wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 14, 2024 – 12:25 pm GMT

PDB ID	:	6TUL
Title	:	Structure of the arginase-2-inhibitory human antigen-binding fragment Fab C0021177
Authors	:	Burschowsky, D.; Addyman, A.; Fiedler, S.; Groves, M.; Haynes, S.; Seewooruthun, C.; Carr, M.
Deposited on	:	2020-01-07
Resolution	:	2.25 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 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:

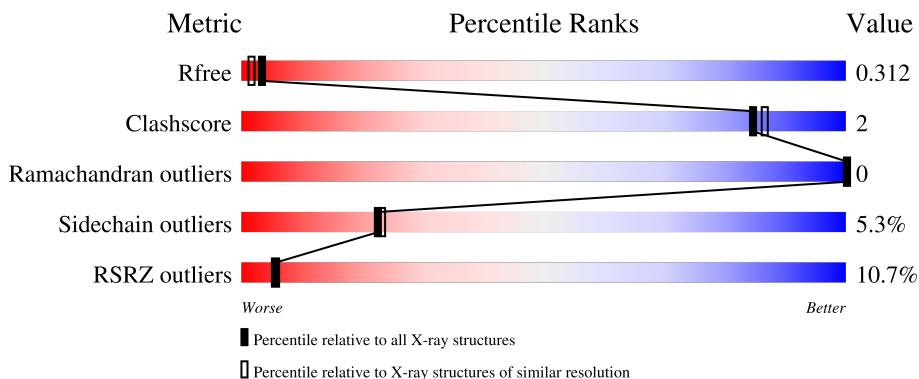|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.25 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		0.312
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		5.3%
RSRZ outliers		10.7%

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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	HHH	233	16% / 84% / 9% · 6%
2	LLL	220	4% / 88% / 8% ·

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 6578 atoms, of which 3249 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 Fab C0021177 heavy chain (IgG1).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	HHH	219	Total	C	H	N	O	S	86	0	0
			3257	1031	1625	281	314	6			

- Molecule 2 is a protein called Fab C0021177 light chain (IgG1).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	LLL	212	Total	C	H	N	O	S	101	0	0
			3095	984	1526	256	325	4			

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).
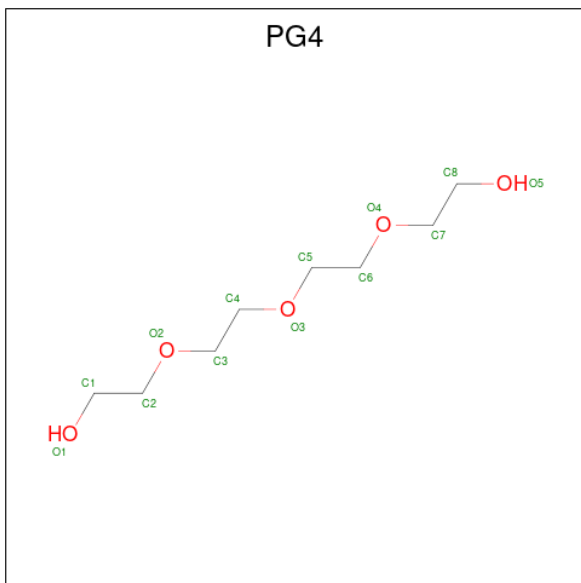
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	HHH	1	Total	C	H	O	1	0
			31	8	18	5		
3	LLL	1	Total	C	H	O	1	0
			31	8	18	5		

- Molecule 4 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).
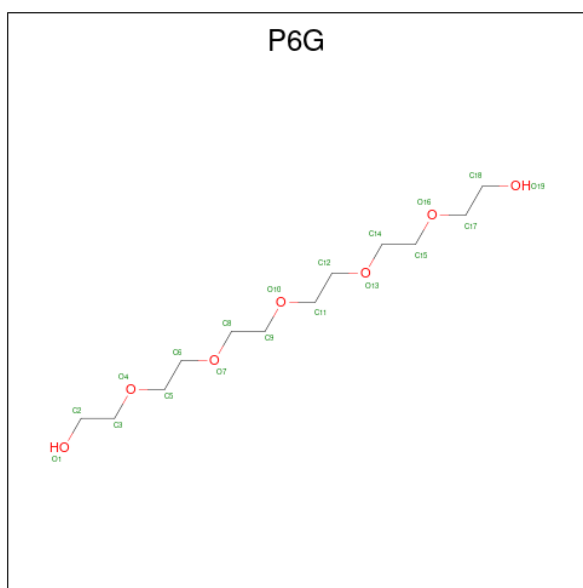
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	HHH	1	Total 45	C 12	H 26	O 7	1	0

- Molecule 5 is D-MALATE (three-letter code: MLT) (formula: $C_4H_6O_5$).
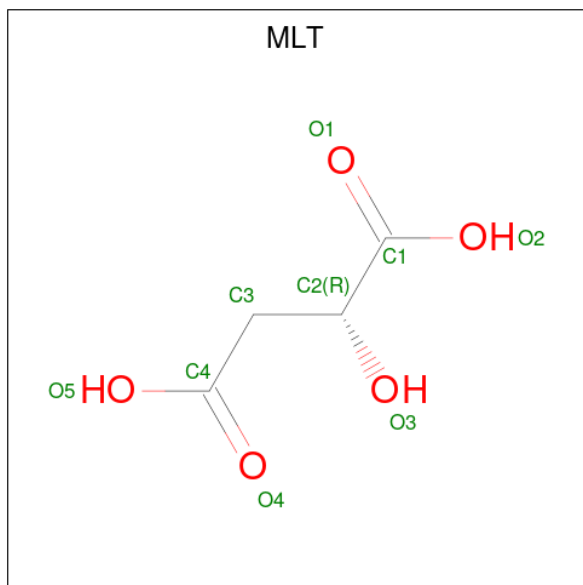
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	HHH	1	Total 13	C 4	H 4	O 5	1	0
5	HHH	1	Total 13	C 4	H 4	O 5	1	0

• Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).

PGE

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	LLL	1	Total 24	C 6	H 14	O 4	1	0
6	LLL	1	Total 24	C 6	H 14	O 4	1	0

• Molecule 7 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	HHH	15	Total 15	O 15	0	0
7	LLL	30	Total 30	O 30	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: Fab C0021177 heavy chain (IgG1)
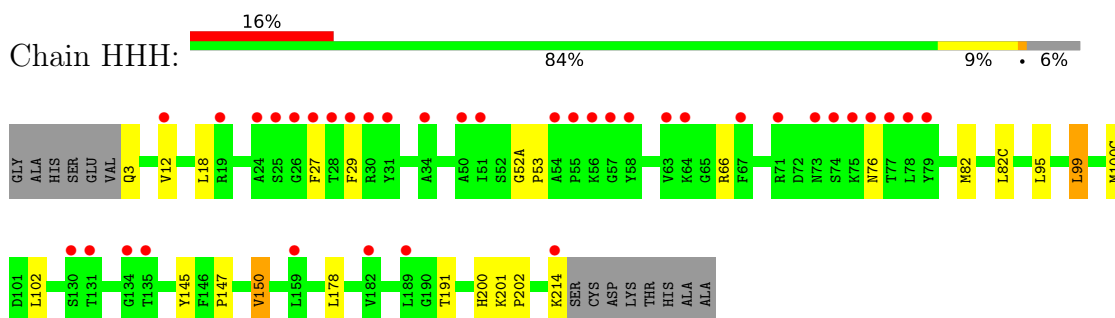
• Molecule 2: Fab C0021177 light chain (IgG1)
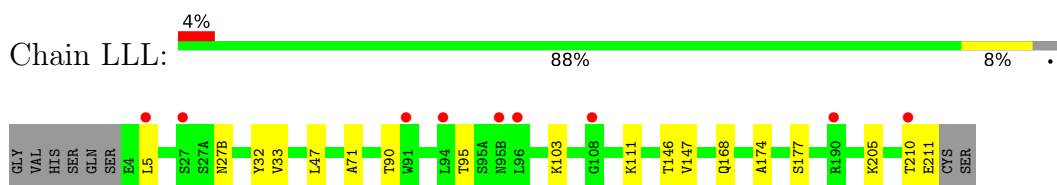
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	53.54Å 69.24Å 106.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.51 – 2.25 47.83 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.51-2.25) 100.0 (47.83-2.25)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.248 , 0.318 0.250 , 0.312	Depositor DCC
R_{free} test set	994 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	53.5	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 45.4	EDS
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6578	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 5.77% 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: PG4, PGE, MLT, P6G

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	HHH	0.66	0/1670	0.75	0/2273
2	LLL	0.66	0/1607	0.72	0/2199
All	All	0.66	0/3277	0.74	0/4472

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	HHH	1632	1625	1622	9	0
2	LLL	1569	1526	1522	7	0
3	HHH	13	18	18	0	0
3	LLL	13	18	18	0	0
4	HHH	19	26	26	0	0
5	HHH	18	8	8	0	0
6	LLL	20	28	28	0	0
7	HHH	15	0	0	0	0
7	LLL	30	0	0	0	0
All	All	3329	3249	3242	15	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 2.

The worst 5 of 15 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:HHH:178:LEU:C	1:HHH:178:LEU:HD12	2.22	0.60
2:LLL:5:LEU:HD11	2:LLL:90:THR:HG22	1.90	0.53
1:HHH:147:PRO:O	1:HHH:200:HIS:HE1	1.92	0.52
1:HHH:12:VAL:HG11	1:HHH:82(C):LEU:HD13	1.97	0.46
2:LLL:168:GLN:HE21	2:LLL:174:ALA:HB2	1.80	0.46

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	HHH	217/233 (93%)	202 (93%)	15 (7%)	0	100	100
2	LLL	210/220 (96%)	203 (97%)	7 (3%)	0	100	100
All	All	427/453 (94%)	405 (95%)	22 (5%)	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	HHH	179/189 (95%)	166 (93%)	13 (7%)	14	12
2	LLL	177/184 (96%)	171 (97%)	6 (3%)	37	45
All	All	356/373 (95%)	337 (95%)	19 (5%)	22	23

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	LLL	95	THR
2	LLL	146	THR
2	LLL	205	LYS
2	LLL	111	LYS
1	HHH	100(C)	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|>2$	Counts	RMSZ	#$\|Z\|>2$
6	PGE	LLL	302	-	9,9,9	0.18	0	8,8,8	0.10	0
6	PGE	LLL	301	-	9,9,9	0.19	0	8,8,8	0.10	0
4	P6G	HHH	302	-	18,18,18	0.50	0	17,17,17	0.22	0
3	PG4	LLL	303	-	12,12,12	0.16	0	11,11,11	0.10	0
5	MLT	HHH	303	-	8,8,8	1.10	0	10,10,10	1.20	1 (10%)
3	PG4	HHH	301	-	12,12,12	0.18	0	11,11,11	0.09	0
5	MLT	HHH	304	-	8,8,8	1.01	0	10,10,10	1.08	1 (10%)

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	PGE	LLL	302	-	-	4/7/7/7	-
6	PGE	LLL	301	-	-	4/7/7/7	-
4	P6G	HHH	302	-	-	6/16/16/16	-
3	PG4	LLL	303	-	-	1/10/10/10	-
5	MLT	HHH	303	-	-	5/8/8/8	-
3	PG4	HHH	301	-	-	4/10/10/10	-
5	MLT	HHH	304	-	-	6/8/8/8	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	HHH	303	MLT	O1-C1-C2	-2.29	118.07	122.54
5	HHH	304	MLT	O2-C1-C2	2.24	117.64	112.72

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	LLL	301	PGE	O2-C3-C4-O3
3	HHH	301	PG4	O3-C5-C6-O4
4	HHH	302	P6G	O4-C5-C6-O7
4	HHH	302	P6G	O13-C14-C15-O16
3	HHH	301	PG4	O4-C7-C8-O5

There are no ring outliers.

No monomer is involved in short contacts.

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 P6G HHH 302	
Bond lengths	Bond angles
Torsions	Rings
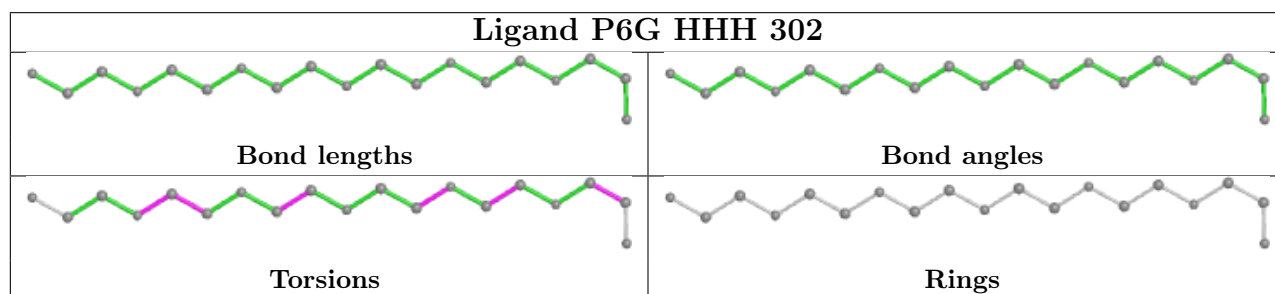
5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	HHH	219/233 (93%)	1.10	37 (16%)	1	1	45, 68, 110, 118	0
2	LLL	212/220 (96%)	0.57	9 (4%)	36	38	46, 61, 82, 103	0
All	All	431/453 (95%)	0.84	46 (10%)	6	5	45, 64, 101, 118	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	LLL	27	SER	6.9
1	HHH	31	TYR	6.3
1	HHH	29	PHE	5.6
1	HHH	28	THR	5.4
1	HHH	134	GLY	5.1

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

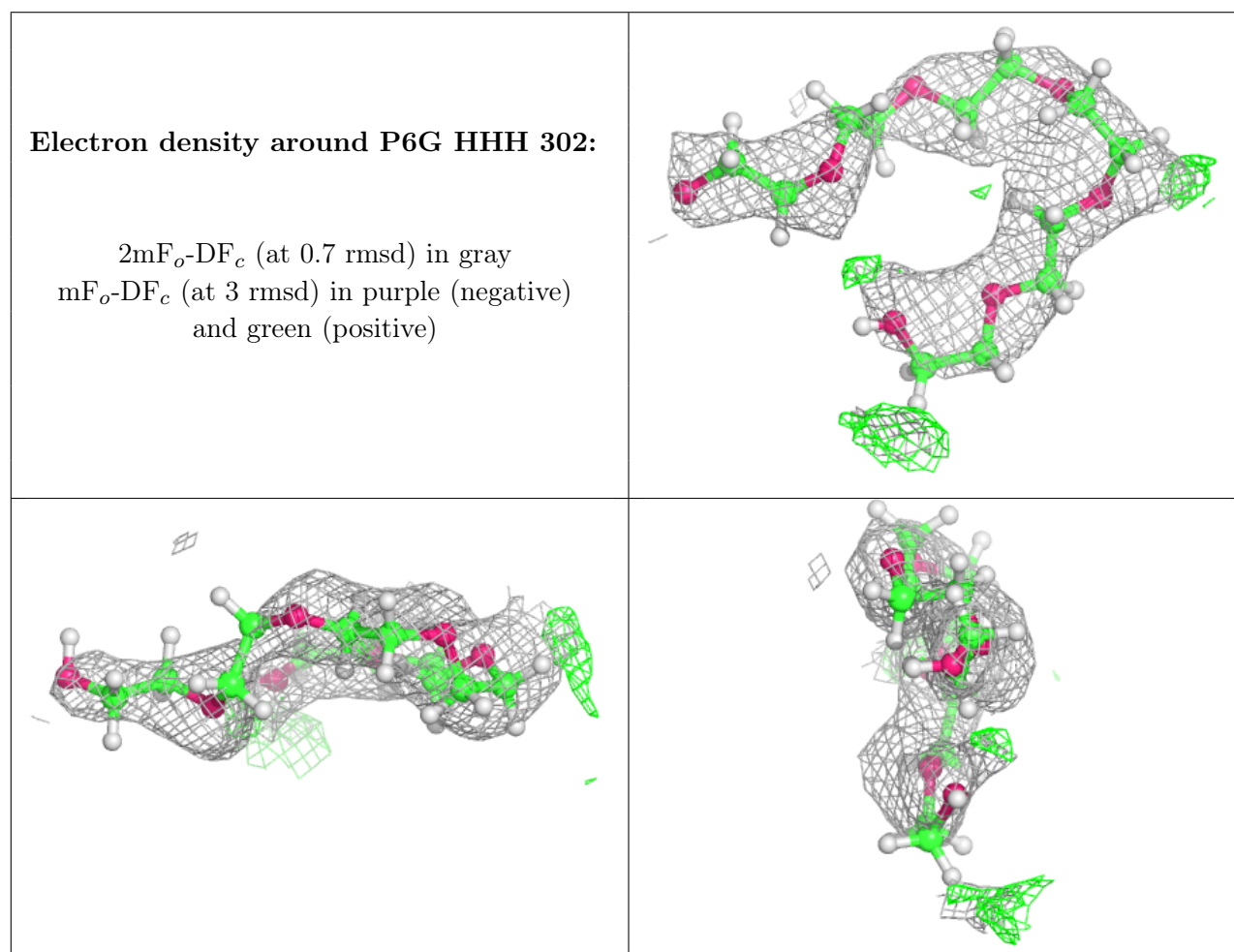There are no non-standard protein/DNA/RNA residues in this entry.

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	PGE	LLL	302	10/10	0.69	0.22	50,87,88,88	1
6	PGE	LLL	301	10/10	0.70	0.21	50,83,84,84	1
3	PG4	HHH	301	13/13	0.75	0.17	50,82,85,85	1
5	MLT	HHH	303	9/9	0.76	0.25	50,100,102,102	1
4	P6G	HHH	302	19/19	0.78	0.19	50,78,82,83	1
3	PG4	LLL	303	13/13	0.81	0.14	50,73,76,76	1
5	MLT	HHH	304	9/9	0.82	0.28	50,102,104,104	1

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 P6G HHH 302:

$2mF_o\text{-}DF_c$ (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.