



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 08:51 am BST

PDB ID : 5TTZ  
Title : Crystal structure of Grp94 bound to isoform-selective inhibitor methyl 2-(2-(1-(4-bromobenzyl)-1H-imidazol-2-yl)ethyl)-3-chloro-4,6-dihydroxybenzoate  
Authors : Lieberman, R.L.; Huard, D.J.E.  
Deposited on : 2016-11-04  
Resolution : 2.71 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

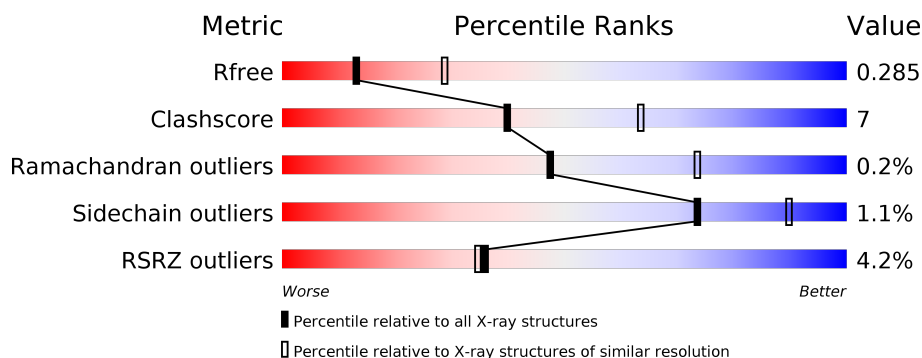
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.71 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	233	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>9%</div> </div> </div>
1	B	233	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>8%</div> </div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3454 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 Endoplasmin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1655	1048	275	326	6			
1	B	215	Total	C	N	O	S	0	0	0
			1652	1044	276	326	6			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	SER	-	expression tag	UNP P41148
A	?	-	GLU	deletion	UNP P41148
A	?	-	THR	deletion	UNP P41148
A	?	-	VAL	deletion	UNP P41148
A	?	-	GLU	deletion	UNP P41148
A	?	-	GLU	deletion	UNP P41148
A	?	-	PRO	deletion	UNP P41148
A	?	-	MET	deletion	UNP P41148
A	?	-	GLU	deletion	UNP P41148
A	?	-	GLU	deletion	UNP P41148
A	?	-	GLU	deletion	UNP P41148
A	?	-	GLU	deletion	UNP P41148
A	?	-	ALA	deletion	UNP P41148
A	?	-	ALA	deletion	UNP P41148
A	?	-	LYS	deletion	UNP P41148
A	?	-	GLU	deletion	UNP P41148
A	?	-	GLU	deletion	UNP P41148
A	?	-	LYS	deletion	UNP P41148
A	?	-	GLU	deletion	UNP P41148
A	?	-	ASP	deletion	UNP P41148
A	?	-	SER	deletion	UNP P41148
A	?	-	ASP	deletion	UNP P41148
A	?	-	ASP	deletion	UNP P41148
A	?	-	GLU	deletion	UNP P41148
A	?	-	ALA	deletion	UNP P41148

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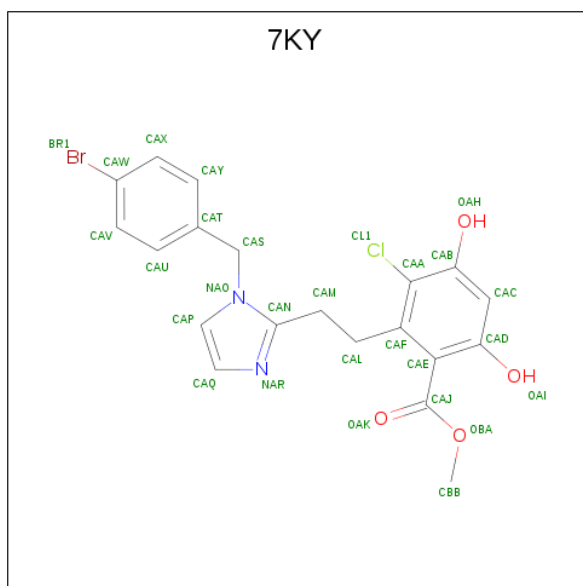
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	deletion	UNP P41148
A	?	-	VAL	deletion	UNP P41148
A	?	-	GLU	deletion	UNP P41148
A	?	-	GLU	deletion	UNP P41148
A	?	-	GLU	deletion	UNP P41148
A	?	-	GLU	deletion	UNP P41148
A	?	-	GLU	deletion	UNP P41148
A	?	-	GLU	deletion	UNP P41148
A	?	-	LYS	deletion	UNP P41148
A	?	-	LYS	deletion	UNP P41148
A	?	-	PRO	deletion	UNP P41148
A	?	-	LYS	deletion	UNP P41148
A	?	-	THR	deletion	UNP P41148
A	324	GLY	LYS	linker	UNP P41148
A	325	GLY	LYS	linker	UNP P41148
A	326	GLY	VAL	linker	UNP P41148
A	327	GLY	GLU	linker	UNP P41148
B	68	SER	-	expression tag	UNP P41148
B	?	-	GLU	deletion	UNP P41148
B	?	-	THR	deletion	UNP P41148
B	?	-	VAL	deletion	UNP P41148
B	?	-	GLU	deletion	UNP P41148
B	?	-	GLU	deletion	UNP P41148
B	?	-	PRO	deletion	UNP P41148
B	?	-	MET	deletion	UNP P41148
B	?	-	GLU	deletion	UNP P41148
B	?	-	GLU	deletion	UNP P41148
B	?	-	GLU	deletion	UNP P41148
B	?	-	GLU	deletion	UNP P41148
B	?	-	ALA	deletion	UNP P41148
B	?	-	ALA	deletion	UNP P41148
B	?	-	LYS	deletion	UNP P41148
B	?	-	GLU	deletion	UNP P41148
B	?	-	GLU	deletion	UNP P41148
B	?	-	LYS	deletion	UNP P41148
B	?	-	GLU	deletion	UNP P41148
B	?	-	ASP	deletion	UNP P41148
B	?	-	SER	deletion	UNP P41148
B	?	-	ASP	deletion	UNP P41148
B	?	-	ASP	deletion	UNP P41148
B	?	-	GLU	deletion	UNP P41148
B	?	-	ALA	deletion	UNP P41148

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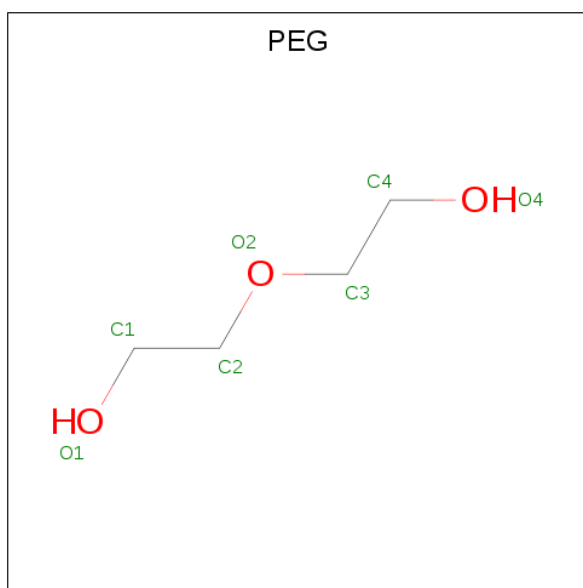
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ALA	deletion	UNP P41148
B	?	-	VAL	deletion	UNP P41148
B	?	-	GLU	deletion	UNP P41148
B	?	-	GLU	deletion	UNP P41148
B	?	-	GLU	deletion	UNP P41148
B	?	-	GLU	deletion	UNP P41148
B	?	-	GLU	deletion	UNP P41148
B	?	-	GLU	deletion	UNP P41148
B	?	-	LYS	deletion	UNP P41148
B	?	-	LYS	deletion	UNP P41148
B	?	-	PRO	deletion	UNP P41148
B	?	-	LYS	deletion	UNP P41148
B	?	-	THR	deletion	UNP P41148
B	324	GLY	LYS	linker	UNP P41148
B	325	GLY	LYS	linker	UNP P41148
B	326	GLY	VAL	linker	UNP P41148
B	327	GLY	GLU	linker	UNP P41148

- Molecule 2 is methyl 2-(2-{1-[(4-bromophenyl)methyl]-1H-imidazol-2-yl}ethyl)-3-chloro-4,6-dihydroxybenzoate (three-letter code: 7KY) (formula: C<sub>20</sub>H<sub>18</sub>BrClN<sub>2</sub>O<sub>4</sub>).



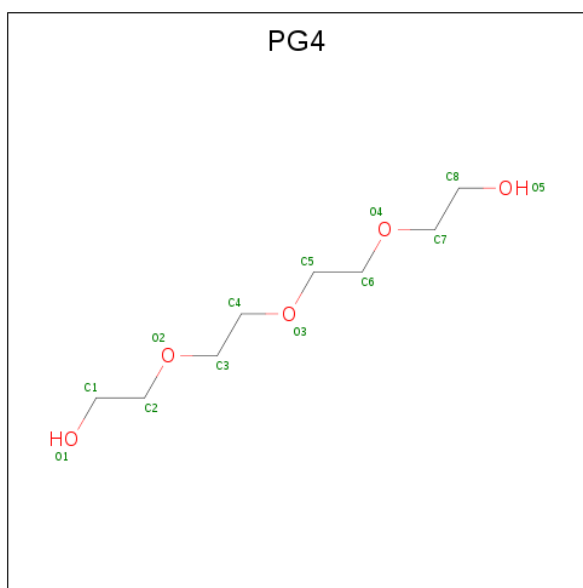
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	Br	C	Cl	N	O	7	0
			28	1	20	1	2	4		
2	B	1	Total	Br	C	Cl	N	O	7	0
			28	1	20	1	2	4		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



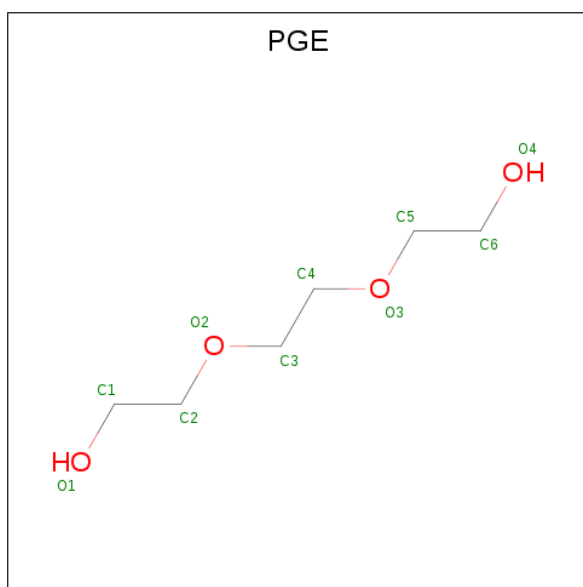
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



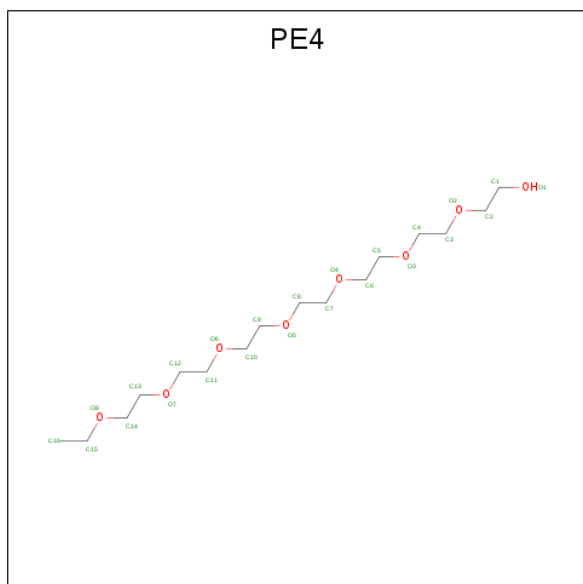
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: C<sub>16</sub>H<sub>34</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			24	16	8		

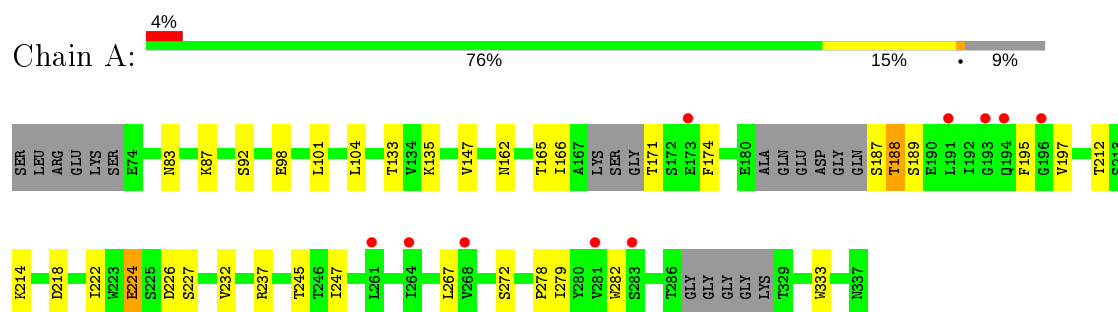
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	18	Total 18	O 18	0	0
7	B	19	Total 19	O 19	0	0

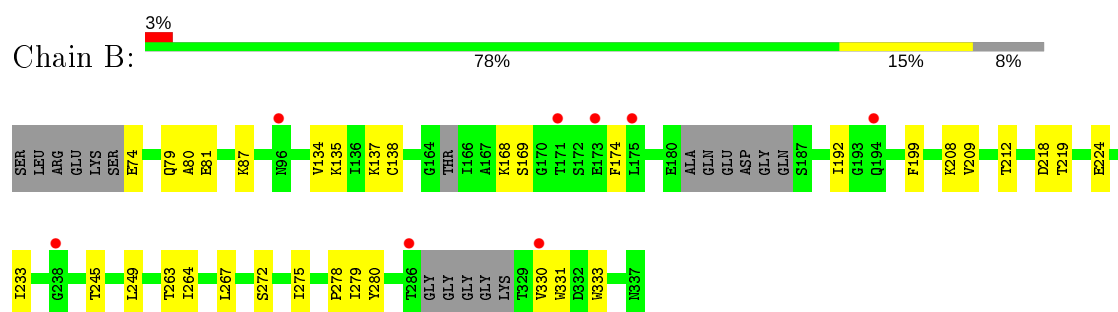
### 3 Residue-property plots [i](#)

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: Endoplasmic



#### • Molecule 1: Endoplasmic



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.24Å 84.42Å 95.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.74 – 2.71 47.74 – 2.71	Depositor EDS
% Data completeness (in resolution range)	97.4 (47.74-2.71) 97.4 (47.74-2.71)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.18 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.199 , 0.285 0.201 , 0.285	Depositor DCC
$R_{free}$ test set	1453 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.2	Xtriage
Anisotropy	0.672	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3454	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.39 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1536e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PE4, 7KY, PG4, PGE, PEG

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	0.47	0/1678	0.63	0/2262
1	B	0.48	0/1674	0.64	0/2252
All	All	0.47	0/3352	0.63	0/4514

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	A	1655	0	1628	22	0
1	B	1652	0	1613	23	0
2	A	28	0	0	1	0
2	B	28	0	0	1	0
3	A	7	0	10	2	0
4	B	13	0	18	3	0
5	B	10	0	14	2	0
6	B	24	0	34	2	0
7	A	18	0	0	2	0
7	B	19	0	0	1	0
All	All	3454	0	3317	49	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 7.

All (49) 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:237:ARG:HH22	3:A:402:PEG:H41	1.48	0.78
1:A:165:THR:OG1	1:A:166:ILE:N	2.16	0.74
1:A:166:ILE:HD11	1:A:195:PHE:HE2	1.53	0.73
3:A:402:PEG:O4	7:A:501:HOH:O	1.94	0.72
1:B:272:SER:HB2	1:B:279:ILE:HD12	1.72	0.71
1:B:87:LYS:HE3	6:B:404:PE4:H92	1.72	0.71
1:A:171:THR:N	7:A:502:HOH:O	2.23	0.71
1:B:208:LYS:NZ	1:B:224:GLU:OE2	2.25	0.69
1:B:79:GLN:NE2	1:B:81:GLU:OE2	2.27	0.68
1:A:226:ASP:O	1:A:227:SER:HB3	1.93	0.67
1:A:187:SER:OG	1:A:188:THR:N	2.33	0.62
1:A:135:LYS:HB3	1:A:333:TRP:CH2	2.35	0.61
1:A:135:LYS:HD2	1:A:333:TRP:CE2	2.37	0.60
5:B:403:PGE:O1	7:B:501:HOH:O	2.15	0.59
1:B:79:GLN:HG2	1:B:80:ALA:N	2.19	0.57
1:B:199:PHE:HB2	2:B:401:7KY:CL1	2.43	0.56
1:A:171:THR:O	1:A:174:PHE:HB3	2.06	0.55
1:B:137:LYS:NZ	4:B:402:PG4:H61	2.23	0.54
1:B:272:SER:HA	1:B:275:ILE:HD13	1.90	0.52
1:B:135:LYS:HD2	1:B:333:TRP:CE2	2.45	0.51
1:B:330:VAL:HG12	1:B:331:TRP:H	1.75	0.50
1:A:101:LEU:HD23	1:A:267:LEU:HB3	1.94	0.49
1:A:83:ASN:O	1:A:87:LYS:HG3	2.13	0.48
1:B:138:CYS:SG	1:B:264:ILE:HG12	2.53	0.48
4:B:402:PG4:H22	5:B:403:PGE:H2	1.95	0.48
1:A:224:GLU:O	1:A:224:GLU:HG3	2.15	0.47
1:A:133:THR:HG22	1:A:278:PRO:HG2	1.97	0.47
1:B:168:LYS:O	1:B:169:SER:OG	2.32	0.47
1:A:272:SER:HB2	1:A:279:ILE:HD12	1.98	0.46
1:A:162:ASN:HB3	2:A:401:7KY:CAS	2.46	0.45
1:B:137:LYS:HZ1	4:B:402:PG4:H61	1.81	0.45
1:B:209:VAL:HG22	1:B:249:LEU:HD22	1.98	0.45
1:A:214:LYS:NZ	1:A:218:ASP:O	2.41	0.44
1:B:74:GLU:CD	1:B:233:ILE:HG22	2.39	0.43
1:B:135:LYS:HB3	1:B:333:TRP:CH2	2.53	0.43
1:B:174:PHE:HZ	1:B:192:ILE:HD13	1.84	0.43
1:B:218:ASP:OD2	1:B:219:THR:N	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:VAL:HG12	1:B:331:TRP:N	2.34	0.43
1:B:263:THR:O	1:B:267:LEU:HD13	2.19	0.42
1:B:134:VAL:HB	1:B:279:ILE:HG23	2.01	0.42
1:B:278:PRO:HB2	1:B:280:TYR:CE2	2.55	0.42
6:B:404:PE4:H111	6:B:404:PE4:H92	1.93	0.42
1:A:92:SER:HB2	1:A:188:THR:HG21	2.02	0.41
1:A:282:TRP:HB2	1:A:333:TRP:CZ3	2.55	0.41
1:A:147:VAL:CG1	1:A:247:ILE:HB	2.51	0.41
1:A:222:ILE:O	1:A:232:VAL:HA	2.21	0.41
1:A:212:THR:O	1:A:245:THR:HA	2.20	0.41
1:A:104:LEU:HA	1:A:104:LEU:HD23	1.86	0.40
1:B:212:THR:O	1:B:245:THR:HA	2.22	0.40

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	A	205/233 (88%)	194 (95%)	10 (5%)	1 (0%)	29	54
1	B	205/233 (88%)	193 (94%)	12 (6%)	0	100	100
All	All	410/466 (88%)	387 (94%)	22 (5%)	1 (0%)	47	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	THR

### 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	183/205 (89%)	179 (98%)	4 (2%)	52	79
1	B	180/205 (88%)	180 (100%)	0	100	100
All	All	363/410 (88%)	359 (99%)	4 (1%)	73	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	GLU
1	A	189	SER
1	A	197	VAL
1	A	224	GLU

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

### 5.3.3 RNA [i](#)

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](#)

6 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	7KY	A	401	-	29,30,30	2.02	6 (20%)	35,42,42	1.04	1 (2%)
6	PE4	B	404	-	23,23,23	0.80	0	22,22,22	0.64	0
3	PEG	A	402	-	6,6,6	0.75	0	5,5,5	0.69	0
5	PGE	B	403	-	9,9,9	0.80	0	8,8,8	0.64	0
2	7KY	B	401	-	29,30,30	2.02	7 (24%)	35,42,42	1.30	6 (17%)
4	PG4	B	402	-	12,12,12	0.87	0	11,11,11	0.48	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
2	7KY	A	401	-	-	6/15/15/15	0/3/3/3
6	PE4	B	404	-	-	10/21/21/21	-
3	PEG	A	402	-	-	4/4/4/4	-
5	PGE	B	403	-	-	4/7/7/7	-
2	7KY	B	401	-	-	7/15/15/15	0/3/3/3
4	PG4	B	402	-	-	5/10/10/10	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	7KY	CAL-CAF	-6.84	1.42	1.52
2	B	401	7KY	CAL-CAF	-6.68	1.42	1.52
2	A	401	7KY	CAS-CAT	-5.32	1.38	1.51
2	B	401	7KY	CAS-CAT	-4.91	1.39	1.51
2	A	401	7KY	CAE-CAJ	-3.84	1.41	1.50
2	B	401	7KY	CAE-CAJ	-3.62	1.42	1.50
2	B	401	7KY	CAP-NAO	-3.14	1.33	1.38
2	A	401	7KY	CAP-NAO	-3.02	1.33	1.38
2	B	401	7KY	CAA-CL1	-2.77	1.66	1.72
2	A	401	7KY	OBA-CAJ	2.74	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	7KY	OBA-CAJ	2.61	1.39	1.33
2	B	401	7KY	CAM-CAN	2.38	1.56	1.50
2	A	401	7KY	CAM-CAN	2.20	1.55	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	7KY	CAL-CAF-CAA	-2.88	116.34	121.77
2	B	401	7KY	CAB-CAC-CAD	-2.77	117.38	120.14
2	B	401	7KY	CAL-CAF-CAE	2.59	125.42	120.65
2	B	401	7KY	CAC-CAD-CAE	2.54	123.88	120.93
2	B	401	7KY	CAC-CAB-CAA	2.16	121.07	119.20
2	B	401	7KY	OAI-CAD-CAE	-2.12	117.18	121.14
2	A	401	7KY	OAI-CAD-CAE	-2.00	117.40	121.14

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	7KY	OAK-CAJ-OBA-CBB
2	A	401	7KY	CAE-CAJ-OBA-CBB
2	B	401	7KY	CAF-CAL-CAM-CAN
2	B	401	7KY	CAT-CAS-NAO-CAP
6	B	404	PE4	C9-C10-O6-C11
6	B	404	PE4	O6-C10-C9-O5
4	B	402	PG4	O3-C5-C6-O4
6	B	404	PE4	O7-C13-C14-O8
6	B	404	PE4	O2-C3-C4-O3
4	B	402	PG4	O1-C1-C2-O2
2	A	401	7KY	CAF-CAL-CAM-CAN
6	B	404	PE4	O3-C5-C6-O4
4	B	402	PG4	O4-C7-C8-O5
5	B	403	PGE	O1-C1-C2-O2
3	A	402	PEG	O1-C1-C2-O2
3	A	402	PEG	O2-C3-C4-O4
6	B	404	PE4	O1-C1-C2-O2
5	B	403	PGE	C6-C5-O3-C4
3	A	402	PEG	C1-C2-O2-C3
5	B	403	PGE	O3-C5-C6-O4
6	B	404	PE4	C11-C12-O7-C13
6	B	404	PE4	C8-C7-O4-C6
6	B	404	PE4	C7-C8-O5-C9

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Mol	Chain	Res	Type	Atoms
2	B	401	7KY	CAD-CAE-CAJ-OAK
5	B	403	PGE	C4-C3-O2-C2
3	A	402	PEG	C4-C3-O2-C2
6	B	404	PE4	C5-C6-O4-C7
4	B	402	PG4	C3-C4-O3-C5
2	A	401	7KY	NAO-CAS-CAT-CAU
2	A	401	7KY	NAO-CAS-CAT-CAY
2	B	401	7KY	CAD-CAE-CAJ-OBA
2	B	401	7KY	CAF-CAE-CAJ-OAK
2	A	401	7KY	CAD-CAE-CAJ-OAK
4	B	402	PG4	C5-C6-O4-C7
2	B	401	7KY	NAO-CAS-CAT-CAY
2	B	401	7KY	NAO-CAS-CAT-CAU

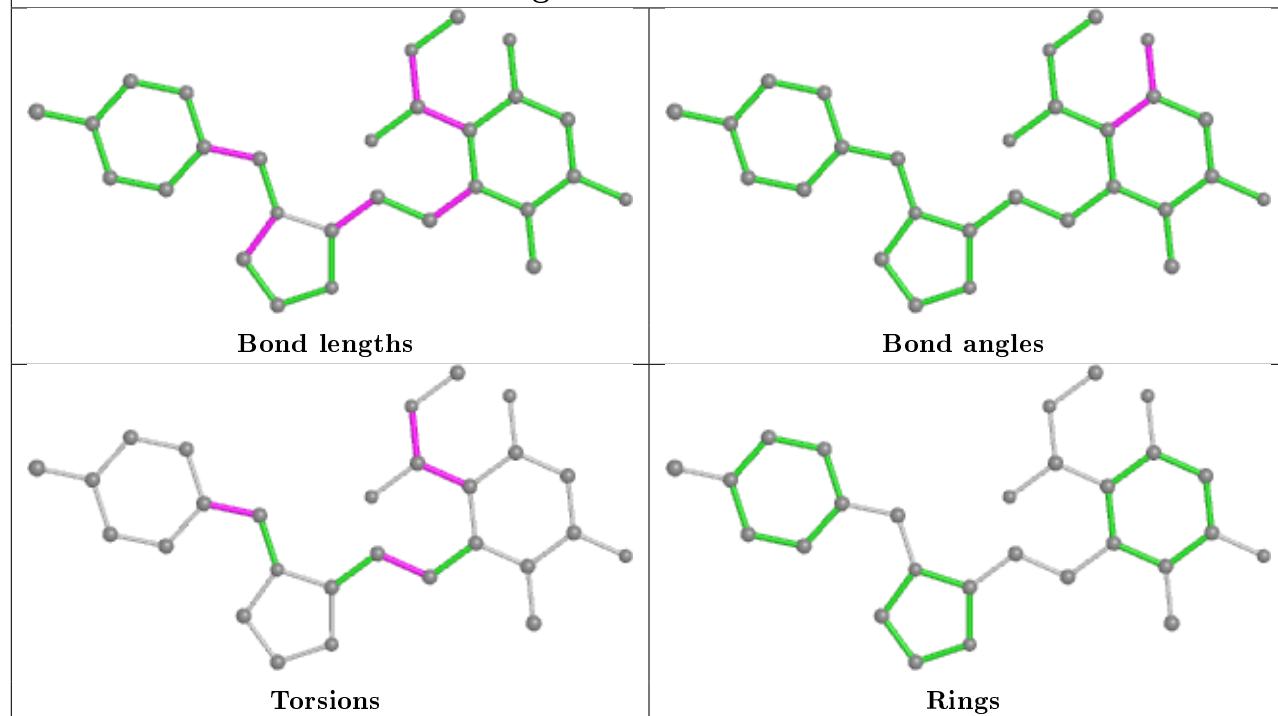
There are no ring outliers.

6 monomers are involved in 10 short contacts:

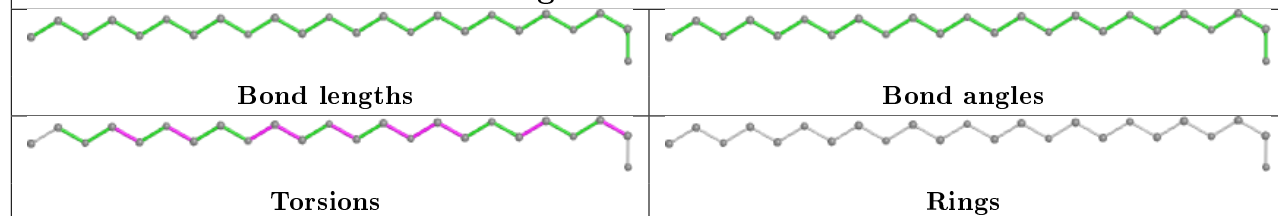
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	7KY	1	0
6	B	404	PE4	2	0
3	A	402	PEG	2	0
5	B	403	PGE	2	0
2	B	401	7KY	1	0
4	B	402	PG4	3	0

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.

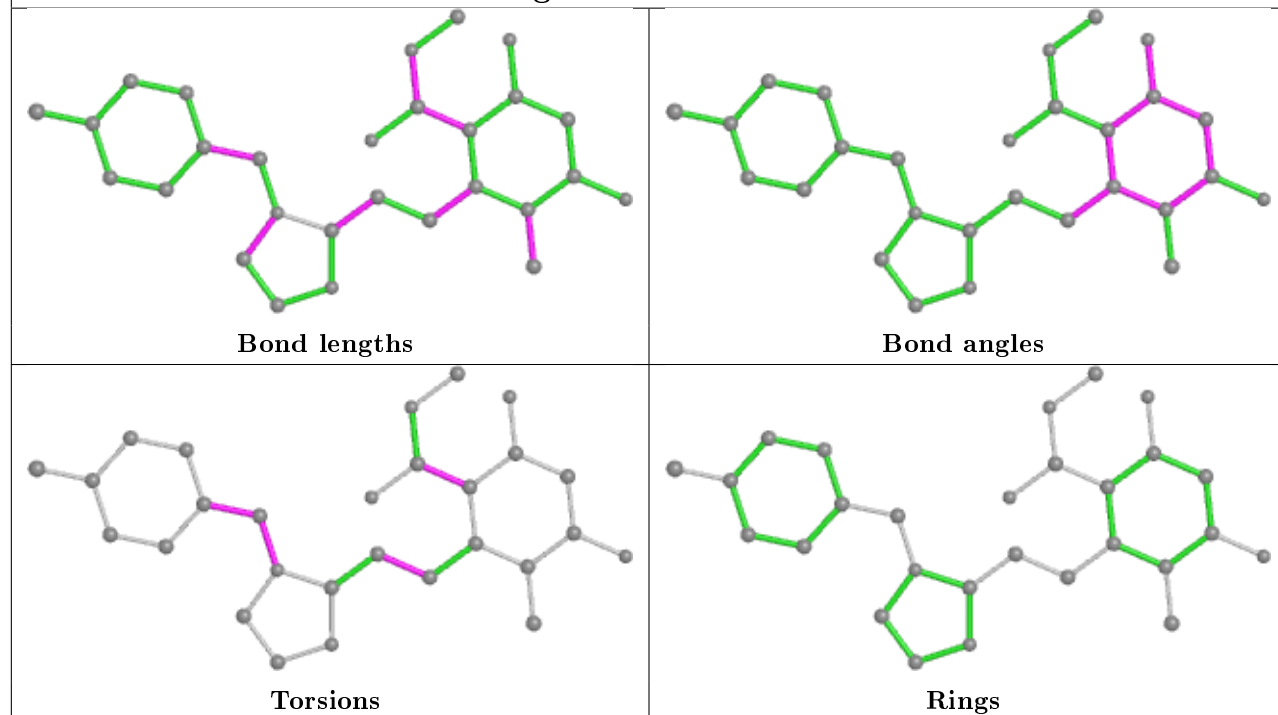
## Ligand 7KY A 401



## Ligand PE4 B 404



## Ligand 7KY B 401



## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	213/233 (91%)	0.19	10 (4%) 31 30	24, 45, 81, 106	0
1	B	215/233 (92%)	0.19	8 (3%) 41 41	25, 44, 83, 106	0
All	All	428/466 (91%)	0.19	18 (4%) 36 35	24, 45, 83, 106	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	175	LEU	4.6
1	B	286	THR	3.9
1	A	261	LEU	3.4
1	A	194	GLN	3.0
1	B	194	GLN	2.9
1	B	173	GLU	2.8
1	A	264	ILE	2.8
1	A	281	VAL	2.7
1	A	191	LEU	2.6
1	A	173	GLU	2.6
1	A	193	GLY	2.5
1	B	330	VAL	2.5
1	A	196	GLY	2.3
1	A	283	SER	2.3
1	B	96	ASN	2.2
1	A	268	VAL	2.2
1	B	171	THR	2.1
1	B	238	GLY	2.0

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

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

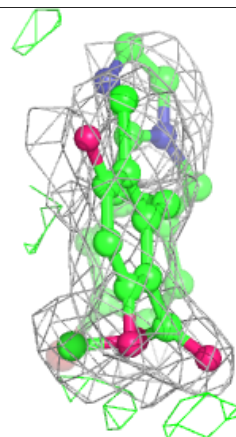
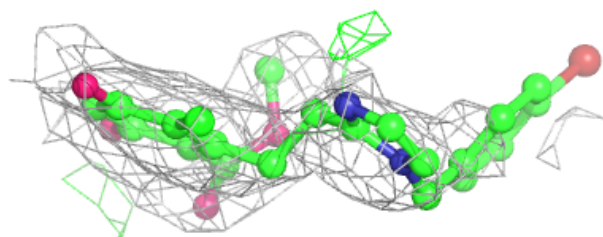
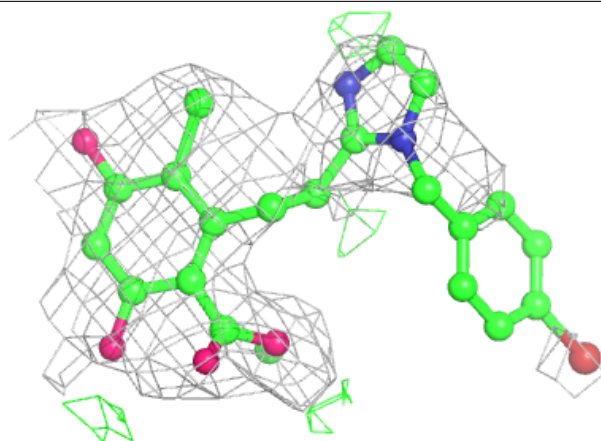
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	7KY	A	401	28/28	0.87	0.28	54,82,87,173	7
2	7KY	B	401	28/28	0.88	0.26	43,76,90,133	7
5	PGE	B	403	10/10	0.89	0.22	37,50,56,59	0
6	PE4	B	404	24/24	0.90	0.25	24,45,79,82	0
4	PG4	B	402	13/13	0.94	0.15	45,52,76,76	0
3	PEG	A	402	7/7	0.97	0.14	29,54,62,64	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.

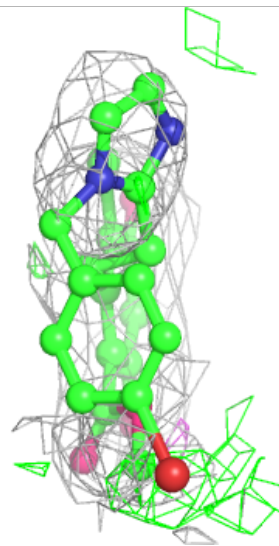
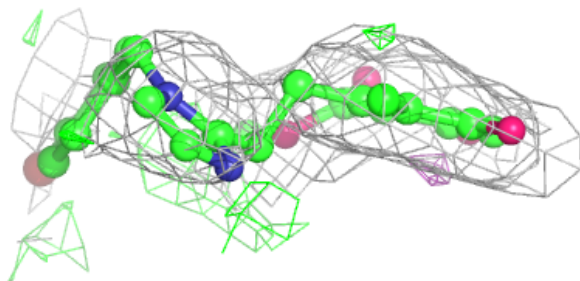
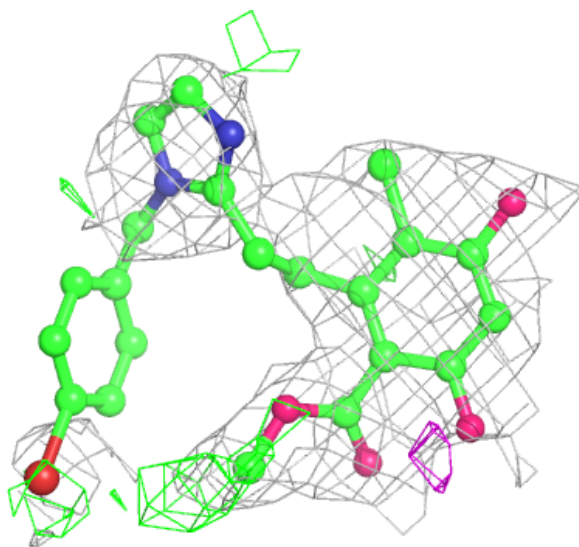
**Electron density around 7KY A 401:**

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



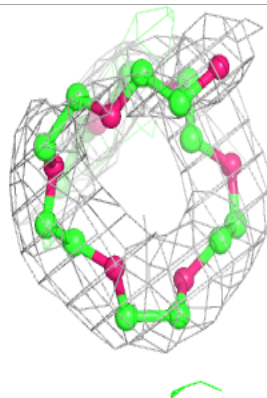
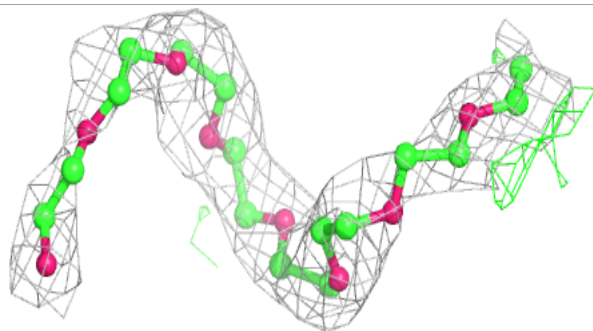
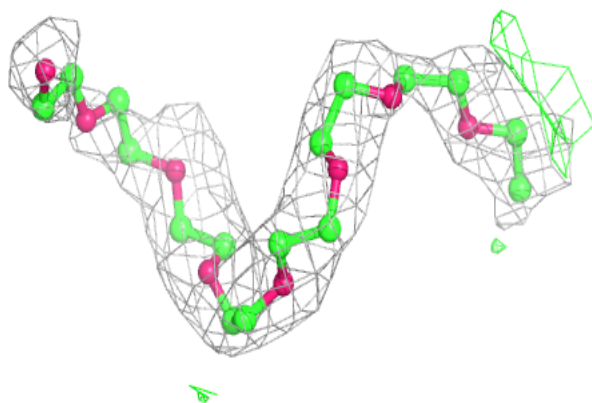
**Electron density around 7KY B 401:**

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



**Electron density around PE4 B 404:**

$2mF_o-DF_c$  (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.