



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2021 – 01:57 PM EDT

PDB ID : 3FYG  
Title : CRYSTAL STRUCTURE OF TETRADECA-(3-FLUOROTYROSYL)-GLUTATHIONE S-TRANSFERASE  
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Deposited on : 1997-08-07  
Resolution : 2.20 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](mailto: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.

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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 : 2.23.2  
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) : 2.23.2

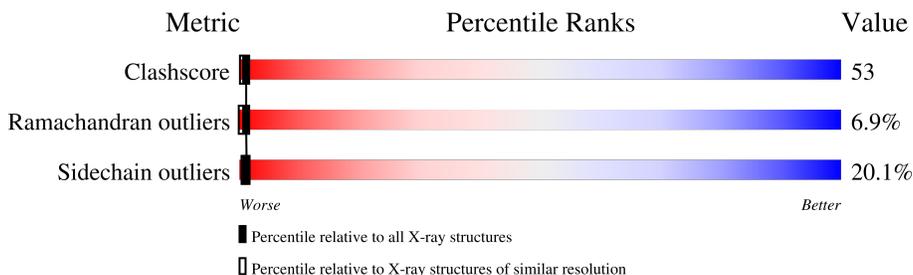
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	217	
1	B	217	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	YOF	A	6	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4173 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 MU CLASS TETRADECA-(3-FLUOROTYROSYL)-GLUTATHIONE S-TRANSFERASE OF ISOENZYME.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	F	N	O	S			
1	A	217	1836	1181	14	303	327	11	0	1	0
1	B	217	1836	1181	14	303	327	11	0	1	0

There are 26 discrepancies between the modelled and reference sequences:

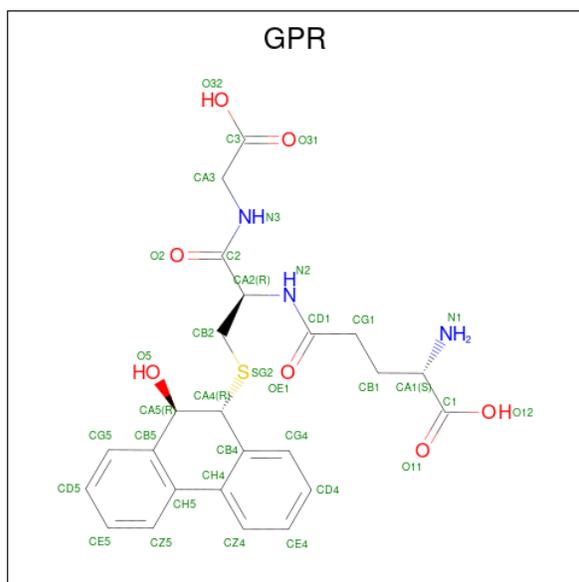
Chain	Residue	Modelled	Actual	Comment	Reference
A	6	YOF	TYR	engineered mutation	UNP P04905
A	22	YOF	TYR	engineered mutation	UNP P04905
A	27	YOF	TYR	engineered mutation	UNP P04905
A	32	YOF	TYR	engineered mutation	UNP P04905
A	40	YOF	TYR	engineered mutation	UNP P04905
A	61	YOF	TYR	engineered mutation	UNP P04905
A	78	YOF	TYR	engineered mutation	UNP P04905
A	137	YOF	TYR	engineered mutation	UNP P04905
A	154	YOF	TYR	engineered mutation	UNP P04905
A	160	YOF	TYR	engineered mutation	UNP P04905
A	166	YOF	TYR	engineered mutation	UNP P04905
A	196	YOF	TYR	engineered mutation	UNP P04905
A	202	YOF	TYR	engineered mutation	UNP P04905
B	6	YOF	TYR	engineered mutation	UNP P04905
B	22	YOF	TYR	engineered mutation	UNP P04905
B	27	YOF	TYR	engineered mutation	UNP P04905
B	32	YOF	TYR	engineered mutation	UNP P04905
B	40	YOF	TYR	engineered mutation	UNP P04905
B	61	YOF	TYR	engineered mutation	UNP P04905
B	78	YOF	TYR	engineered mutation	UNP P04905
B	137	YOF	TYR	engineered mutation	UNP P04905
B	154	YOF	TYR	engineered mutation	UNP P04905
B	160	YOF	TYR	engineered mutation	UNP P04905
B	166	YOF	TYR	engineered mutation	UNP P04905

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Chain	Residue	Modelled	Actual	Comment	Reference
B	196	YOF	TYR	engineered mutation	UNP P04905
B	202	YOF	TYR	engineered mutation	UNP P04905

- Molecule 2 is (9R,10R)-9-(S-GLUTATHIONYL)-10-HYDROXY-9,10-DIHYDROPHENANTHRENE (three-letter code: GPR) (formula: C<sub>24</sub>H<sub>27</sub>N<sub>3</sub>O<sub>7</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	Total	C	N	O	S	0	0
			35	24	3	7	1		
2	B	1	Total	C	N	O	S	0	0
			35	24	3	7	1		

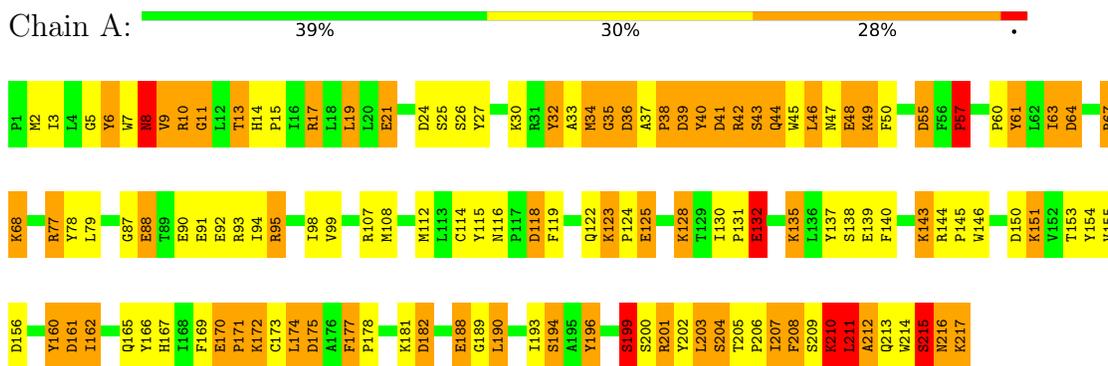
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	210	Total	O	0	0
			210	210		
3	B	221	Total	O	0	0
			221	221		

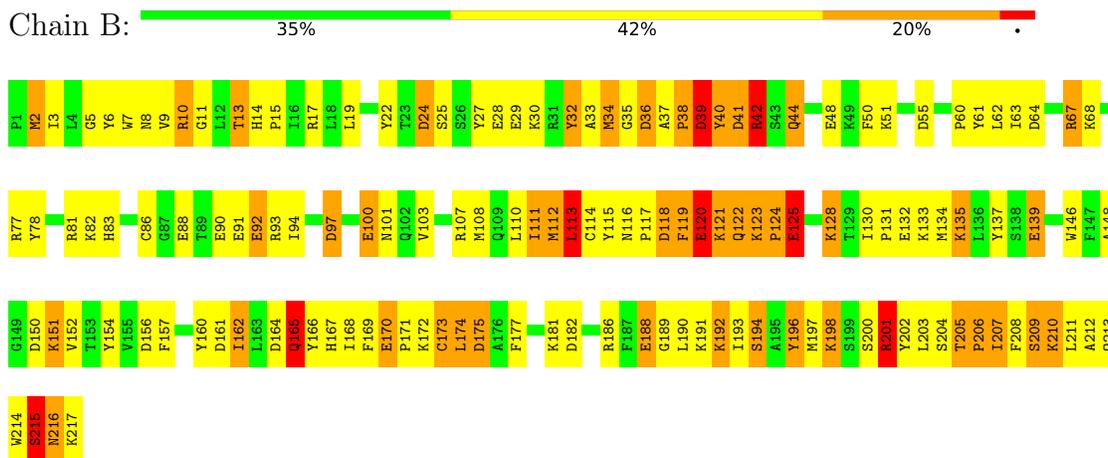
### 3 Residue-property plots

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. 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. 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: MU CLASS TETRADECA-(3-FLUOROTYROSYL)-GLUTATHIONE S-TRANSFERASE OF ISOENZYME



- Molecule 1: MU CLASS TETRADECA-(3-FLUOROTYROSYL)-GLUTATHIONE S-TRANSFERASE OF ISOENZYME



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.43Å 88.42Å 57.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 39.26 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.20) 96.9 (39.26-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.33 (at 2.20Å)	Xtrriage
Refinement program	TNT 5E	Depositor
R, $R_{free}$	0.170 , (Not available) 0.270 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.8	Xtrriage
Anisotropy	0.281	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 225.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.011 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	4173	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: YOF, GPR

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	1.09	10/1685 (0.6%)	1.47	25/2242 (1.1%)
1	B	1.11	17/1685 (1.0%)	1.50	30/2242 (1.3%)
All	All	1.10	27/3370 (0.8%)	1.48	55/4484 (1.2%)

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	GLU	CD-OE2	9.44	1.36	1.25
1	B	198	LYS	CD-CE	9.41	1.74	1.51
1	B	132	GLU	CD-OE2	8.13	1.34	1.25
1	B	120	GLU	CD-OE2	8.05	1.34	1.25
1	B	91	GLU	CD-OE2	6.90	1.33	1.25

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	77	ARG	NE-CZ-NH1	10.14	125.37	120.30
1	B	64	ASP	CB-CG-OD1	9.60	126.94	118.30
1	B	150	ASP	CB-CG-OD2	-9.08	110.13	118.30
1	A	77	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	B	93	ARG	NE-CZ-NH1	8.35	124.47	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	1836	0	1775	213	0
1	B	1836	0	1777	173	0
2	A	35	0	25	2	0
2	B	35	0	25	6	0
3	A	210	0	0	11	1
3	B	221	0	0	21	0
All	All	4173	0	3602	389	1

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 53.

The worst 5 of 389 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:B:198:LYS:CE	1:B:198:LYS:CD	1.74	1.57
1:B:10:ARG:HD3	1:B:207:ILE:HG13	1.34	1.06
1:A:143:LYS:H	1:A:143:LYS:HD2	1.22	1.03
1:B:11:GLY:H	1:B:207:ILE:HA	1.20	1.03
1:B:33:ALA:H	1:B:44:GLN:NE2	1.56	1.02

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:649:HOH:O	3:A:649:HOH:O 2_655	1.90	0.30

## 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	202/217 (93%)	176 (87%)	9 (4%)	17 (8%)	1	0
1	B	202/217 (93%)	173 (86%)	18 (9%)	11 (5%)	2	0
All	All	404/434 (93%)	349 (86%)	27 (7%)	28 (7%)	1	0

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	38	PRO
1	A	39	ASP
1	A	210	LYS
1	A	211	LEU

### 5.3.2 Protein sidechains [i](#)

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	184/184 (100%)	148 (80%)	36 (20%)	1	1
1	B	184/184 (100%)	146 (79%)	38 (21%)	1	1
All	All	368/368 (100%)	294 (80%)	74 (20%)	1	1

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	151	LYS
1	B	210	LYS
1	B	165	GLN
1	B	200	SER
1	A	194	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	8	ASN

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Mol	Chain	Res	Type
1	B	44	GLN
1	B	216	ASN
1	A	14	HIS
1	A	8	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

28 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$
1	YOF	A	6	1	12,13,14	1.19	1 (8%)	12,17,19	1.97	2 (16%)
1	YOF	B	40	1	12,13,14	1.09	1 (8%)	12,17,19	1.19	1 (8%)
1	YOF	A	137	1	12,13,14	0.77	0	12,17,19	1.46	2 (16%)
1	YOF	B	22	1	12,13,14	0.90	0	12,17,19	1.00	0
1	YOF	B	202	1	12,13,14	0.82	0	12,17,19	0.91	0
1	YOF	B	78	1	12,13,14	0.83	0	12,17,19	1.58	4 (33%)
1	YOF	B	27	1	12,13,14	0.95	1 (8%)	12,17,19	0.99	1 (8%)
1	YOF	A	196	1	12,13,14	1.15	1 (8%)	12,17,19	0.82	0
1	YOF	B	196	1	12,13,14	0.91	0	12,17,19	2.51	4 (33%)
1	YOF	A	32	1	12,13,14	0.76	0	12,17,19	1.20	2 (16%)
1	YOF	A	166	1	12,13,14	1.05	1 (8%)	12,17,19	1.21	0
1	YOF	A	160	1	12,13,14	0.72	0	12,17,19	1.25	1 (8%)
1	YOF	A	27	1	12,13,14	1.14	0	12,17,19	1.51	3 (25%)
1	YOF	A	22	1	12,13,14	0.69	0	12,17,19	1.11	0
1	YOF	A	40	1	12,13,14	1.26	1 (8%)	12,17,19	1.26	1 (8%)
1	YOF	A	61	1	12,13,14	1.42	2 (16%)	12,17,19	1.45	1 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	YOF	B	154[B]	-	12,13,14	0.86	0	12,17,19	1.17	1 (8%)
1	YOF	A	154[B]	-	12,13,14	0.93	0	12,17,19	0.93	1 (8%)
1	YOF	B	137	1	12,13,14	0.84	0	12,17,19	1.19	1 (8%)
1	YOF	B	6	1	12,13,14	0.99	0	12,17,19	1.47	2 (16%)
1	YOF	A	78	1	12,13,14	0.97	0	12,17,19	1.42	2 (16%)
1	YOF	B	61	1	12,13,14	0.67	0	12,17,19	1.41	1 (8%)
1	YOF	A	202	1	12,13,14	0.85	0	12,17,19	1.29	1 (8%)
1	YOF	B	154[A]	-	12,13,14	0.74	0	12,17,19	1.09	1 (8%)
1	YOF	A	154[A]	-	12,13,14	0.95	0	12,17,19	1.12	1 (8%)
1	YOF	B	32	1	12,13,14	0.84	0	12,17,19	1.15	2 (16%)
1	YOF	B	166	1	12,13,14	1.05	0	12,17,19	1.10	1 (8%)
1	YOF	B	160	1	12,13,14	0.90	0	12,17,19	1.36	1 (8%)

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
1	YOF	A	6	1	-	2/5/6/8	0/1/1/1
1	YOF	B	40	1	-	5/5/6/8	0/1/1/1
1	YOF	A	137	1	-	1/5/6/8	0/1/1/1
1	YOF	B	22	1	-	0/5/6/8	0/1/1/1
1	YOF	B	202	1	-	0/5/6/8	0/1/1/1
1	YOF	B	78	1	-	0/5/6/8	0/1/1/1
1	YOF	B	27	1	-	0/5/6/8	0/1/1/1
1	YOF	A	196	1	-	2/5/6/8	0/1/1/1
1	YOF	B	196	1	-	2/5/6/8	0/1/1/1
1	YOF	A	32	1	-	0/5/6/8	0/1/1/1
1	YOF	A	166	1	-	2/5/6/8	0/1/1/1
1	YOF	A	160	1	-	0/5/6/8	0/1/1/1
1	YOF	A	27	1	-	0/5/6/8	0/1/1/1
1	YOF	A	22	1	-	0/5/6/8	0/1/1/1
1	YOF	A	40	1	-	0/5/6/8	0/1/1/1
1	YOF	A	61	1	-	0/5/6/8	0/1/1/1
1	YOF	B	154[B]	-	-	1/5/6/8	0/1/1/1
1	YOF	A	154[B]	-	-	0/5/6/8	0/1/1/1
1	YOF	B	137	1	-	0/5/6/8	0/1/1/1
1	YOF	B	6	1	-	2/5/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	YOF	A	78	1	-	0/5/6/8	0/1/1/1
1	YOF	B	61	1	-	0/5/6/8	0/1/1/1
1	YOF	A	202	1	-	0/5/6/8	0/1/1/1
1	YOF	B	154[A]	-	-	1/5/6/8	0/1/1/1
1	YOF	A	154[A]	-	-	0/5/6/8	0/1/1/1
1	YOF	B	32	1	-	0/5/6/8	0/1/1/1
1	YOF	B	166	1	-	2/5/6/8	0/1/1/1
1	YOF	B	160	1	-	0/5/6/8	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	40	YOF	CZ-CE1	3.16	1.41	1.39
1	B	40	YOF	CZ-CE1	2.76	1.41	1.39
1	A	61	YOF	CE2-CD2	2.37	1.43	1.38
1	A	6	YOF	CZ-CE1	2.33	1.41	1.39
1	A	61	YOF	CB-CA	-2.31	1.48	1.53

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	YOF	CG-CD1-CE1	5.59	123.00	119.37
1	B	196	YOF	CB-CA-C	-4.41	103.21	111.47
1	B	196	YOF	CD2-CE2-CZ	-4.25	116.14	120.50
1	A	202	YOF	CG-CD1-CE1	4.06	122.00	119.37
1	B	196	YOF	CG-CB-CA	-3.78	106.44	114.10

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	166	YOF	C-CA-CB-CG
1	B	40	YOF	O-C-CA-CB
1	B	166	YOF	C-CA-CB-CG
1	B	40	YOF	N-CA-CB-CG
1	B	166	YOF	N-CA-CB-CG

There are no ring outliers.

11 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	6	YOF	8	0
1	B	40	YOF	5	0
1	B	22	YOF	1	0
1	B	202	YOF	3	0
1	A	196	YOF	1	0
1	B	196	YOF	1	0
1	A	32	YOF	1	0
1	A	160	YOF	1	0
1	A	40	YOF	5	0
1	A	61	YOF	1	0
1	B	32	YOF	3	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 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
2	GPR	B	218	-	29,37,37	2.45	10 (34%)	37,51,51	1.78	9 (24%)
2	GPR	A	218	-	29,37,37	3.33	7 (24%)	37,51,51	2.23	9 (24%)

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	GPR	B	218	-	-	1/21/43/43	0/3/3/3
2	GPR	A	218	-	-	3/21/43/43	0/3/3/3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	218	GPR	CB2-SG2	-15.97	1.65	1.82
2	B	218	GPR	CB2-SG2	-8.08	1.73	1.82
2	B	218	GPR	CG4-CB4	4.63	1.45	1.39
2	B	218	GPR	CG5-CB5	4.18	1.45	1.39
2	A	218	GPR	O5-CA5	3.91	1.50	1.42

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	218	GPR	CB2-CA2-C2	-7.52	93.40	109.73
2	A	218	GPR	CD4-CG4-CB4	-6.17	113.17	121.01
2	A	218	GPR	CG4-CB4-CH4	4.42	125.14	119.32
2	B	218	GPR	CB2-CA2-N2	-4.28	99.44	111.00
2	B	218	GPR	CD4-CG4-CB4	-4.24	115.62	121.01

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	218	GPR	N1-CA1-CB1-CG1
2	A	218	GPR	C1-CA1-CB1-CG1
2	B	218	GPR	OE1-CD1-N2-CA2
2	A	218	GPR	OE1-CD1-N2-CA2

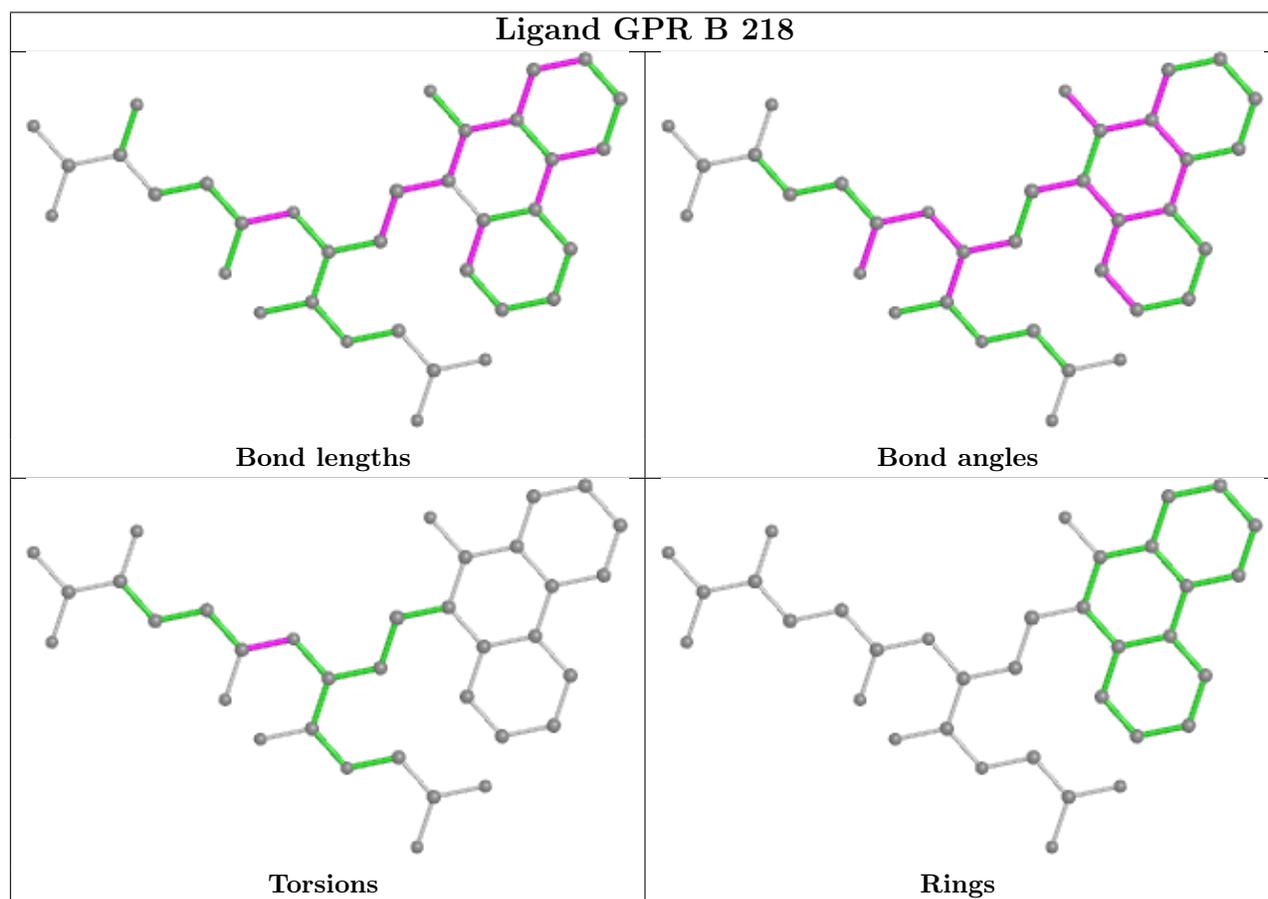
There are no ring outliers.

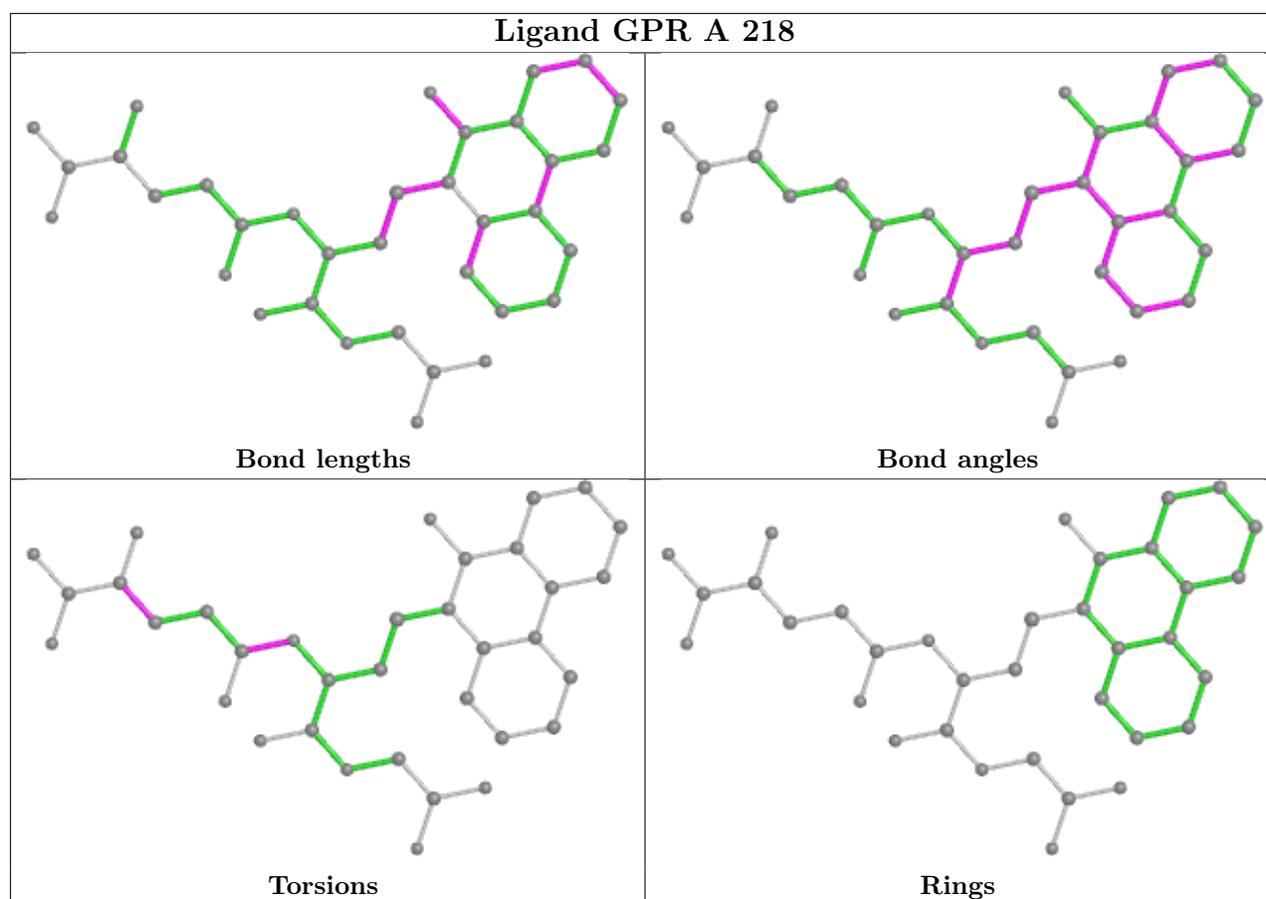
2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	218	GPR	6	0
2	A	218	GPR	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

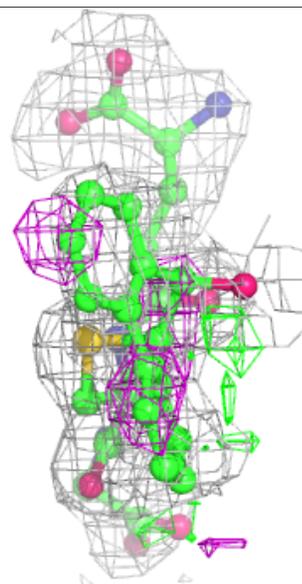
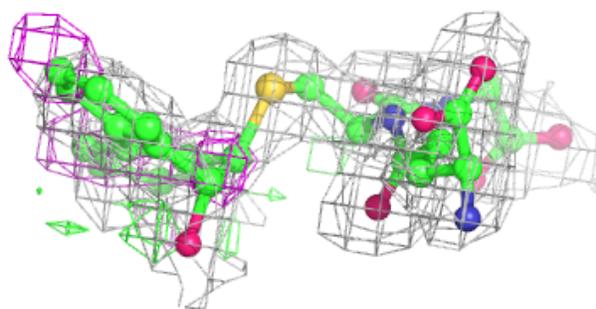
### 6.4 Ligands

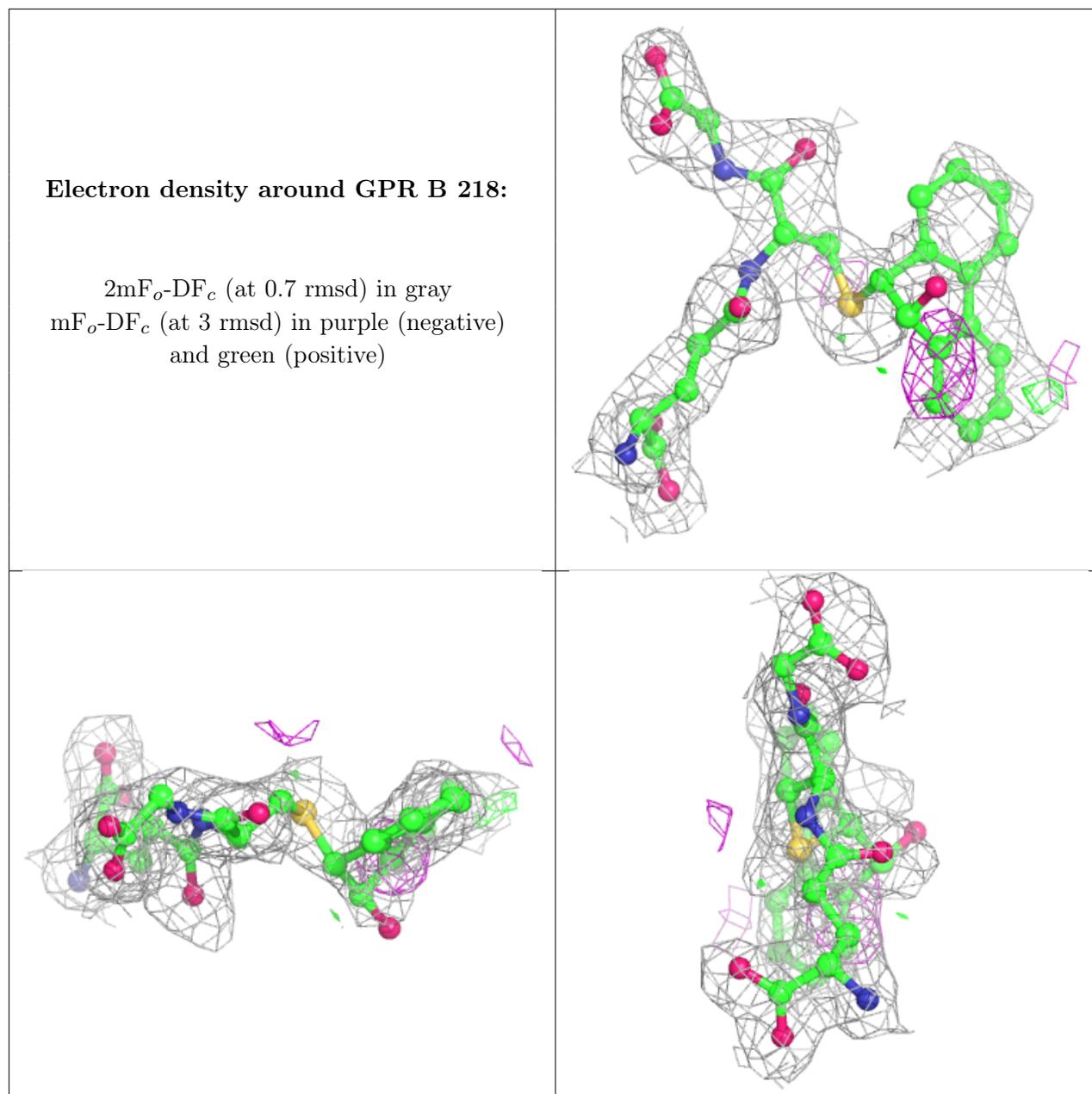
Unable to reproduce the depositors R factor - this section is therefore empty.

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 GPR A 218:**

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





## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.