	129 (97%)	4 (3%)	41	50
4	A	111/150 (74%)	108 (97%)	3 (3%)	44	55
4	E	81/150 (54%)	79 (98%)	2 (2%)	47	58
All	All	766/952 (80%)	736 (96%)	30 (4%)	32	40

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	23	THR
4	A	163	ILE
1	H	53	ASP
4	E	62	GLU
3	F	170	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
4	E	94	HIS
4	E	95	HIS
4	A	95	HIS
4	E	25	GLN
4	E	43	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
6	GDP	A	201	7	24,30,30	1.91	5 (20%)	30,47,47	1.86	9 (30%)
6	GDP	E	201	7	24,30,30	1.24	2 (8%)	30,47,47	1.64	9 (30%)
5	X53	B	401	-	61,78,78	4.04	18 (29%)	61,113,113	1.81	14 (22%)
5	X53	F	401	-	61,78,78	4.13	17 (27%)	61,113,113	1.81	13 (21%)

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
6	GDP	A	201	7	-	4/12/32/32	0/3/3/3
6	GDP	E	201	7	-	5/12/32/32	0/3/3/3
5	X53	B	401	-	-	5/37/92/92	0/9/9/9
5	X53	F	401	-	-	4/37/92/92	0/9/9/9

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	401	X53	C32-C21	-17.53	1.37	1.50
5	B	401	X53	C32-C21	-17.24	1.38	1.50
5	F	401	X53	C62-C65	-15.16	1.33	1.48
5	B	401	X53	C62-C65	-14.99	1.33	1.48
5	F	401	X53	C23-S24	-12.37	1.53	1.72

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	401	X53	N6-C5-N4	-5.95	120.06	126.00
5	F	401	X53	N6-C5-N4	-5.50	120.50	126.00
5	B	401	X53	C1-N6-C5	5.26	120.89	115.08
5	F	401	X53	C1-N6-C5	4.98	120.58	115.08
5	F	401	X53	C2-C1-N6	-4.29	118.63	123.96

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	401	X53	C44-C43-C45-C47
5	F	401	X53	C45-C43-C44-N48

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Mol	Chain	Res	Type	Atoms
5	F	401	X53	C45-C43-C44-O49
6	E	201	GDP	C5'-O5'-PA-O1A
6	E	201	GDP	C5'-O5'-PA-O2A

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	201	GDP	4	0
6	E	201	GDP	5	0
5	B	401	X53	5	0
5	F	401	X53	5	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 then 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.

Ligand GDP A 201

Bond lengths

Bond angles

Torsions

Rings

Ligand GDP E 201

Bond lengths

Bond angles

Torsions

Rings

Ligand X53 B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand X53 F 401

Bond lengths

Bond angles

Torsions

Rings
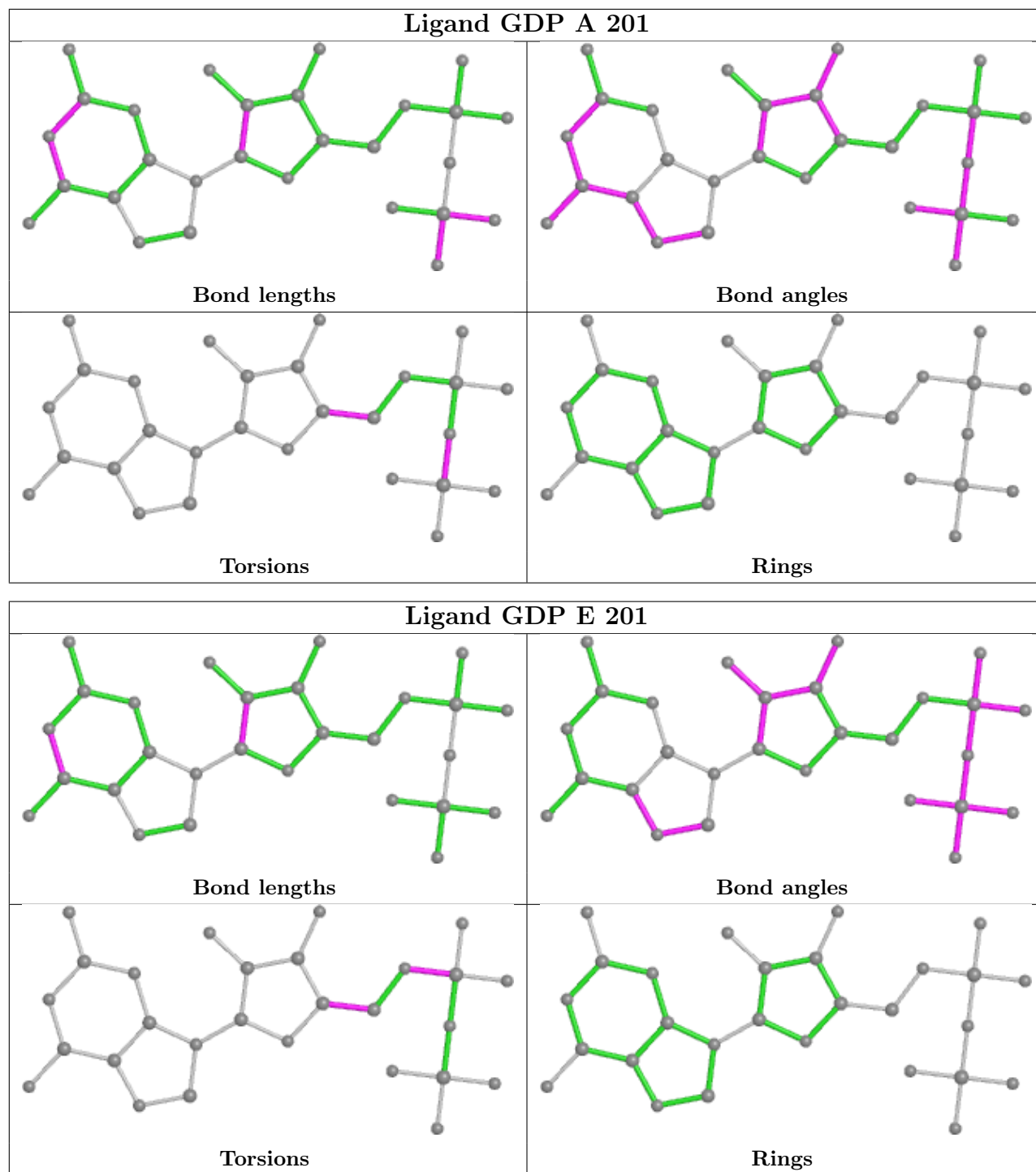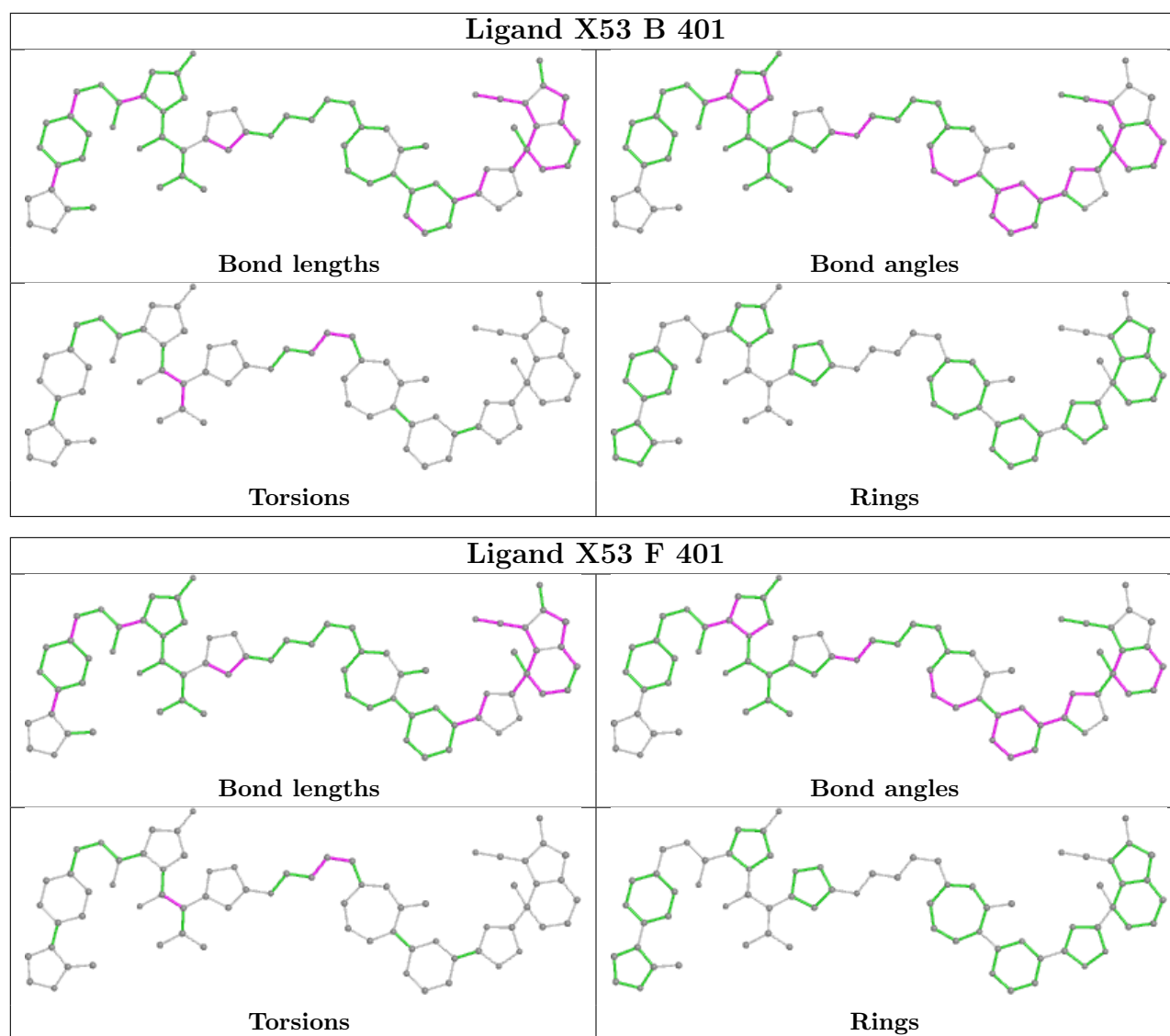
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	D	102/104 (98%)	0.75	12 (11%)	4	7	47, 82, 103, 113	0
1	H	103/104 (99%)	0.37	3 (2%)	51	62	34, 55, 69, 86	0
2	C	85/97 (87%)	0.33	2 (2%)	59	68	35, 57, 71, 74	0
2	G	86/97 (88%)	0.38	2 (2%)	60	70	29, 49, 62, 69	0
3	B	148/162 (91%)	0.25	1 (0%)	87	92	23, 39, 62, 89	0
3	F	148/162 (91%)	0.35	4 (2%)	54	64	25, 45, 67, 78	0
4	A	166/170 (97%)	0.45	13 (7%)	13	19	39, 78, 91, 105	0
4	E	144/170 (84%)	0.58	15 (10%)	6	10	44, 81, 97, 100	0
All	All	982/1066 (92%)	0.43	52 (5%)	26	38	23, 58, 94, 113	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	79	PHE	4.7
4	E	152	VAL	4.5
1	D	50	LEU	4.4
1	D	77	LEU	4.4
4	A	46	ILE	4.4

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

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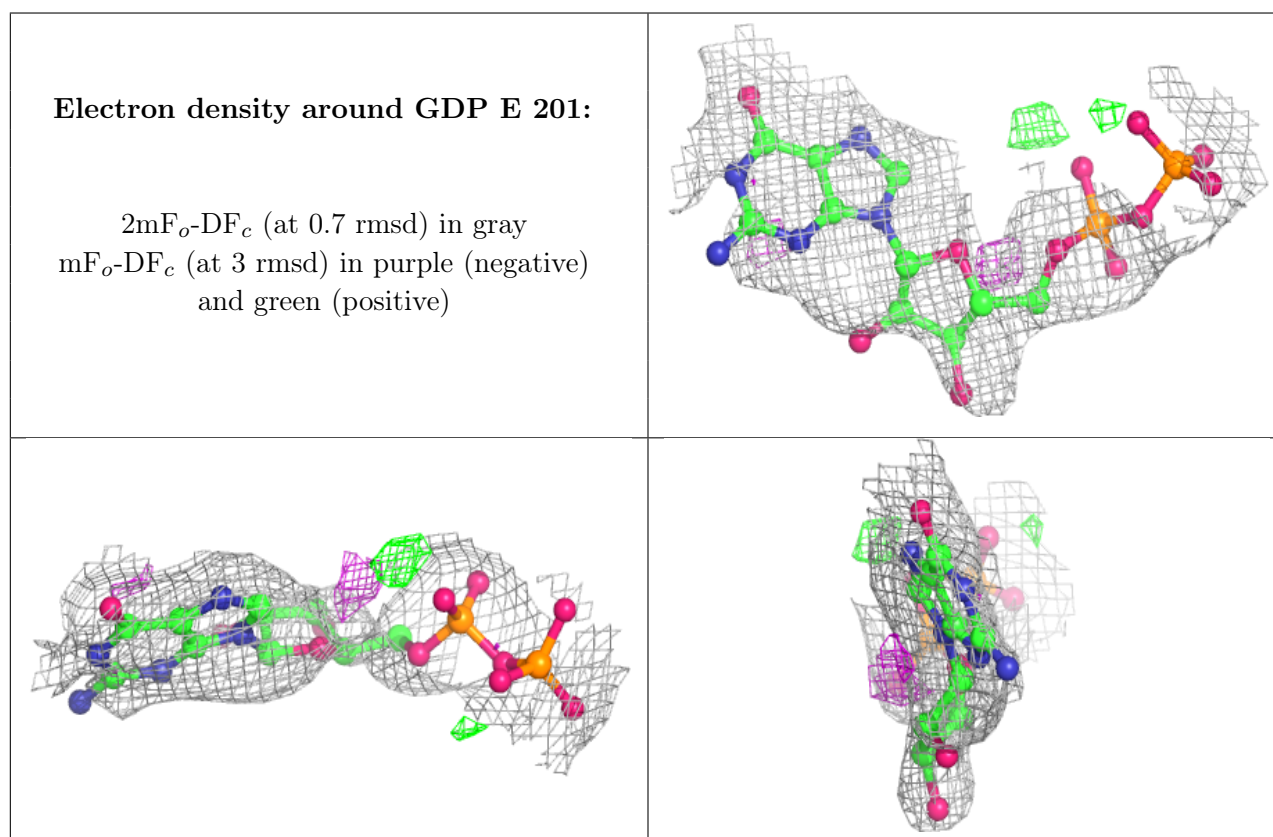
6.3   Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4   Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
6	GDP	E	201	28/28	0.76	0.21	91,105,112,114	0
6	GDP	A	201	28/28	0.91	0.13	71,84,88,93	0
5	X53	F	401	70/70	0.94	0.15	33,54,83,91	0
7	MG	E	202	1/1	0.94	0.06	88,88,88,88	0
5	X53	B	401	70/70	0.95	0.15	28,47,69,75	0
7	MG	A	202	1/1	0.98	0.28	55,55,55,55	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.
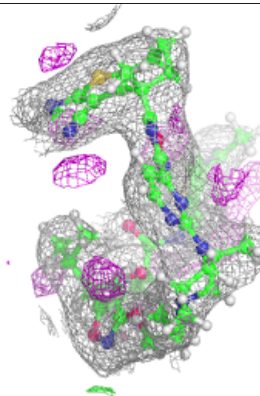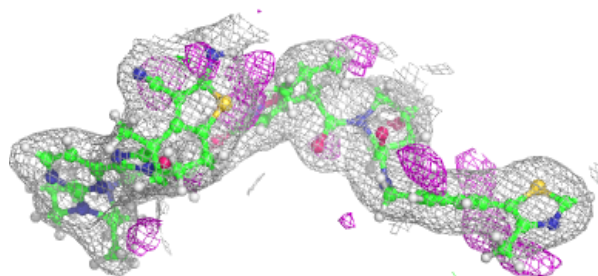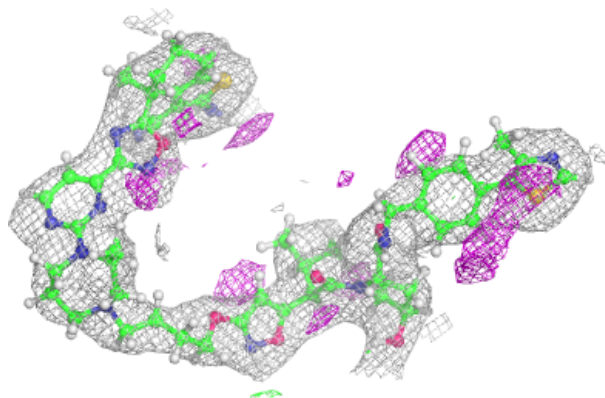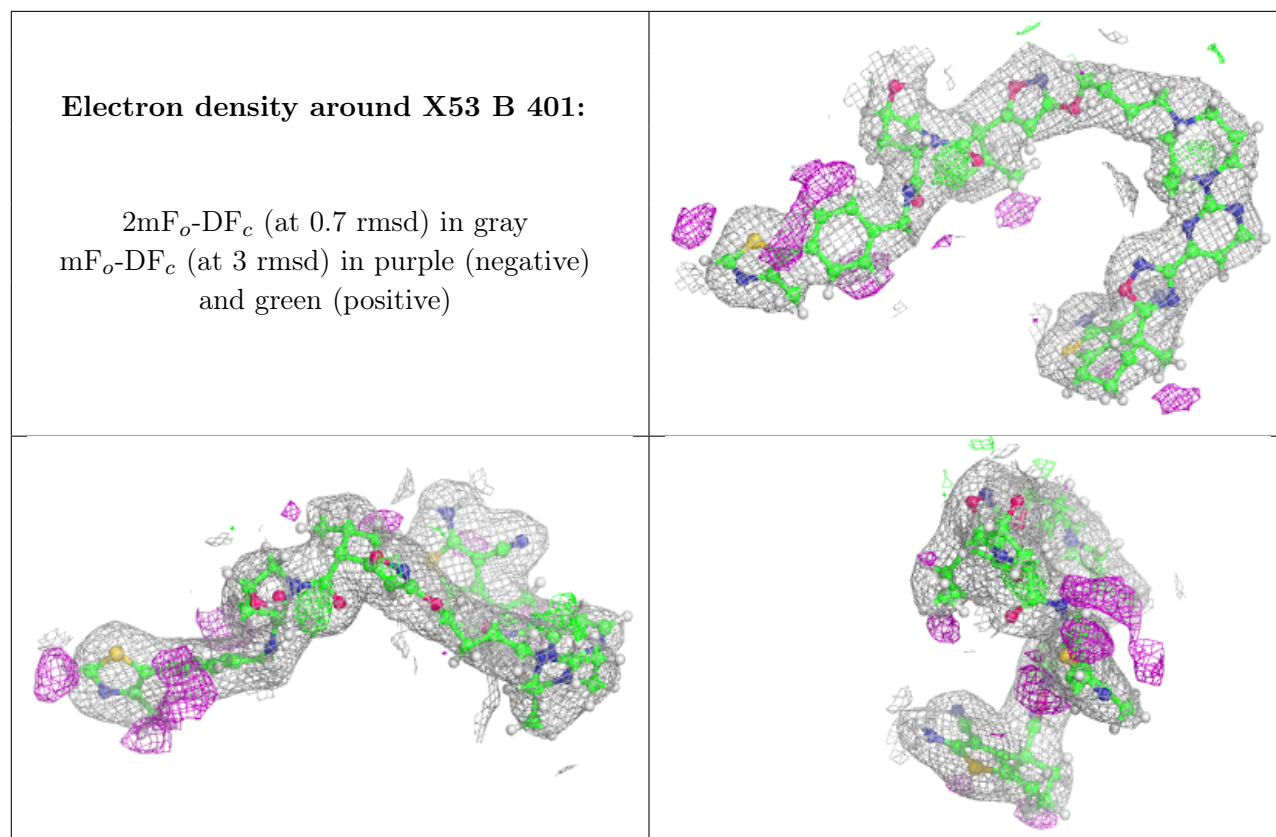
Electron density around GDP E 201:

$2mF_o$-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 A 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
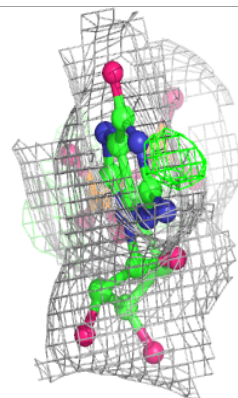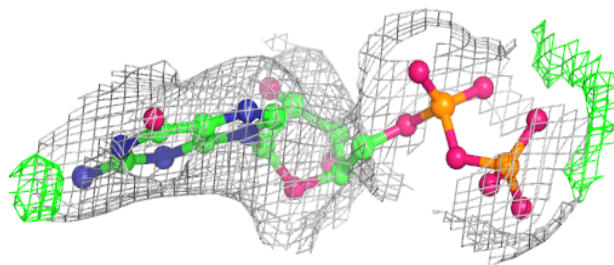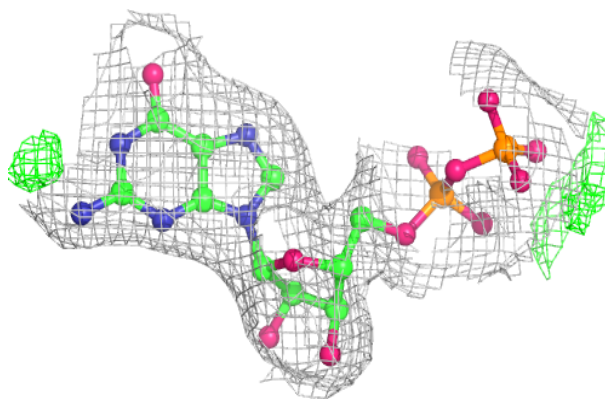
Electron density around X53 F 401:

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

Electron density around X53 B 401:

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

6.5　Other polymers ⓘ

There are no such residues in this entry.