



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 08:04 pm BST

PDB ID : 2ZNX  
Title : 5-Fluorotryptophan Incorporated ScFv10 Complexed to Hen Egg Lysozyme  
Authors : DeSantis, M.E.; Acchione, M.; Li, M.; Walter, R.L.; Wlodawer, A.; Smith-Gill, S.  
Deposited on : 2008-05-02  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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	:	2.11
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

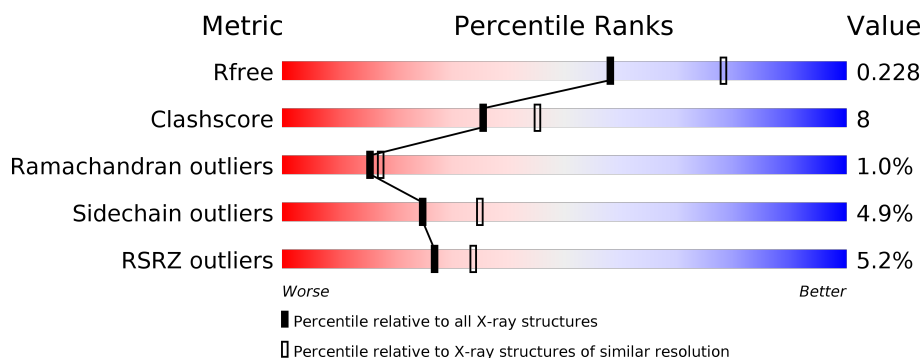
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	242	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>17%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	242	<div> <div>6%</div> <div> <div></div> <div>75%</div> <div>14%</div> <div>••</div> <div>9%</div> </div> </div>
2	Y	129	<div> <div>5%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div>•</div> </div> </div>
2	Z	129	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>•</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5793 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 ScFv.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	221	Total	C	F	N	O	S	0	0	0
			1723	1077	6	281	353	6			
1	B	221	Total	C	F	N	O	S	0	0	0
			1723	1077	6	281	353	6			

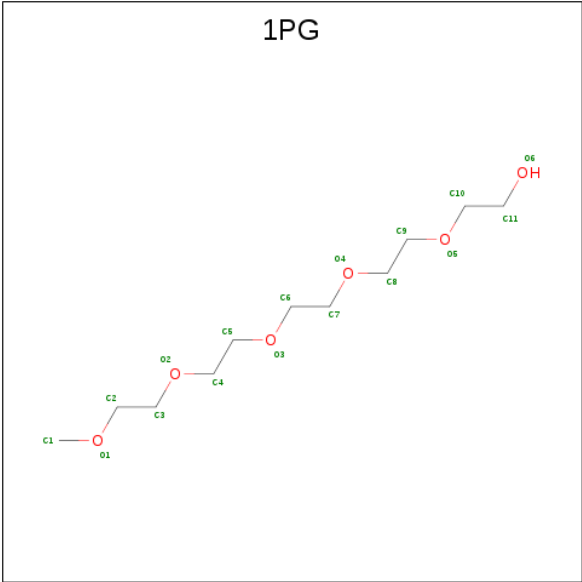
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	237	HIS	-	EXPRESSION TAG	PDB 2ZNX
A	238	HIS	-	EXPRESSION TAG	PDB 2ZNX
A	239	HIS	-	EXPRESSION TAG	PDB 2ZNX
A	240	HIS	-	EXPRESSION TAG	PDB 2ZNX
A	241	HIS	-	EXPRESSION TAG	PDB 2ZNX
A	242	HIS	-	EXPRESSION TAG	PDB 2ZNX
B	237	HIS	-	EXPRESSION TAG	PDB 2ZNX
B	238	HIS	-	EXPRESSION TAG	PDB 2ZNX
B	239	HIS	-	EXPRESSION TAG	PDB 2ZNX
B	240	HIS	-	EXPRESSION TAG	PDB 2ZNX
B	241	HIS	-	EXPRESSION TAG	PDB 2ZNX
B	242	HIS	-	EXPRESSION TAG	PDB 2ZNX

- Molecule 2 is a protein called Lysozyme C.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	Y	129	Total	C	N	O	S		0	0	0
			1001	613	193	185	10				
2	Z	129	Total	C	N	O	S		0	0	0
			1001	613	193	185	10				

- Molecule 3 is 2-(2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHANOL (three-letter code: 1PG) (formula: C<sub>11</sub>H<sub>24</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			17	11	6		
3	B	1	Total	C	O	0	0
			17	11	6		

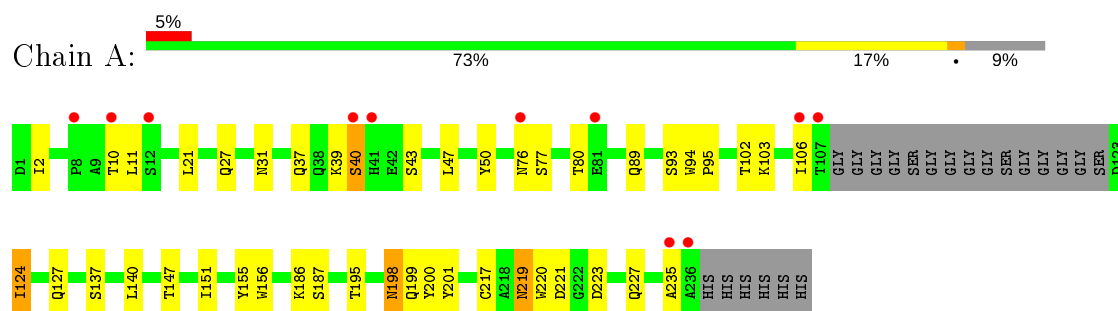
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	97	Total	O	0	0
			97	97		
4	Y	51	Total	O	0	0
			51	51		
4	B	107	Total	O	0	0
			107	107		
4	Z	56	Total	O	0	0
			56	56		

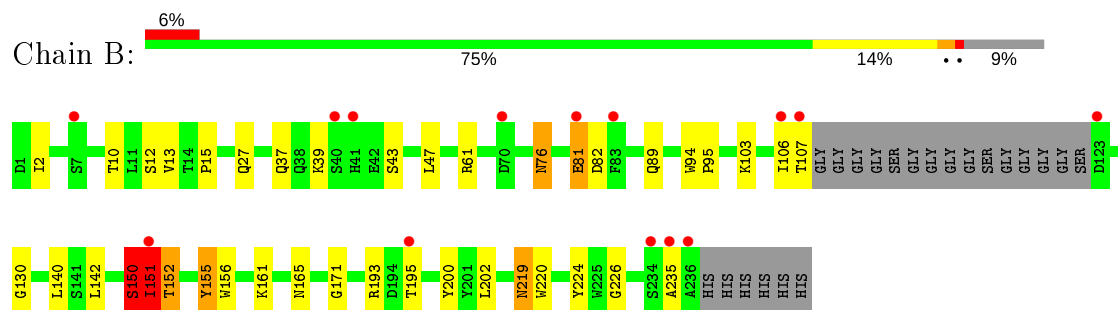
### 3 Residue-property plots [i](#)

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.

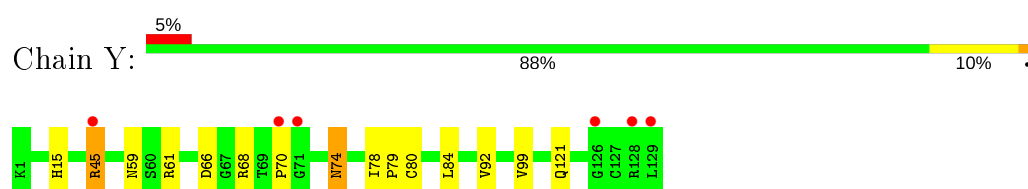
- Molecule 1: ScFv



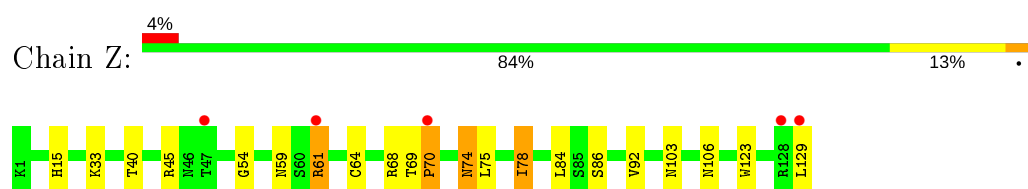
- Molecule 1: ScFv



- Molecule 2: Lysozyme C



- Molecule 2: Lysozyme C



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.24Å 149.24Å 81.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 44.23 – 2.30	Depositor EDS
% Data completeness (in resolution range)	83.0 (50.00-2.30) 99.9 (44.23-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.71 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.4.0057	Depositor
R, $R_{free}$	0.193 , 0.232 0.192 , 0.228	Depositor DCC
$R_{free}$ test set	2051 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.6	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 36.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5793	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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: FTR, 1PG

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	0.52	0/1657	0.67	0/2239
1	B	0.58	0/1657	0.69	0/2239
2	Y	0.57	0/1021	0.63	0/1379
2	Z	0.57	0/1021	0.63	0/1379
All	All	0.56	0/5356	0.66	0/7236

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	150	SER	Peptide

### 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	1723	0	1612	27	0
1	B	1723	0	1611	31	0
2	Y	1001	0	959	11	0
2	Z	1001	0	959	14	0
3	A	17	0	24	5	0
3	B	17	0	24	7	0
4	A	97	0	0	3	1
4	B	107	0	0	2	1
4	Y	51	0	0	0	0
4	Z	56	0	0	0	0
All	All	5793	0	5189	86	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 8.

All (86) 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)
3:B:243:1PG:H42	3:B:243:1PG:H13	1.24	1.11
2:Y:45:ARG:HG3	2:Y:45:ARG:HH11	1.16	1.07
3:A:243:1PG:H42	3:A:243:1PG:H13	1.53	0.91
3:B:243:1PG:C1	3:B:243:1PG:H42	2.08	0.84
1:A:89:GLN:HE22	3:A:243:1PG:H22	1.43	0.82
1:A:127:GLN:HE22	1:A:227:GLN:HE21	1.33	0.74
2:Y:45:ARG:CG	2:Y:45:ARG:HH11	1.98	0.74
2:Y:45:ARG:HG3	2:Y:45:ARG:NH1	1.96	0.73
2:Z:74:ASN:HD21	2:Z:78:ILE:H	1.38	0.69
2:Y:74:ASN:HD21	2:Y:78:ILE:H	1.39	0.69
1:B:61:ARG:NH2	1:B:82:ASP:OD1	2.30	0.63
1:B:89:GLN:HE22	3:B:243:1PG:H22	1.63	0.63
1:A:10:THR:HG22	1:A:103:LYS:HB3	1.81	0.63
1:B:220:FTR:F	3:B:243:1PG:H81	1.93	0.59
1:B:151:ILE:HG21	2:Z:75:LEU:HD21	1.85	0.59
1:A:89:GLN:HE22	3:A:243:1PG:C2	2.13	0.58
1:B:37:GLN:HB2	1:B:47:LEU:HD11	1.86	0.58
1:B:15:PRO:HG3	1:B:106:ILE:HD11	1.87	0.57
1:A:187:SER:HB3	4:A:244:HOH:O	2.04	0.56
3:B:243:1PG:H101	4:B:293:HOH:O	2.04	0.56
1:B:155:TYR:HB2	1:B:220:FTR:HB2	1.88	0.55
1:A:2:ILE:HG12	1:A:27:GLN:HG3	1.89	0.55
1:A:151:ILE:H	1:A:198:ASN:HD21	1.53	0.54
1:B:10:THR:HG22	1:B:103:LYS:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ILE:HD11	1:A:195:THR:HA	1.90	0.53
1:A:200:TYR:OH	1:A:217:CYS:HB2	2.08	0.53
1:B:94:FTR:CD2	1:B:95:PRO:HA	2.40	0.52
1:A:186:LYS:O	1:A:187:SER:HB3	2.08	0.52
1:A:156:FTR:HB2	1:A:200:TYR:CZ	2.45	0.52
2:Y:45:ARG:CG	2:Y:45:ARG:NH1	2.64	0.52
2:Y:59:ASN:ND2	2:Y:61:ARG:H	2.07	0.52
2:Z:59:ASN:ND2	2:Z:61:ARG:HB2	2.25	0.52
2:Y:45:ARG:HH22	2:Y:68:ARG:CZ	2.22	0.52
1:B:89:GLN:HE22	3:B:243:1PG:C2	2.23	0.51
1:A:127:GLN:NE2	1:A:227:GLN:HE21	2.04	0.51
2:Z:59:ASN:HD21	2:Z:61:ARG:HB2	1.76	0.51
1:B:130:GLY:HA3	1:B:142:LEU:HD23	1.94	0.50
1:A:155:TYR:HB2	1:A:220:FTR:HB2	1.94	0.49
1:A:80:THR:HA	1:A:106:ILE:HG12	1.93	0.49
1:B:161:LYS:HE2	1:B:165:ASN:HA	1.95	0.48
1:B:156:FTR:HB2	1:B:200:TYR:CZ	2.49	0.48
2:Z:40:THR:O	2:Z:54:GLY:HA2	2.14	0.48
1:A:124:ILE:HA	1:A:147:THR:O	2.14	0.47
1:A:94:FTR:CD2	1:A:95:PRO:HA	2.44	0.47
1:B:150:SER:OG	1:B:151:ILE:N	2.47	0.47
1:B:2:ILE:HG12	1:B:27:GLN:HG2	1.96	0.47
1:B:155:TYR:HB2	1:B:220:FTR:CB	2.44	0.47
3:A:243:1PG:H81	4:A:248:HOH:O	2.15	0.47
1:B:43:SER:HB3	1:B:226:GLY:O	2.15	0.47
2:Z:64:CYS:HA	2:Z:74:ASN:ND2	2.30	0.46
1:A:221:ASP:O	3:A:243:1PG:H41	2.16	0.46
1:A:219:ASN:HD21	1:A:223:ASP:H	1.64	0.46
2:Z:59:ASN:ND2	2:Z:61:ARG:H	2.14	0.46
1:B:94:FTR:HH2	1:B:171:GLY:HA2	1.97	0.45
1:A:31:ASN:O	1:A:50:TYR:HA	2.17	0.45
1:A:155:TYR:HB2	1:A:220:FTR:CB	2.47	0.45
1:B:142:LEU:HD12	1:B:202:LEU:HD23	1.98	0.45
2:Y:45:ARG:HH12	2:Y:68:ARG:HH12	1.63	0.45
1:B:219:ASN:ND2	1:B:224:TYR:H	2.15	0.45
1:A:2:ILE:HD12	1:A:93:SER:HB2	1.99	0.45
2:Y:78:ILE:HG13	2:Y:79:PRO:HD2	1.99	0.45
1:A:21:LEU:HD22	1:A:102:THR:HG21	1.97	0.44
1:B:151:ILE:HG21	2:Z:75:LEU:CD2	2.47	0.44
2:Z:33:LYS:HG2	2:Z:123:TRP:CH2	2.53	0.43
1:B:13:VAL:O	1:B:107:THR:HB	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:GLN:HB2	1:A:47:LEU:HD11	2.00	0.43
1:B:61:ARG:HB2	1:B:76:ASN:HB3	2.00	0.43
1:B:219:ASN:HD21	1:B:224:TYR:H	1.64	0.43
1:B:61:ARG:HH21	1:B:82:ASP:CG	2.22	0.42
2:Z:15:HIS:HB3	2:Z:92:VAL:HG11	2.02	0.42
3:B:243:1PG:H82	4:B:267:HOH:O	2.20	0.42
1:B:39:LYS:HE2	1:B:81:GLU:O	2.20	0.42
1:A:198:ASN:ND2	4:A:308:HOH:O	2.52	0.42
1:A:39:LYS:O	1:A:40:SER:C	2.58	0.41
2:Y:15:HIS:HB3	2:Y:92:VAL:HG11	2.02	0.41
1:B:155:TYR:N	1:B:155:TYR:CD1	2.88	0.41
1:B:195:THR:O	1:B:195:THR:HG22	2.19	0.41
1:A:151:ILE:H	1:A:198:ASN:ND2	2.17	0.41
2:Z:129:LEU:HA	2:Z:129:LEU:HD23	1.95	0.41
2:Z:69:THR:HA	2:Z:70:PRO:HD2	1.83	0.41
1:B:152:THR:O	1:B:193:ARG:HD2	2.21	0.41
1:B:151:ILE:CG2	2:Z:75:LEU:HD21	2.51	0.41
1:B:155:TYR:N	1:B:155:TYR:HD1	2.20	0.40
2:Z:103:ASN:O	2:Z:106:ASN:HB2	2.22	0.40
1:A:199:GLN:NE2	1:A:201:TYR:OH	2.53	0.40
2:Y:66:ASP:HB3	2:Y:80:CYS:SG	2.62	0.40

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)
4:A:338:HOH:O	4:B:272:HOH:O[3_455]	2.18	0.02

## 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	211/242 (87%)	203 (96%)	6 (3%)	2 (1%)	17	20
1	B	211/242 (87%)	198 (94%)	10 (5%)	3 (1%)	11	11
2	Y	127/129 (98%)	125 (98%)	1 (1%)	1 (1%)	19	23
2	Z	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	19	23
All	All	676/742 (91%)	648 (96%)	21 (3%)	7 (1%)	15	17

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Y	70	PRO
1	B	235	ALA
2	Z	70	PRO
1	B	150	SER
1	A	40	SER
1	A	235	ALA
1	B	151	ILE

### 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	190/199 (96%)	181 (95%)	9 (5%)	26	37
1	B	190/199 (96%)	182 (96%)	8 (4%)	30	42
2	Y	105/105 (100%)	100 (95%)	5 (5%)	25	36
2	Z	105/105 (100%)	98 (93%)	7 (7%)	16	21
All	All	590/608 (97%)	561 (95%)	29 (5%)	25	35

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	43	SER
1	A	76	ASN
1	A	77	SER

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Mol	Chain	Res	Type
1	A	124	ILE
1	A	137	SER
1	A	140	LEU
1	A	198	ASN
1	A	219	ASN
2	Y	45	ARG
2	Y	74	ASN
2	Y	84	LEU
2	Y	99	VAL
2	Y	121	GLN
1	B	12	SER
1	B	76	ASN
1	B	81	GLU
1	B	140	LEU
1	B	151	ILE
1	B	152	THR
1	B	155	TYR
1	B	219	ASN
2	Z	45	ARG
2	Z	61	ARG
2	Z	68	ARG
2	Z	74	ASN
2	Z	78	ILE
2	Z	84	LEU
2	Z	86	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	127	GLN
1	A	198	ASN
1	A	199	GLN
1	A	219	ASN
1	A	227	GLN
2	Y	59	ASN
2	Y	74	ASN
2	Y	113	ASN
1	B	89	GLN
1	B	205	ASN
1	B	219	ASN
2	Z	46	ASN

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Mol	Chain	Res	Type
2	Z	59	ASN
2	Z	74	ASN
2	Z	113	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	FTR	B	220	1	14,16,17	1.37	1 (7%)	14,22,24	1.45	2 (14%)
1	FTR	B	35	1	14,16,17	1.31	1 (7%)	14,22,24	1.50	3 (21%)
1	FTR	A	156	1	14,16,17	1.35	2 (14%)	14,22,24	1.65	2 (14%)
1	FTR	A	94	1	14,16,17	1.17	1 (7%)	14,22,24	1.97	3 (21%)
1	FTR	B	94	1	14,16,17	1.29	2 (14%)	14,22,24	2.11	2 (14%)
1	FTR	B	225	1	14,16,17	1.35	3 (21%)	14,22,24	1.81	4 (28%)
1	FTR	A	35	1	14,16,17	1.30	2 (14%)	14,22,24	1.60	3 (21%)
1	FTR	A	158	1	14,16,17	1.22	1 (7%)	14,22,24	1.38	2 (14%)
1	FTR	B	158	1	14,16,17	1.16	0	14,22,24	1.52	2 (14%)
1	FTR	B	156	1	14,16,17	1.35	3 (21%)	14,22,24	1.40	3 (21%)
1	FTR	A	220	1	14,16,17	1.25	2 (14%)	14,22,24	1.67	4 (28%)
1	FTR	A	225	1	14,16,17	1.23	0	14,22,24	1.48	4 (28%)

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	FTR	B	220	1	-	0/4/6/8	0/2/2/2
1	FTR	B	35	1	-	0/4/6/8	0/2/2/2
1	FTR	A	156	1	-	0/4/6/8	0/2/2/2
1	FTR	A	94	1	-	0/4/6/8	0/2/2/2
1	FTR	B	94	1	-	0/4/6/8	0/2/2/2
1	FTR	B	225	1	-	0/4/6/8	0/2/2/2
1	FTR	A	35	1	-	0/4/6/8	0/2/2/2
1	FTR	A	158	1	-	0/4/6/8	0/2/2/2
1	FTR	B	158	1	-	0/4/6/8	0/2/2/2
1	FTR	B	156	1	-	0/4/6/8	0/2/2/2
1	FTR	A	220	1	-	0/4/6/8	0/2/2/2
1	FTR	A	225	1	-	1/4/6/8	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	220	FTR	CE3-CZ3	2.72	1.40	1.36
1	A	35	FTR	CE3-CZ3	2.67	1.40	1.36
1	B	35	FTR	CE3-CZ3	2.56	1.40	1.36
1	A	156	FTR	CE3-CZ3	2.52	1.40	1.36
1	A	156	FTR	CZ2-CH2	2.51	1.41	1.36
1	B	156	FTR	CE3-CZ3	2.37	1.40	1.36
1	B	156	FTR	CZ2-CH2	2.34	1.41	1.36
1	A	158	FTR	CE3-CZ3	2.28	1.39	1.36
1	A	220	FTR	CD2-CE2	2.19	1.48	1.42
1	B	225	FTR	CH2-CZ3	2.15	1.41	1.37
1	B	94	FTR	CH2-CZ3	2.14	1.41	1.37
1	A	220	FTR	CE3-CZ3	2.13	1.39	1.36
1	B	225	FTR	CD2-CE2	2.12	1.48	1.42
1	A	94	FTR	CE3-CZ3	2.08	1.39	1.36
1	B	156	FTR	CH2-CZ3	2.04	1.41	1.37
1	A	35	FTR	CD2-CE2	2.03	1.48	1.42
1	B	225	FTR	CE3-CZ3	2.02	1.39	1.36
1	B	94	FTR	CE3-CZ3	2.01	1.39	1.36

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	FTR	CG-CB-CA	-6.42	104.61	114.53
1	A	94	FTR	CG-CB-CA	-5.59	105.88	114.53
1	B	225	FTR	CB-CA-C	-3.71	104.51	111.47
1	A	156	FTR	CG-CB-CA	-3.54	109.05	114.53
1	B	220	FTR	CZ3-CE3-CD2	-3.42	116.12	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	FTR	CZ2-CH2-CZ3	3.14	122.33	118.74
1	B	225	FTR	CZ3-CE3-CD2	-3.01	116.44	118.80
1	B	225	FTR	CE3-CD2-CE2	2.98	122.33	118.26
1	A	220	FTR	CZ3-CE3-CD2	-2.83	116.58	118.80
1	A	220	FTR	CE3-CD2-CE2	2.78	122.07	118.26
1	A	35	FTR	CB-CA-C	-2.76	106.30	111.47
1	A	94	FTR	CE3-CD2-CE2	2.75	122.02	118.26
1	B	158	FTR	CZ2-CH2-CZ3	2.68	121.81	118.74
1	A	35	FTR	CZ2-CH2-CZ3	2.66	121.78	118.74
1	B	220	FTR	CE3-CD2-CE2	2.62	121.84	118.26
1	B	94	FTR	CE3-CD2-CE2	2.58	121.79	118.26
1	A	225	FTR	CE3-CD2-CE2	2.55	121.74	118.26
1	B	225	FTR	CZ2-CH2-CZ3	2.46	121.55	118.74
1	B	35	FTR	CG-CB-CA	-2.45	110.75	114.53
1	B	158	FTR	CE3-CD2-CE2	2.44	121.59	118.26
1	B	156	FTR	CG-CB-CA	-2.41	110.79	114.53
1	B	156	FTR	CE3-CD2-CE2	2.38	121.51	118.26
1	A	35	FTR	CE3-CD2-CE2	2.31	121.42	118.26
1	B	35	FTR	CB-CA-C	-2.25	107.24	111.47
1	A	220	FTR	CB-CA-C	2.21	115.62	111.47
1	A	225	FTR	CZ2-CH2-CZ3	2.21	121.26	118.74
1	A	156	FTR	CE3-CD2-CE2	2.18	121.24	118.26
1	A	158	FTR	CE3-CD2-CE2	2.18	121.23	118.26
1	B	35	FTR	CE3-CD2-CE2	2.15	121.19	118.26
1	A	94	FTR	CZ2-CH2-CZ3	2.14	121.19	118.74
1	A	158	FTR	CZ2-CH2-CZ3	2.11	121.15	118.74
1	A	225	FTR	CG-CB-CA	-2.08	111.30	114.53
1	A	225	FTR	CZ3-CE3-CD2	-2.07	117.18	118.80
1	B	156	FTR	CZ2-CH2-CZ3	2.04	121.08	118.74

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	225	FTR	O-C-CA-CB

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	220	FTR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	156	FTR	1	0
1	A	94	FTR	1	0
1	B	94	FTR	2	0
1	B	156	FTR	1	0
1	A	220	FTR	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	$\# Z  > 2$
3	1PG	B	243	-	16,16,16	0.67	0	15,15,15	0.56	0
3	1PG	A	243	-	16,16,16	0.59	0	15,15,15	0.37	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
3	1PG	B	243	-	-	10/14/14/14	-
3	1PG	A	243	-	-	8/14/14/14	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:



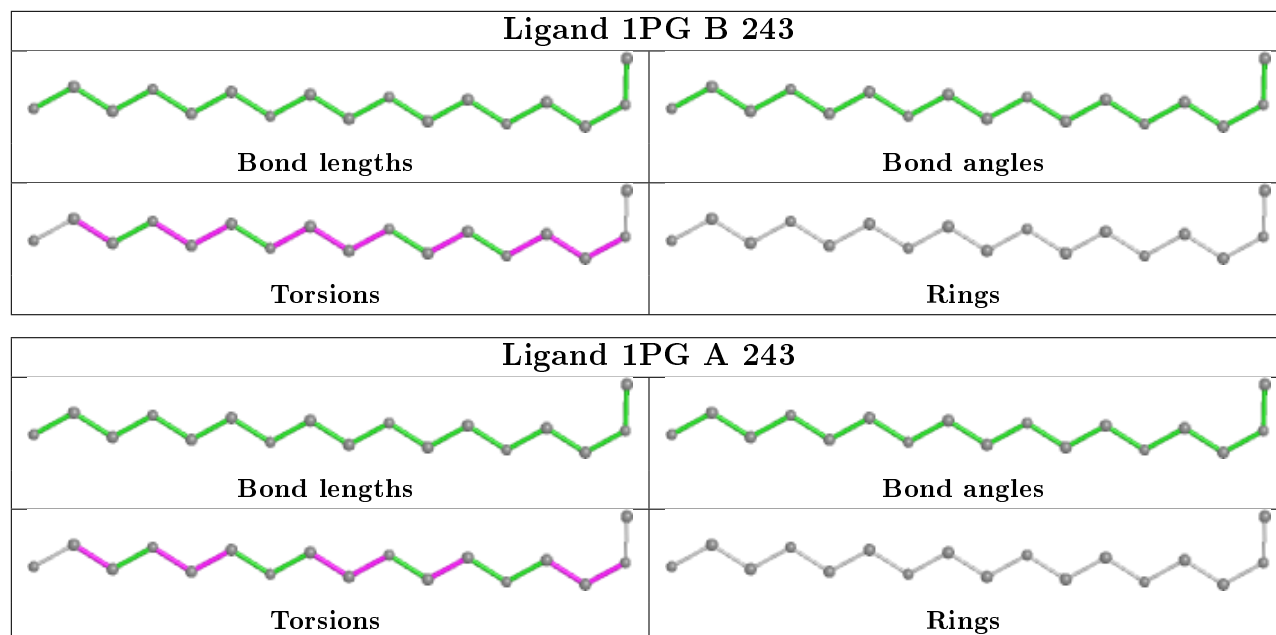
Mol	Chain	Res	Type	Atoms
3	B	243	1PG	O4-C8-C9-O5
3	A	243	1PG	O4-C8-C9-O5
3	A	243	1PG	O5-C10-C11-O6
3	A	243	1PG	O2-C4-C5-O3
3	A	243	1PG	O1-C2-C3-O2
3	B	243	1PG	O5-C10-C11-O6
3	A	243	1PG	C7-C6-O3-C5
3	A	243	1PG	C8-C9-O5-C10
3	B	243	1PG	C6-C7-O4-C8
3	A	243	1PG	O3-C6-C7-O4
3	B	243	1PG	O3-C6-C7-O4
3	B	243	1PG	O1-C2-C3-O2
3	B	243	1PG	O2-C4-C5-O3
3	B	243	1PG	C7-C6-O3-C5
3	B	243	1PG	C8-C9-O5-C10
3	B	243	1PG	C2-C3-O2-C4
3	B	243	1PG	C3-C2-O1-C1
3	A	243	1PG	C3-C2-O1-C1

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	243	1PG	7	0
3	A	243	1PG	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	215/242 (88%)	0.17	11 (5%) 28 35	14, 26, 45, 54	0
1	B	215/242 (88%)	0.15	14 (6%) 18 24	14, 26, 43, 54	0
2	Y	129/129 (100%)	-0.03	6 (4%) 31 38	15, 23, 39, 59	0
2	Z	129/129 (100%)	-0.09	5 (3%) 39 46	14, 23, 39, 58	0
All	All	688/742 (92%)	0.08	36 (5%) 27 34	14, 24, 43, 59	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	236	ALA	17.5
1	A	41	HIS	5.6
2	Z	70	PRO	5.5
1	A	236	ALA	5.4
1	A	40	SER	5.1
2	Y	129	LEU	5.0
2	Z	129	LEU	4.7
2	Y	71	GLY	4.7
2	Y	128	ARG	4.6
1	B	41	HIS	4.5
1	B	235	ALA	4.4
1	B	195	THR	4.4
2	Z	128	ARG	4.3
1	A	107	THR	3.9
1	B	107	THR	3.5
2	Y	70	PRO	3.3
1	B	83	PHE	3.1
1	A	106	ILE	3.1
1	B	123	ASP	3.0
1	B	106	ILE	2.8
2	Z	47	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	151	ILE	2.8
2	Y	126	GLY	2.7
1	B	81	GLU	2.6
1	A	235	ALA	2.4
1	A	76	ASN	2.4
2	Y	45	ARG	2.4
1	A	81	GLU	2.4
1	A	10	THR	2.4
1	A	12	SER	2.3
1	B	40	SER	2.3
1	B	234	SER	2.2
1	B	7	SER	2.2
1	B	70	ASP	2.1
1	A	8	PRO	2.0
2	Z	61	ARG	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	FTR	B	94	15/16	0.95	0.13	18,19,21,25	0
1	FTR	B	225	15/16	0.96	0.12	18,21,24,25	0
1	FTR	A	225	15/16	0.96	0.12	19,20,24,25	0
1	FTR	A	94	15/16	0.97	0.11	18,19,20,22	0
1	FTR	B	220	15/16	0.97	0.11	15,16,18,18	0
1	FTR	B	35	15/16	0.97	0.11	18,20,23,27	0
1	FTR	A	35	15/16	0.97	0.10	18,20,24,28	0
1	FTR	B	156	15/16	0.97	0.13	16,17,18,21	0
1	FTR	A	220	15/16	0.97	0.12	16,18,19,22	0
1	FTR	A	156	15/16	0.97	0.14	14,17,18,21	0
1	FTR	B	158	15/16	0.98	0.12	14,16,17,20	0
1	FTR	A	158	15/16	0.98	0.12	15,16,17,20	0

## 6.3 Carbohydrates [i](#)

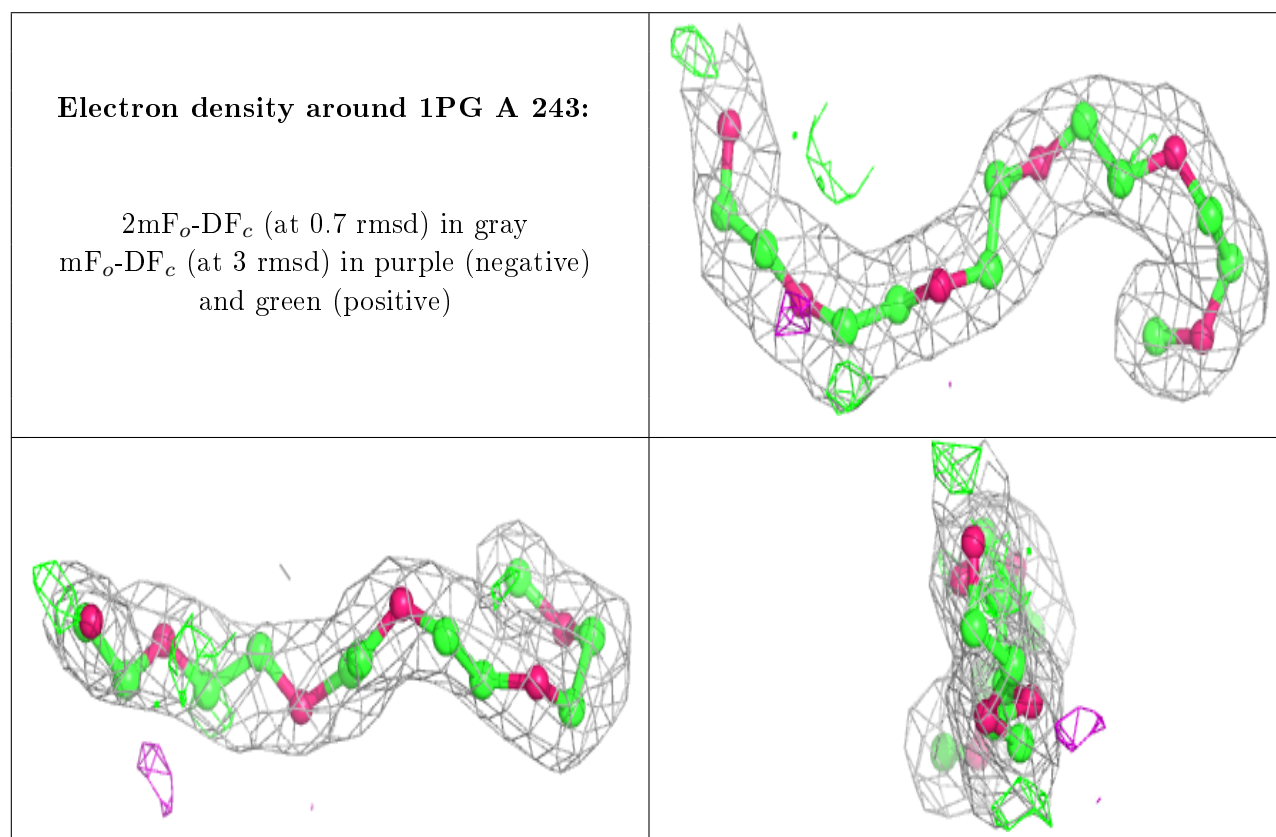
There are no carbohydrates in this entry.

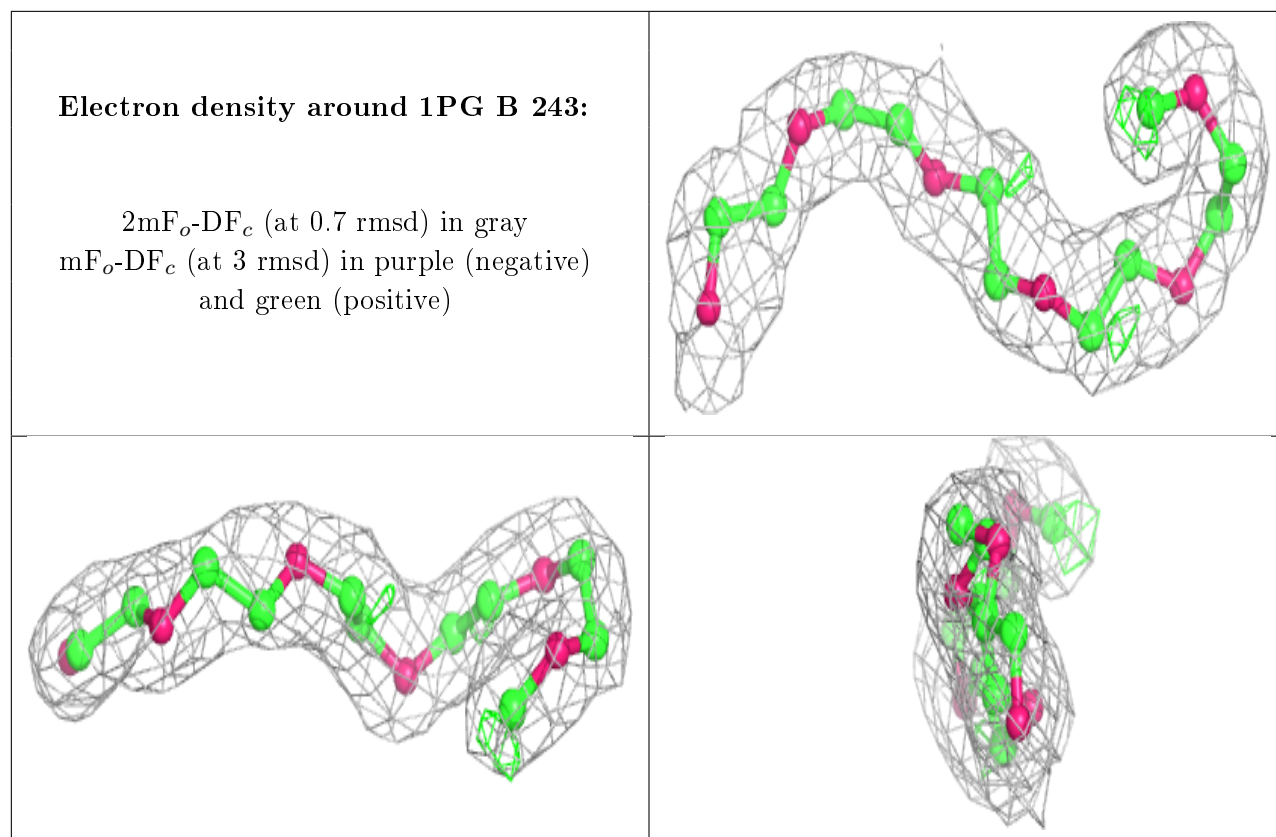
## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	1PG	A	243	17/17	0.90	0.18	28,33,38,39	0
3	1PG	B	243	17/17	0.92	0.15	18,25,31,32	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.