



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 10:46 pm BST

PDB ID : 4K81
Title : Crystal structure of the Grb14 RA and PH domains in complex with GTP-loaded H-Ras
Authors : Qamra, R.; Hubbard, S.R.
Deposited on : 2013-04-17
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

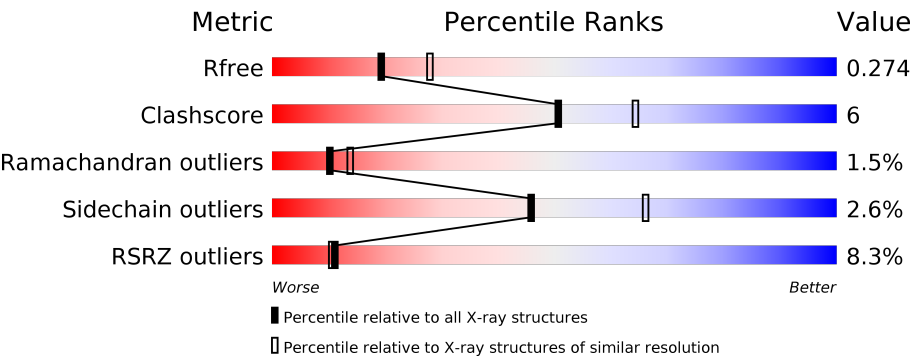
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on 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	258	<div><div>3%</div><div><div></div><div>77%</div><div>17%</div><div>• 5%</div></div></div>
1	C	258	<div><div>5%</div><div><div></div><div>76%</div><div>17%</div><div>• 5%</div></div></div>
1	E	258	<div><div>6%</div><div><div></div><div>82%</div><div>12%</div><div>• 5%</div></div></div>
1	G	258	<div><div>26%</div><div><div></div><div>76%</div><div>17%</div><div>• 5%</div></div></div>
2	B	171	<div><div>2%</div><div><div></div><div>89%</div><div>10%</div><div>•</div></div></div>
2	D	171	<div><div>%</div><div><div></div><div>89%</div><div>11%</div><div>•</div></div></div>

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Mol	Chain	Length	Quality of chain
2	F	171	<div><div></div><div>2%</div><div>81%</div><div>19%</div><div></div></div>
2	H	171	<div><div></div><div>13%</div><div>80%</div><div>20%</div><div></div></div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13867 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 Growth factor receptor-bound protein 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total 2023	C 1312	N 340	O 361	S 10	0	0	0
1	C	244	Total 2023	C 1312	N 340	O 361	S 10	0	0	0
1	E	244	Total 2023	C 1312	N 340	O 361	S 10	0	0	0
1	G	244	Total 2023	C 1312	N 340	O 361	S 10	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	99	GLY	-	EXPRESSION TAG	UNP Q14449
A	100	HIS	-	EXPRESSION TAG	UNP Q14449
A	101	MET	-	EXPRESSION TAG	UNP Q14449
A	102	ALA	-	EXPRESSION TAG	UNP Q14449
A	103	SER	-	EXPRESSION TAG	UNP Q14449
A	104	GLY	-	EXPRESSION TAG	UNP Q14449
A	105	SER	-	EXPRESSION TAG	UNP Q14449
A	272	ALA	LYS	ENGINEERED MUTATION	UNP Q14449
A	273	ALA	GLU	ENGINEERED MUTATION	UNP Q14449
C	99	GLY	-	EXPRESSION TAG	UNP Q14449
C	100	HIS	-	EXPRESSION TAG	UNP Q14449
C	101	MET	-	EXPRESSION TAG	UNP Q14449
C	102	ALA	-	EXPRESSION TAG	UNP Q14449
C	103	SER	-	EXPRESSION TAG	UNP Q14449
C	104	GLY	-	EXPRESSION TAG	UNP Q14449
C	105	SER	-	EXPRESSION TAG	UNP Q14449
C	272	ALA	LYS	ENGINEERED MUTATION	UNP Q14449
C	273	ALA	GLU	ENGINEERED MUTATION	UNP Q14449
E	99	GLY	-	EXPRESSION TAG	UNP Q14449
E	100	HIS	-	EXPRESSION TAG	UNP Q14449
E	101	MET	-	EXPRESSION TAG	UNP Q14449

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Chain	Residue	Modelled	Actual	Comment	Reference
E	102	ALA	-	EXPRESSION TAG	UNP Q14449
E	103	SER	-	EXPRESSION TAG	UNP Q14449
E	104	GLY	-	EXPRESSION TAG	UNP Q14449
E	105	SER	-	EXPRESSION TAG	UNP Q14449
E	272	ALA	LYS	ENGINEERED MUTATION	UNP Q14449
E	273	ALA	GLU	ENGINEERED MUTATION	UNP Q14449
G	99	GLY	-	EXPRESSION TAG	UNP Q14449
G	100	HIS	-	EXPRESSION TAG	UNP Q14449
G	101	MET	-	EXPRESSION TAG	UNP Q14449
G	102	ALA	-	EXPRESSION TAG	UNP Q14449
G	103	SER	-	EXPRESSION TAG	UNP Q14449
G	104	GLY	-	EXPRESSION TAG	UNP Q14449
G	105	SER	-	EXPRESSION TAG	UNP Q14449
G	272	ALA	LYS	ENGINEERED MUTATION	UNP Q14449
G	273	ALA	GLU	ENGINEERED MUTATION	UNP Q14449

- Molecule 2 is a protein called GTPase HRas.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	171	Total	C	N	O	S	0	0	0
			1352	842	233	269	8			
2	D	171	Total	C	N	O	S	0	0	0
			1352	842	233	269	8			
2	F	171	Total	C	N	O	S	0	0	0
			1352	842	233	269	8			
2	H	171	Total	C	N	O	S	0	0	0
			1352	842	233	269	8			

There are 24 discrepancies between the modelled and reference sequences:

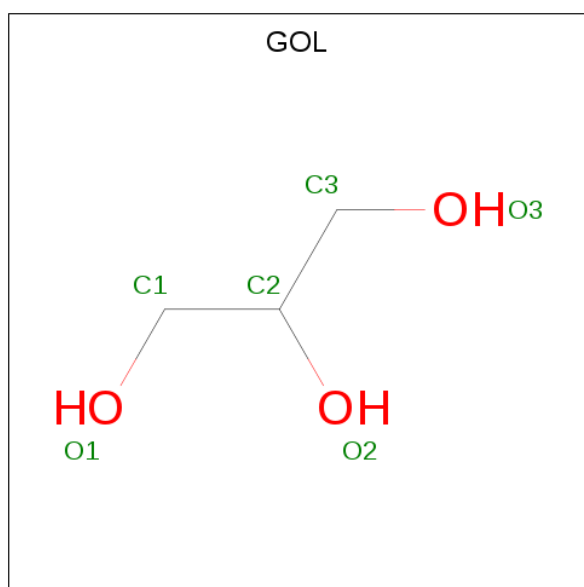
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	EXPRESSION TAG	UNP P01112
B	-3	ALA	-	EXPRESSION TAG	UNP P01112
B	-2	MET	-	EXPRESSION TAG	UNP P01112
B	-1	GLY	-	EXPRESSION TAG	UNP P01112
B	0	SER	-	EXPRESSION TAG	UNP P01112
B	12	VAL	GLY	ENGINEERED MUTATION	UNP P01112
D	-4	GLY	-	EXPRESSION TAG	UNP P01112
D	-3	ALA	-	EXPRESSION TAG	UNP P01112
D	-2	MET	-	EXPRESSION TAG	UNP P01112
D	-1	GLY	-	EXPRESSION TAG	UNP P01112
D	0	SER	-	EXPRESSION TAG	UNP P01112

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Chain	Residue	Modelled	Actual	Comment	Reference
D	12	VAL	GLY	ENGINEERED MUTATION	UNP P01112
F	-4	GLY	-	EXPRESSION TAG	UNP P01112
F	-3	ALA	-	EXPRESSION TAG	UNP P01112
F	-2	MET	-	EXPRESSION TAG	UNP P01112
F	-1	GLY	-	EXPRESSION TAG	UNP P01112
F	0	SER	-	EXPRESSION TAG	UNP P01112
F	12	VAL	GLY	ENGINEERED MUTATION	UNP P01112
H	-4	GLY	-	EXPRESSION TAG	UNP P01112
H	-3	ALA	-	EXPRESSION TAG	UNP P01112
H	-2	MET	-	EXPRESSION TAG	UNP P01112
H	-1	GLY	-	EXPRESSION TAG	UNP P01112
H	0	SER	-	EXPRESSION TAG	UNP P01112
H	12	VAL	GLY	ENGINEERED MUTATION	UNP P01112

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



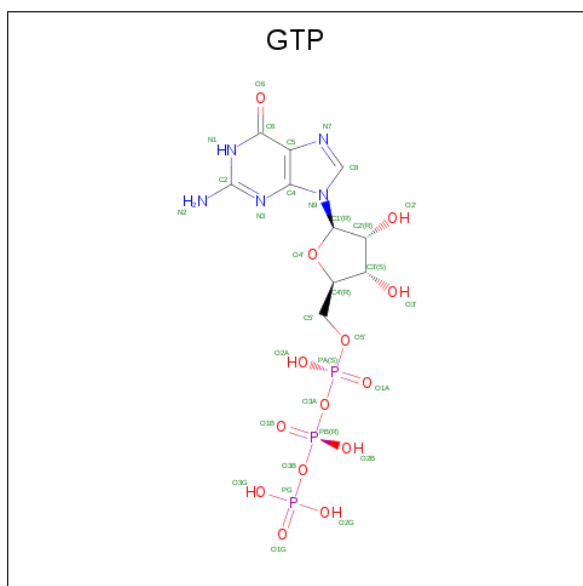
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	F	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	H	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Mg 1	0	0
5	D	1	Total 1	Mg 1	0	0
5	F	1	Total 1	Mg 1	0	0

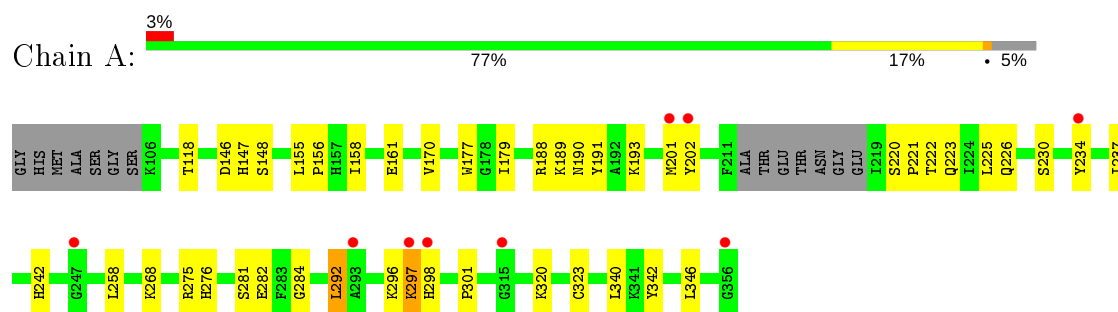
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	46	Total 46	O 46	0	0
6	B	24	Total 24	O 24	0	0
6	C	25	Total 25	O 25	0	0
6	D	21	Total 21	O 21	0	0
6	E	33	Total 33	O 33	0	0
6	F	16	Total 16	O 16	0	0
6	G	10	Total 10	O 10	0	0
6	H	6	Total 6	O 6	0	0

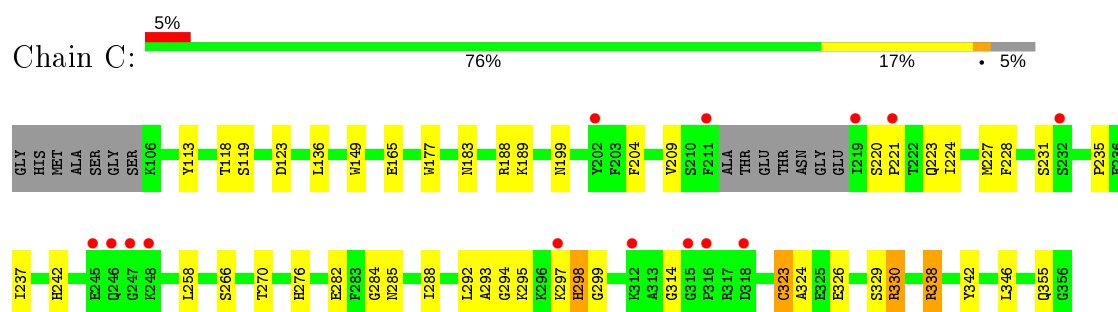
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

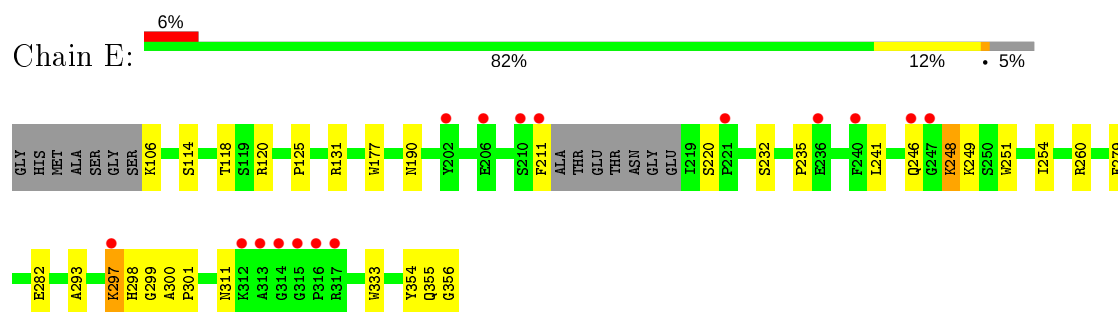
- Molecule 1: Growth factor receptor-bound protein 14



- Molecule 1: Growth factor receptor-bound protein 14

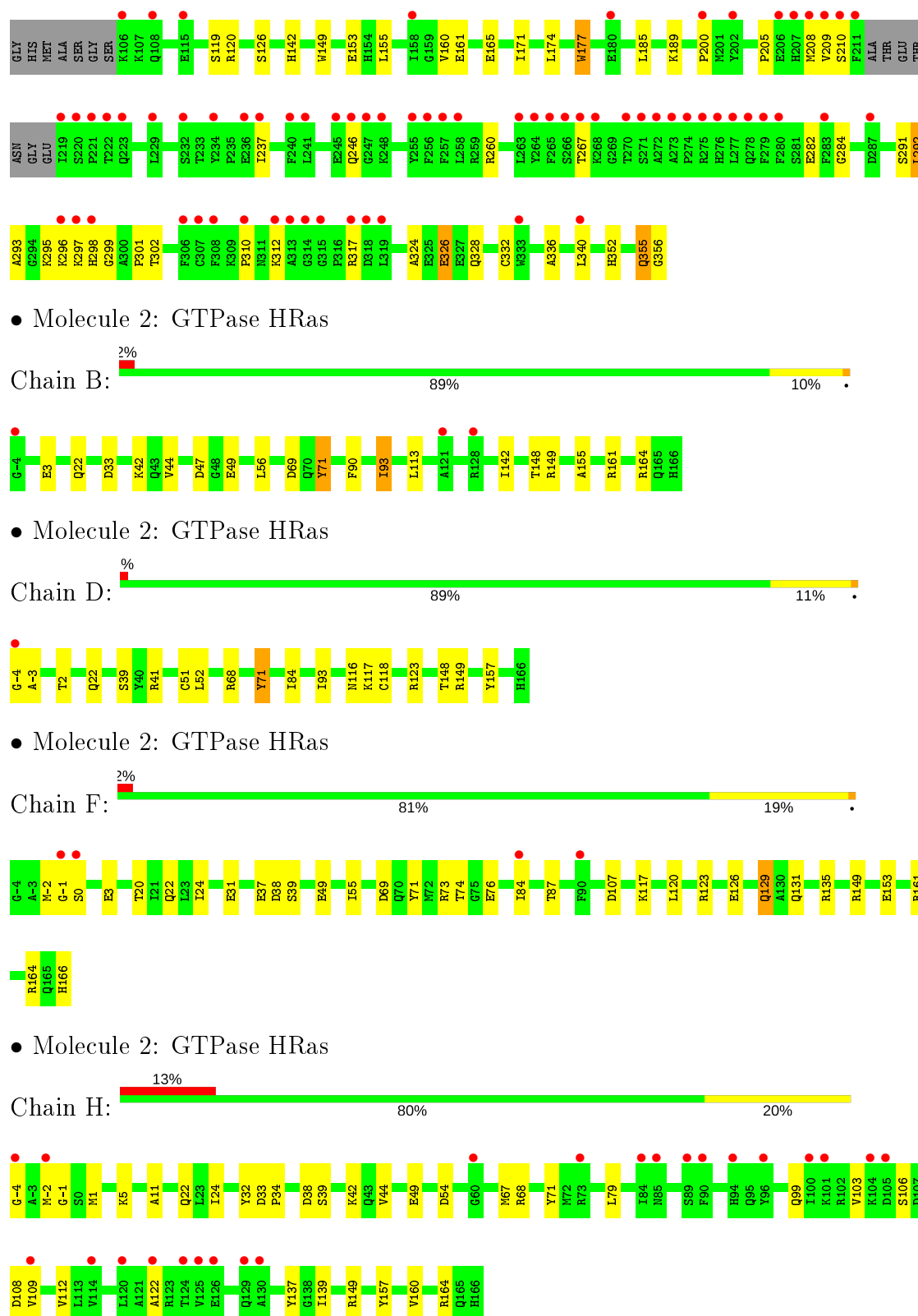


- Molecule 1: Growth factor receptor-bound protein 14



- Molecule 1: Growth factor receptor-bound protein 14





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.73Å 115.59Å 103.11Å 90.00° 96.75° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 46.81 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.40) 99.6 (46.81-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.219 , 0.277 0.217 , 0.274	Depositor DCC
R_{free} test set	3628 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	51.7	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13867	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.62	0/2083	0.68	0/2808
1	C	0.56	1/2083 (0.0%)	0.64	1/2808 (0.0%)
1	E	0.58	2/2083 (0.1%)	0.64	0/2808
1	G	0.51	1/2083 (0.0%)	0.53	0/2808
2	B	0.48	0/1371	0.63	0/1850
2	D	0.51	0/1371	0.66	0/1850
2	F	0.43	0/1371	0.59	0/1850
2	H	0.36	0/1371	0.53	0/1850
All	All	0.52	4/13816 (0.0%)	0.62	1/18632 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	177	TRP	CD2-CE2	5.25	1.47	1.41
1	G	177	TRP	CD2-CE2	5.23	1.47	1.41
1	C	149	TRP	CD2-CE2	5.22	1.47	1.41
1	E	251	TRP	CD2-CE2	5.01	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	338	ARG	NE-CZ-NH2	-5.27	117.67	120.30

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	2023	0	1974	31	0
1	C	2023	0	1974	28	0
1	E	2023	0	1974	15	0
1	G	2023	0	1974	24	0
2	B	1352	0	1326	14	0
2	D	1352	0	1326	16	0
2	F	1352	0	1325	19	0
2	H	1352	0	1326	19	0
3	A	24	0	32	4	0
3	B	6	0	8	1	0
3	C	12	0	16	0	0
3	E	12	0	16	0	0
4	B	32	0	12	0	0
4	D	32	0	12	0	0
4	F	32	0	12	1	0
4	H	32	0	12	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
6	A	46	0	0	6	0
6	B	24	0	0	2	0
6	C	25	0	0	0	0
6	D	21	0	0	0	0
6	E	33	0	0	1	0
6	F	16	0	0	2	0
6	G	10	0	0	0	0
6	H	6	0	0	1	0
All	All	13867	0	13319	154	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 6.

The worst 5 of 154 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:TYR:HB2	6:A:540:HOH:O	1.56	1.03
1:C:330:ARG:HG2	1:C:330:ARG:HH11	1.28	0.96
1:E:356:GLY:HA2	6:E:507:HOH:O	1.72	0.86
2:D:84:ILE:HD12	2:D:123:ARG:HG2	1.63	0.80
1:A:346:LEU:HG	6:A:540:HOH:O	1.82	0.78

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	240/258 (93%)	223 (93%)	15 (6%)	2 (1%)	19	29
1	C	240/258 (93%)	222 (92%)	14 (6%)	4 (2%)	9	11
1	E	240/258 (93%)	222 (92%)	13 (5%)	5 (2%)	7	8
1	G	240/258 (93%)	213 (89%)	19 (8%)	8 (3%)	4	3
2	B	169/171 (99%)	163 (96%)	6 (4%)	0	100	100
2	D	169/171 (99%)	166 (98%)	2 (1%)	1 (1%)	25	36
2	F	169/171 (99%)	161 (95%)	6 (4%)	2 (1%)	13	19
2	H	169/171 (99%)	160 (95%)	7 (4%)	2 (1%)	13	19
All	All	1636/1716 (95%)	1530 (94%)	82 (5%)	24 (2%)	10	14

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	293	ALA
1	E	248	LYS
1	C	298	HIS
2	D	-3	ALA
1	E	293	ALA

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	219/228 (96%)	215 (98%)	4 (2%)	59	76
1	C	219/228 (96%)	210 (96%)	9 (4%)	30	48
1	E	219/228 (96%)	215 (98%)	4 (2%)	59	76
1	G	219/228 (96%)	215 (98%)	4 (2%)	59	76
2	B	147/147 (100%)	144 (98%)	3 (2%)	55	74
2	D	147/147 (100%)	143 (97%)	4 (3%)	44	65
2	F	147/147 (100%)	141 (96%)	6 (4%)	30	48
2	H	147/147 (100%)	143 (97%)	4 (3%)	44	65
All	All	1464/1500 (98%)	1426 (97%)	38 (3%)	46	66

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	51	CYS
1	E	220	SER
2	H	49	GLU
2	D	93	ILE
1	E	254	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	311	ASN
1	E	345	GLN
2	F	150	GLN
1	E	246	GLN
1	G	328	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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	GTP	H	200	5	26,34,34	1.14	2 (7%)	33,54,54	1.95	8 (24%)
3	GOL	C	400	-	5,5,5	0.38	0	5,5,5	0.60	0
3	GOL	B	201	-	5,5,5	0.43	0	5,5,5	0.58	0
3	GOL	E	401	-	5,5,5	0.29	0	5,5,5	0.90	0
4	GTP	B	202	5	26,34,34	1.12	2 (7%)	33,54,54	1.82	9 (27%)
3	GOL	A	401	-	5,5,5	0.40	0	5,5,5	0.68	0
3	GOL	C	401	-	5,5,5	0.21	0	5,5,5	0.49	0
3	GOL	E	400	-	5,5,5	0.31	0	5,5,5	0.51	0
3	GOL	A	402	-	5,5,5	0.36	0	5,5,5	0.46	0
4	GTP	D	200	5	26,34,34	1.17	2 (7%)	33,54,54	1.88	8 (24%)
4	GTP	F	200	5	26,34,34	1.26	2 (7%)	33,54,54	1.99	9 (27%)
3	GOL	A	404	-	5,5,5	0.61	0	5,5,5	0.89	0
3	GOL	A	403	-	5,5,5	0.59	0	5,5,5	0.64	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
4	GTP	H	200	5	-	2/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	400	-	-	2/4/4/4	-
3	GOL	B	201	-	-	2/4/4/4	-
3	GOL	E	401	-	-	2/4/4/4	-
4	GTP	B	202	5	-	2/18/38/38	0/3/3/3
3	GOL	A	401	-	-	2/4/4/4	-
3	GOL	C	401	-	-	2/4/4/4	-
3	GOL	E	400	-	-	2/4/4/4	-
3	GOL	A	402	-	-	4/4/4/4	-
4	GTP	D	200	5	-	2/18/38/38	0/3/3/3
4	GTP	F	200	5	-	2/18/38/38	0/3/3/3
3	GOL	A	404	-	-	0/4/4/4	-
3	GOL	A	403	-	-	0/4/4/4	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	200	GTP	C6-C5	4.71	1.49	1.41
4	D	200	GTP	C6-C5	4.24	1.48	1.41
4	H	200	GTP	C6-C5	4.18	1.48	1.41
4	B	202	GTP	C6-C5	4.10	1.48	1.41
4	D	200	GTP	C5-C4	2.70	1.48	1.40

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	200	GTP	C2-N3-C4	5.11	121.20	115.36
4	F	200	GTP	C5-C6-N1	-4.77	116.91	123.43
4	D	200	GTP	C2-N3-C4	4.74	120.77	115.36
4	F	200	GTP	C2-N3-C4	4.65	120.66	115.36
4	B	202	GTP	C5-C6-N1	-4.63	117.09	123.43

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	400	GOL	C1-C2-C3-O3
3	B	201	GOL	O1-C1-C2-C3
3	A	401	GOL	C1-C2-C3-O3
3	C	401	GOL	O1-C1-C2-C3

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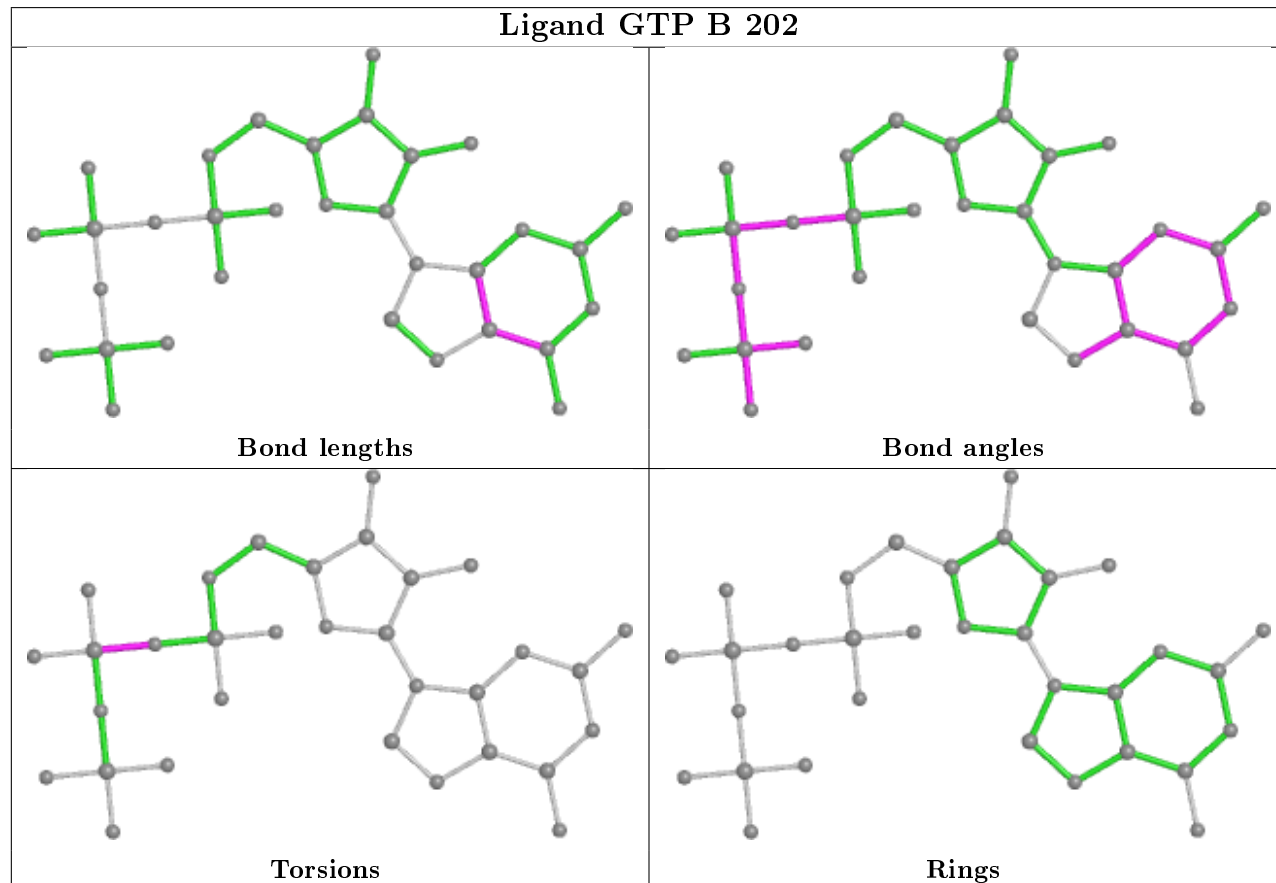
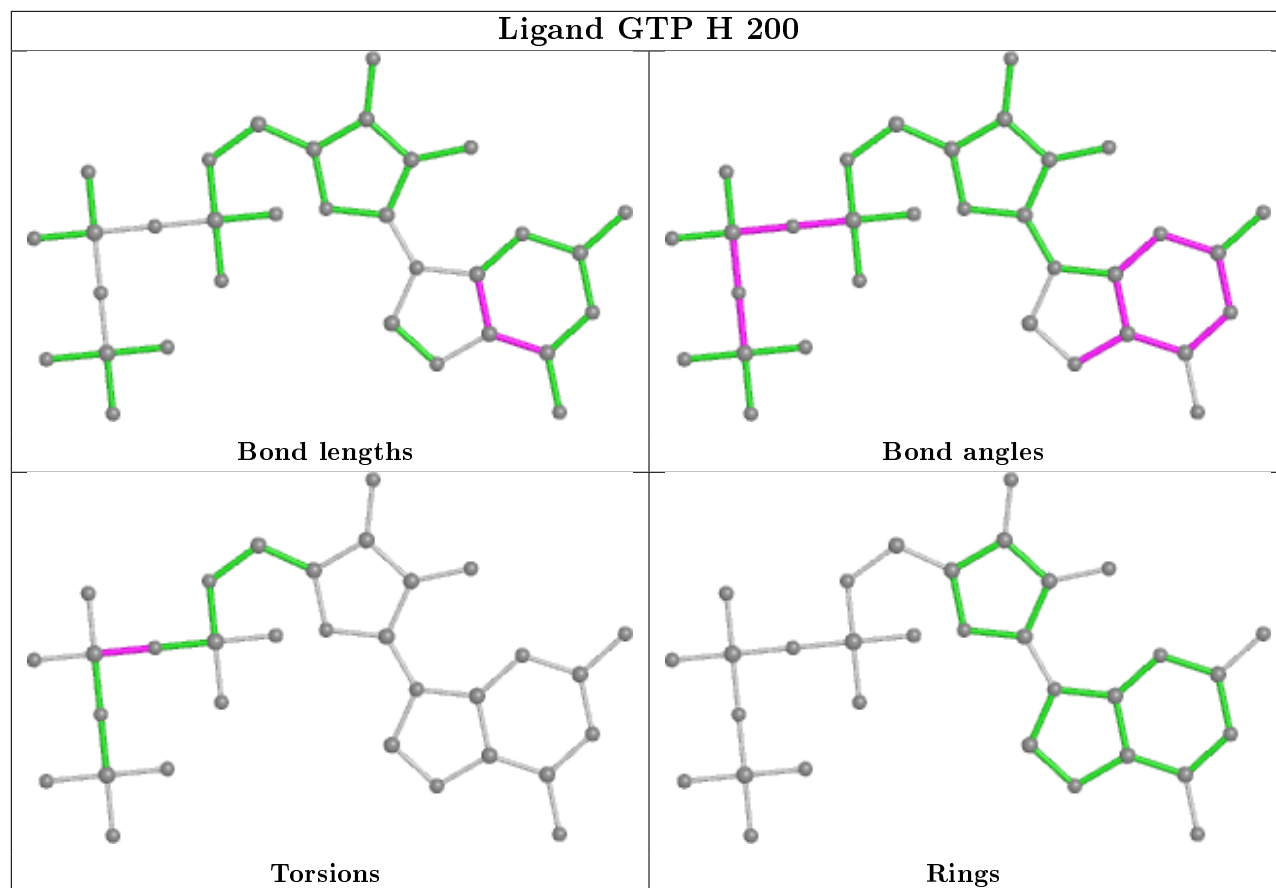
Mol	Chain	Res	Type	Atoms
3	A	402	GOL	O1-C1-C2-C3

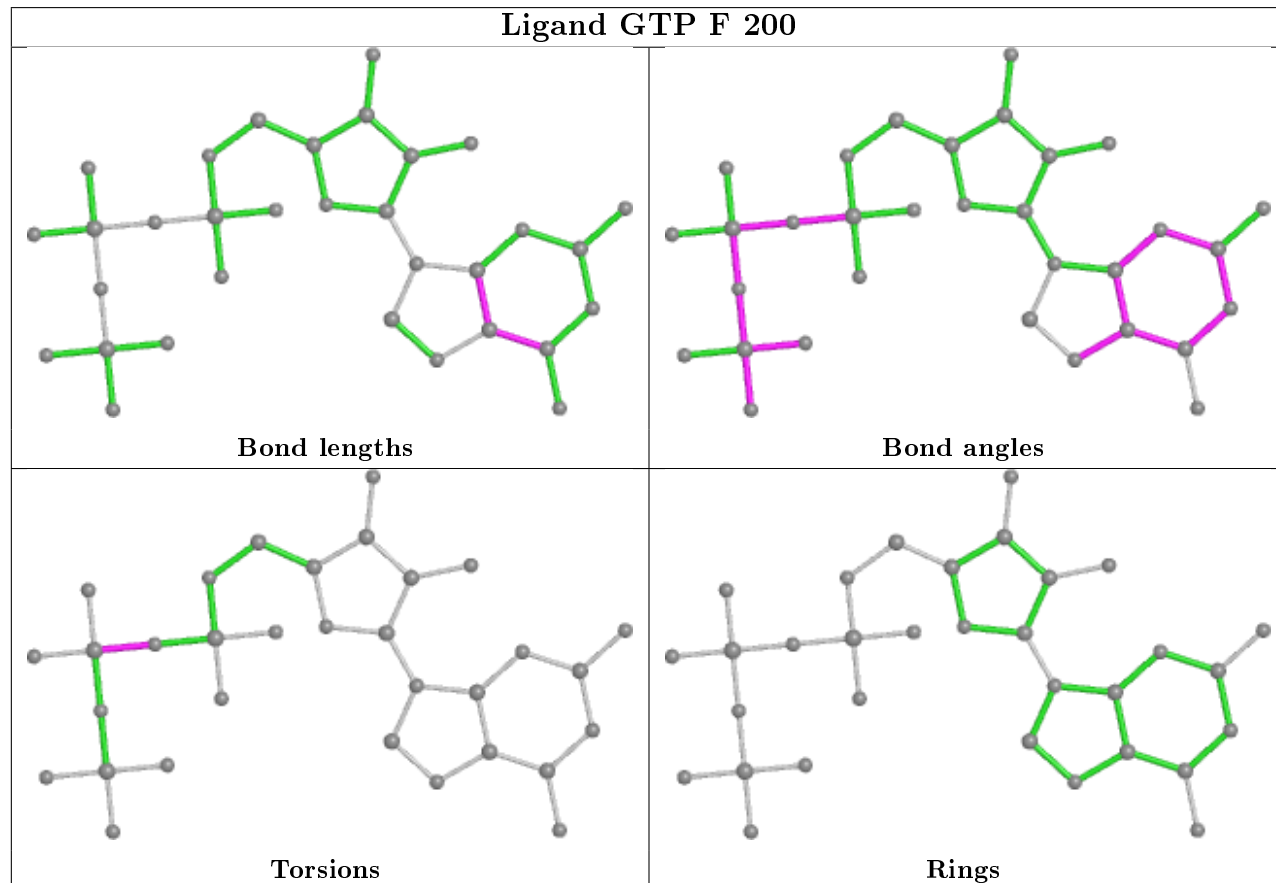
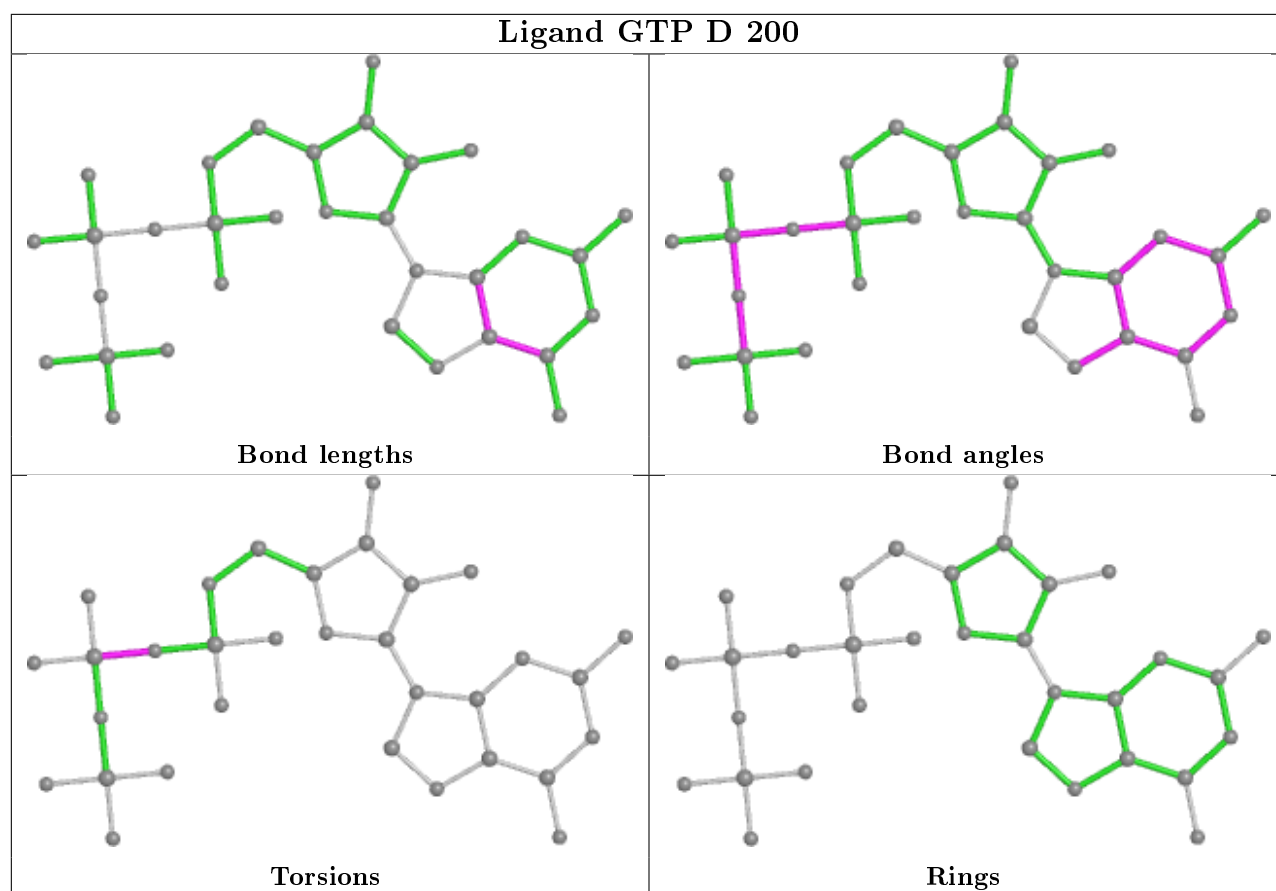
There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	201	GOL	1	0
3	A	401	GOL	2	0
3	A	402	GOL	1	0
4	F	200	GTP	1	0
3	A	404	GOL	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	244/258 (94%)	0.19	9 (3%) 41 41	26, 46, 87, 107	0
1	C	244/258 (94%)	0.33	14 (5%) 23 22	34, 57, 111, 127	0
1	E	244/258 (94%)	0.37	16 (6%) 18 17	29, 55, 95, 136	0
1	G	244/258 (94%)	1.45	68 (27%) 0 0	43, 93, 159, 187	0
2	B	171/171 (100%)	0.12	3 (1%) 68 66	29, 52, 85, 112	0
2	D	171/171 (100%)	0.02	1 (0%) 89 88	29, 47, 73, 103	0
2	F	171/171 (100%)	0.30	4 (2%) 60 58	38, 63, 95, 121	0
2	H	171/171 (100%)	1.06	23 (13%) 3 2	47, 90, 156, 196	0
All	All	1660/1716 (96%)	0.50	138 (8%) 11 10	26, 60, 129, 196	0

The worst 5 of 138 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	257	PHE	9.2
1	G	271	SER	8.5
1	G	297	LYS	8.2
1	G	246	GLN	7.0
1	G	265	PHE	6.9

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 carbohydrates in this entry.

6.4 Ligands ⓘ

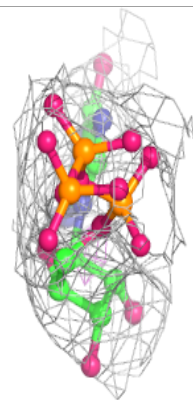
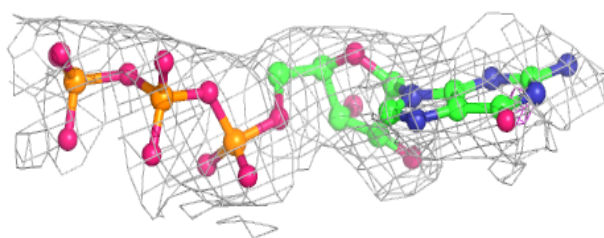
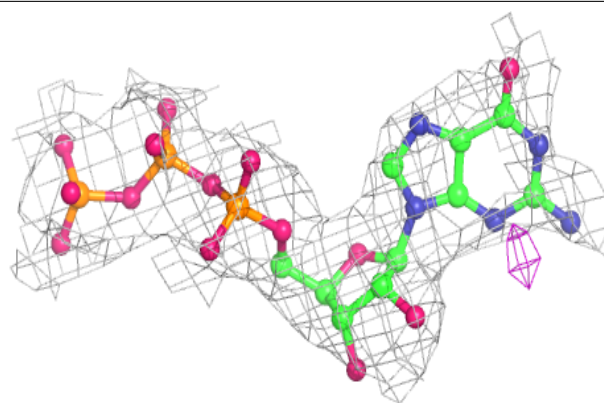
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	C	400	6/6	0.75	0.38	65,67,68,70	0
3	GOL	A	403	6/6	0.78	0.34	49,51,55,56	0
3	GOL	A	404	6/6	0.84	0.15	44,50,54,55	0
5	MG	H	201	1/1	0.84	0.21	63,63,63,63	0
3	GOL	E	401	6/6	0.87	0.20	41,43,44,45	0
5	MG	D	201	1/1	0.90	0.18	45,45,45,45	0
3	GOL	B	201	6/6	0.91	0.19	46,54,55,61	0
3	GOL	C	401	6/6	0.91	0.18	40,43,44,44	0
3	GOL	A	402	6/6	0.92	0.18	32,34,34,37	0
3	GOL	A	401	6/6	0.93	0.25	46,47,48,51	0
4	GTP	H	200	32/32	0.94	0.18	69,80,91,93	0
3	GOL	E	400	6/6	0.95	0.15	41,43,44,47	0
4	GTP	B	202	32/32	0.97	0.15	34,41,52,53	0
5	MG	B	203	1/1	0.97	0.16	40,40,40,40	0
4	GTP	F	200	32/32	0.97	0.15	39,56,66,66	0
5	MG	F	201	1/1	0.97	0.22	54,54,54,54	0
4	GTP	D	200	32/32	0.98	0.13	38,46,50,51	0

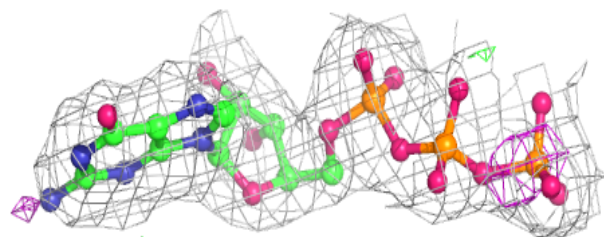
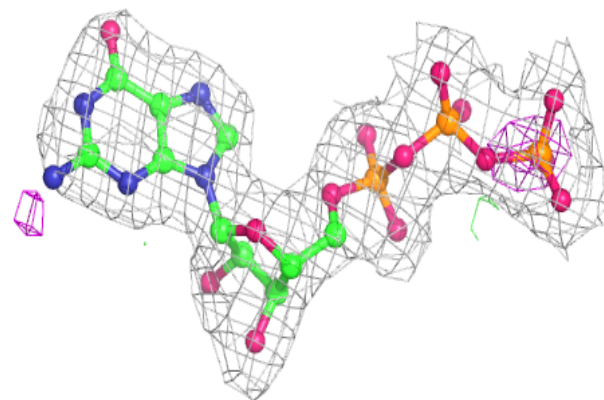
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GTP H 200:

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

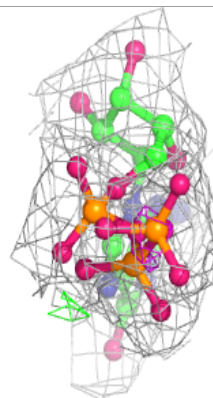
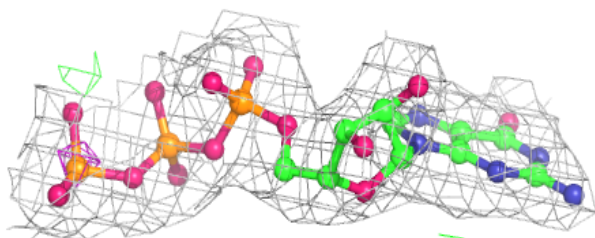
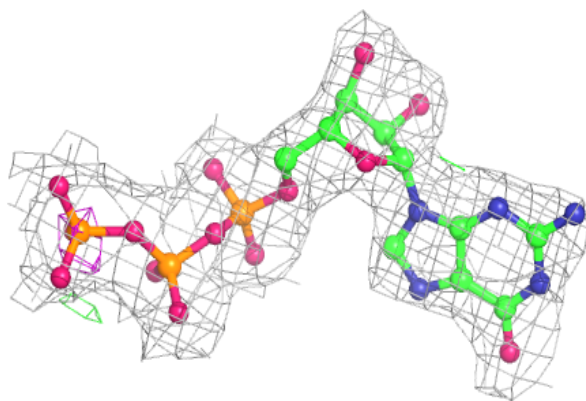
**Electron density around GTP B 202:**

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

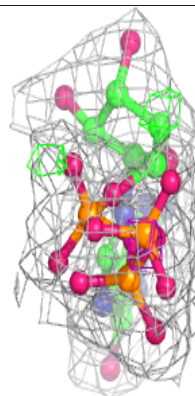
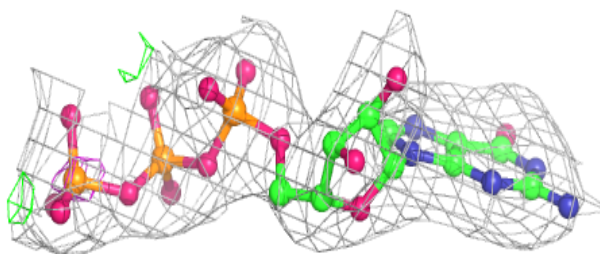
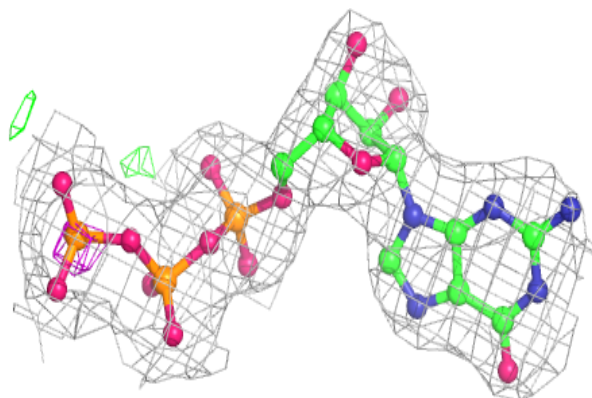


Electron density around GTP F 200:

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

**Electron density around GTP D 200:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.