



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 04:40 pm BST

PDB ID : 5LGR  
Title : Crystal structure of mouse CARM1 in complex with ligand P1C3u  
Authors : Marechal, N.; Troffer-Charlier, N.; Cura, V.; Bonnefond, L.; Cavarelli, J.  
Deposited on : 2016-07-08  
Resolution : 2.00 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

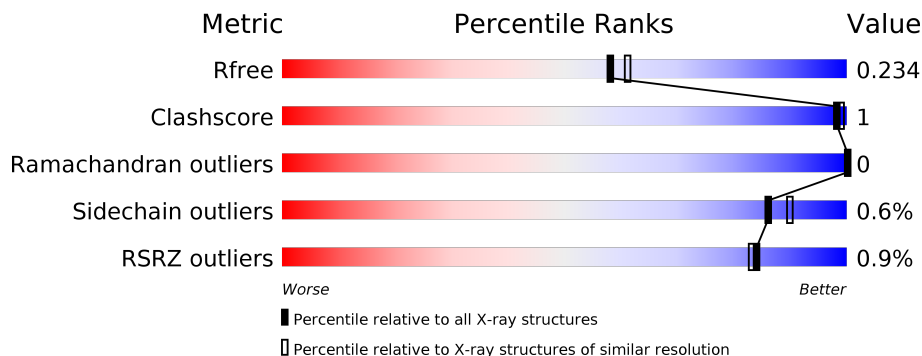
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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.



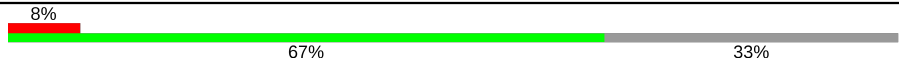
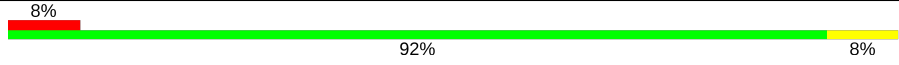
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	361	94% (5% not modelled)
1	B	361	93% (5% not modelled)
1	C	361	94% (5% not modelled)
1	D	361	92% (5% not modelled)
2	E	12	8% poor fit, 92% quality, 8% not modelled
2	F	12	100% quality

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Mol	Chain	Length	Quality of chain
2	G	12	 <p>8% 67% 33%</p>
2	H	12	 <p>8% 92% 8%</p>

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 23651 atoms, of which 11340 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 Histone-arginine methyltransferase CARM1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	344	Total	C	H	N	O	S	0	5	0
			5485	1785	2718	459	509	14			
1	B	343	Total	C	H	N	O	S	0	0	0
			5460	1778	2705	457	506	14			
1	C	344	Total	C	H	N	O	S	0	6	0
			5496	1791	2722	459	510	14			
1	D	343	Total	C	H	N	O	S	0	3	0
			5481	1787	2714	458	508	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	GLY	-	expression tag	UNP Q9WVG6
A	128	HIS	-	expression tag	UNP Q9WVG6
A	129	MET	-	expression tag	UNP Q9WVG6
B	127	GLY	-	expression tag	UNP Q9WVG6
B	128	HIS	-	expression tag	UNP Q9WVG6
B	129	MET	-	expression tag	UNP Q9WVG6
C	127	GLY	-	expression tag	UNP Q9WVG6
C	128	HIS	-	expression tag	UNP Q9WVG6
C	129	MET	-	expression tag	UNP Q9WVG6
D	127	GLY	-	expression tag	UNP Q9WVG6
D	128	HIS	-	expression tag	UNP Q9WVG6
D	129	MET	-	expression tag	UNP Q9WVG6

- Molecule 2 is a protein called Polyadenylate-binding protein 1.

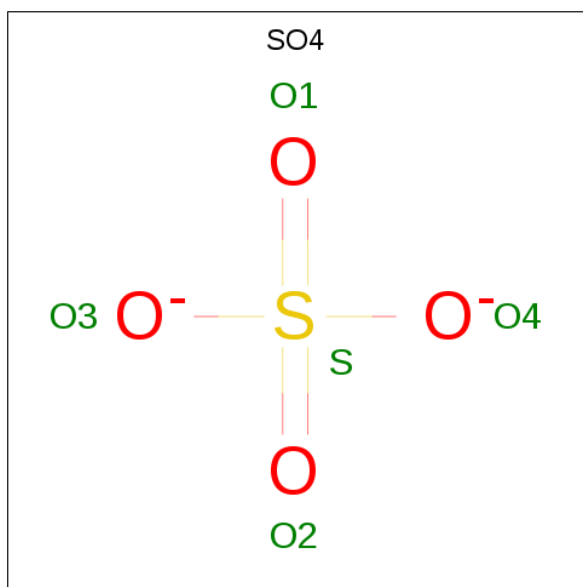
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	E	11	Total	C	H	N	O	S	0	0	0
			155	47	78	16	13	1			
2	F	12	Total	C	H	N	O	S	0	0	0
			175	56	87	17	14	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	8	Total	C	H	N	O	0	0	0
			107	33	55	11	8			
2	H	12	Total	C	H	N	O	S	0	0
			175	56	87	17	14	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



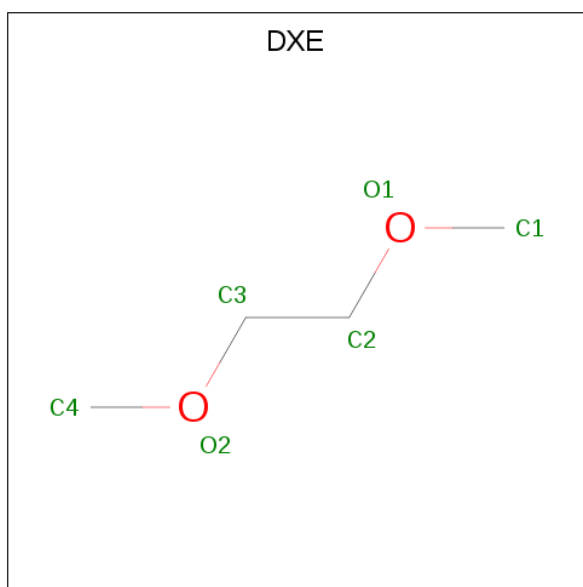
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



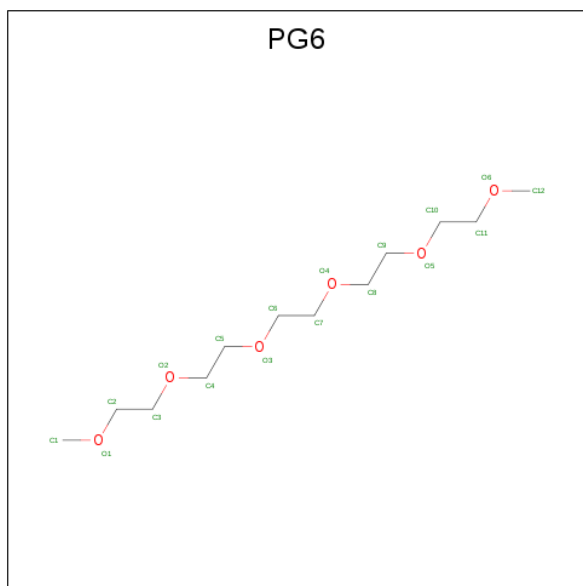
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	10	2	6	2	0	0
4	A	1	10	2	6	2	0	0
4	B	1	10	2	6	2	0	0
4	C	1	10	2	6	2	0	0
4	D	1	10	2	6	2	0	0
4	E	1	10	2	6	2	0	0

- Molecule 5 is 1,2-DIMETHOXYETHANE (three-letter code: DXE) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>).



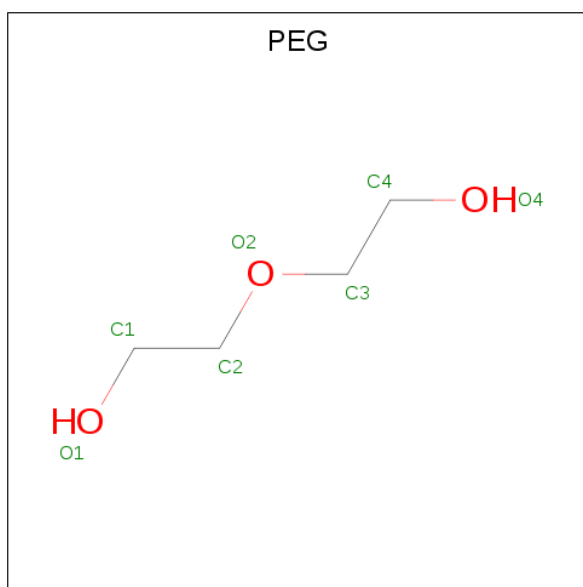
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	A	1	16	4	10	2	0	0

- Molecule 6 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANE (three-letter code: PG6) (formula:  $C_{12}H_{26}O_6$ ).



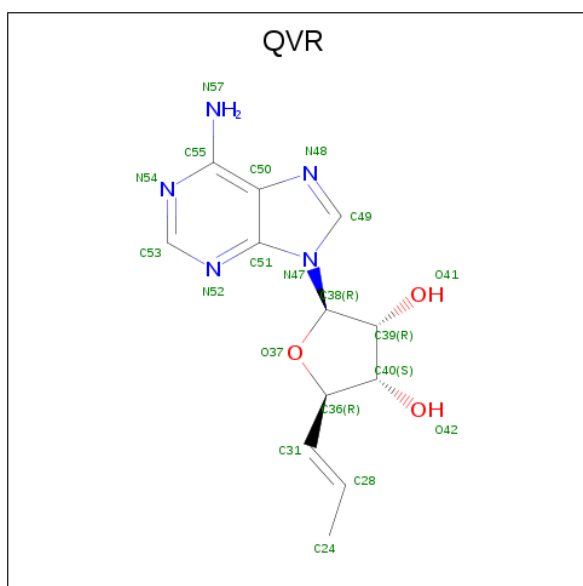
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
6	B	1	44	12	26	6	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
7	C	1	17	4	10	3	0	0

- Molecule 8 is (2 {R},3 {R},4 {S},5 {R})-2-(6-aminopurin-9-yl)-5-[( {E})-prop-1-enyl]oxolan e-3,4-diol (three-letter code: QVR) (formula: C<sub>12</sub>H<sub>15</sub>N<sub>5</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
8	E	1	34	12	14	5	3	0	0
8	F	1	34	12	14	5	3	0	0

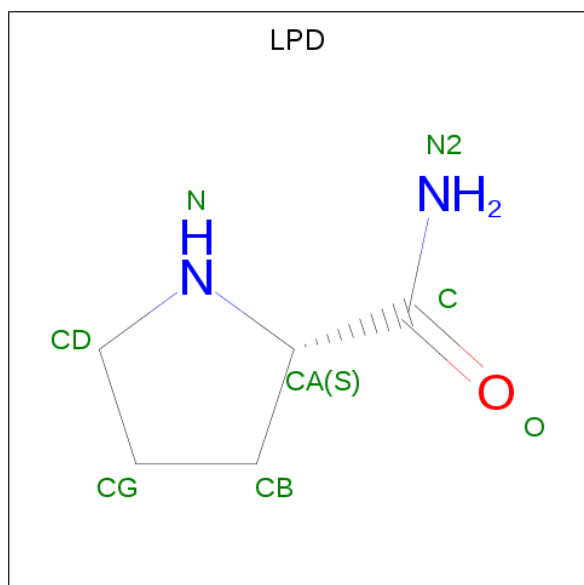
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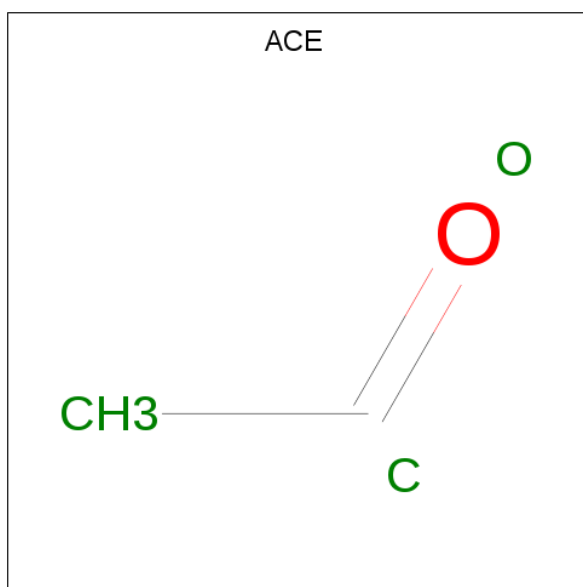
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	G	1	Total	C	H	N	O	0	0
			34	12	14	5	3		
8	H	1	Total	C	H	N	O	0	0
			34	12	14	5	3		

- Molecule 9 is L-PROLINAMIDE (three-letter code: LPD) (formula: C<sub>5</sub>H<sub>10</sub>N<sub>2</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	E	1	Total	C	H	N	O	0	0
			17	5	9	2	1		
9	F	1	Total	C	H	N	O	0	0
			17	5	9	2	1		
9	G	1	Total	C	H	N	O	0	0
			17	5	9	2	1		
9	H	1	Total	C	H	N	O	0	0
			17	5	9	2	1		

- Molecule 10 is ACETYL GROUP (three-letter code: ACE) (formula: C<sub>2</sub>H<sub>4</sub>O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	F	1	Total C O 3 2 1	0	0
10	H	1	Total C O 3 2 1	0	0

- Molecule 11 is water.

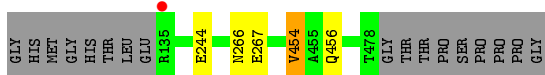
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	218	Total O 218 218	0	0
11	B	218	Total O 218 218	0	0
11	C	163	Total O 163 163	0	0
11	D	143	Total O 143 143	0	0
11	E	6	Total O 6 6	0	0
11	F	9	Total O 9 9	0	0
11	G	2	Total O 2 2	0	0
11	H	6	Total O 6 6	0	0

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

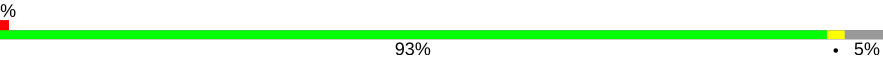
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Histone-arginine methyltransferase CARM1

Chain A: 



- Molecule 1: Histone-arginine methyltransferase CARM1

Chain B: 



- Molecule 1: Histone-arginine methyltransferase CARM1

Chain C: 

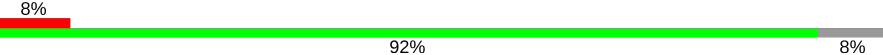


- Molecule 1: Histone-arginine methyltransferase CARM1

Chain D: 



- Molecule 2: Polyadenylate-binding protein 1

Chain E: 



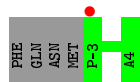
- Molecule 2: Polyadenylate-binding protein 1

Chain F:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Polyadenylate-binding protein 1

Chain G:  8% 67% 33%



- Molecule 2: Polyadenylate-binding protein 1

Chain H:  8% 92% 8%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.83Å 98.54Å 208.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.05 – 2.00 46.05 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.05-2.00) 99.9 (46.05-2.00)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 2.00Å)	Xtrriage
Refinement program	PHENIX dev_2386	Depositor
R, $R_{free}$	0.192 , 0.234 0.192 , 0.234	Depositor DCC
$R_{free}$ test set	5220 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.7	Xtrriage
Anisotropy	0.557	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 44.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	23651	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.94 % 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 2.5407e-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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: LPD, ACE, EDO, PG6, SO4, DXE, PEG, QVR

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	0.26	0/2840	0.47	1/3848 (0.0%)
1	B	0.25	0/2825	0.45	1/3827 (0.0%)
1	C	0.25	0/2851	0.44	0/3862
1	D	0.25	0/2837	0.43	0/3842
2	E	0.38	0/78	0.48	0/105
2	F	0.33	0/90	0.56	0/121
2	G	0.37	0/53	0.57	0/71
2	H	0.35	0/90	0.63	0/121
All	All	0.25	0/11664	0.45	2/15797 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	454	VAL	CG1-CB-CG2	6.94	122.00	110.90
1	B	260	MET	C-N-CA	5.15	133.12	122.30

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	2767	2718	2707	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2755	2705	2705	2	0
1	C	2774	2722	2704	2	0
1	D	2767	2714	2703	6	0
2	E	77	78	80	0	0
2	F	88	87	87	0	0
2	G	52	55	57	0	0
2	H	88	87	87	0	0
3	A	5	0	0	0	0
4	A	8	12	12	0	0
4	B	4	6	6	1	0
4	C	4	6	6	0	0
4	D	4	6	6	0	0
4	E	4	6	6	0	0
5	A	6	10	10	0	0
6	B	18	26	26	0	0
7	C	7	10	10	0	0
8	E	20	14	0	0	0
8	F	20	14	0	0	0
8	G	20	14	0	0	0
8	H	20	14	0	0	0
9	E	8	9	9	0	0
9	F	8	9	9	0	0
9	G	8	9	9	0	0
9	H	8	9	9	0	0
10	F	3	0	3	0	0
10	H	3	0	3	0	0
11	A	218	0	0	1	1
11	B	218	0	0	2	0
11	C	163	0	0	0	2
11	D	143	0	0	1	1
11	E	6	0	0	0	0
11	F	9	0	0	0	0
11	G	2	0	0	0	0
11	H	6	0	0	0	0
All	All	12311	11340	11254	13	3

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 1.

All (13) 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)
4:B:501:EDO:O1	11:B:601:HOH:O	2.14	0.65
1:A:456:GLN:OE1	11:A:601:HOH:O	2.15	0.64
1:C:149:GLN:OE1	1:D:149:GLN:NE2	2.32	0.62
1:D:306:GLU:OE2	11:D:601:HOH:O	2.19	0.51
1:D:459:GLN:OE1	1:D:459:GLN:N	2.48	0.47
1:B:266:ASN:O	1:B:267:GLU:HB2	2.15	0.46
1:D:266:ASN:O	1:D:267:GLU:HB2	2.14	0.46
1:D:204:ALA:O	1:D:235:ARG:NH1	2.48	0.46
1:D:169:ARG:NE	1:D:258:GLU:OE1	2.35	0.45
1:A:266:ASN:O	1:A:267:GLU:HB2	2.16	0.45
1:C:266:ASN:O	1:C:267:GLU:HB2	2.18	0.43
1:B:450:ASP:OD2	11:B:602:HOH:O	2.22	0.41
1:A:244:GLU:OE1	1:A:244:GLU:N	2.50	0.40

All (3) 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)
11:C:675:HOH:O	11:C:675:HOH:O[2_655]	2.09	0.11
11:A:690:HOH:O	11:A:790:HOH:O[2_655]	2.15	0.05
11:C:727:HOH:O	11:D:719:HOH:O[2_655]	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	343/361 (95%)	333 (97%)	10 (3%)	0	100	100
1	B	341/361 (94%)	329 (96%)	12 (4%)	0	100	100
1	C	343/361 (95%)	332 (97%)	11 (3%)	0	100	100
1	D	341/361 (94%)	331 (97%)	10 (3%)	0	100	100
2	E	9/12 (75%)	9 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	10/12 (83%)	9 (90%)	1 (10%)	0	100	100
2	G	6/12 (50%)	6 (100%)	0	0	100	100
2	H	10/12 (83%)	10 (100%)	0	0	100	100
All	All	1403/1492 (94%)	1359 (97%)	44 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	301/313 (96%)	300 (100%)	1 (0%)	92	95
1	B	299/313 (96%)	296 (99%)	3 (1%)	76	81
1	C	302/313 (96%)	301 (100%)	1 (0%)	92	95
1	D	300/313 (96%)	299 (100%)	1 (0%)	92	95
2	E	7/8 (88%)	7 (100%)	0	100	100
2	F	8/8 (100%)	8 (100%)	0	100	100
2	G	4/8 (50%)	4 (100%)	0	100	100
2	H	8/8 (100%)	7 (88%)	1 (12%)	4	2
All	All	1229/1284 (96%)	1222 (99%)	7 (1%)	86	90

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	454	VAL
1	B	169	ARG
1	B	308	PHE
1	B	328	ARG
1	C	467	LEU
1	D	441	LEU
2	H	1	ARG

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](#)

20 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
9	LPD	G	101	2	8,8,8	0.27	0	10,10,10	0.47	0
4	EDO	C	501	-	3,3,3	0.48	0	2,2,2	0.35	0
8	QVR	E	101	2	19,22,22	0.61	0	19,32,32	0.72	1 (5%)
9	LPD	F	103	2	8,8,8	0.29	0	10,10,10	0.39	0
6	PG6	B	502	-	17,17,17	0.51	0	16,16,16	0.40	0
4	EDO	D	501	-	3,3,3	0.48	0	2,2,2	0.34	0
10	ACE	F	101	2	1,2,2	0.82	0	1,1,1	0.24	0
7	PEG	C	502	-	6,6,6	0.49	0	5,5,5	0.44	0
8	QVR	G	102	2	19,22,22	0.63	0	19,32,32	0.73	1 (5%)
4	EDO	E	103	-	3,3,3	0.48	0	2,2,2	0.33	0
8	QVR	F	102	2	19,22,22	0.62	0	19,32,32	0.72	1 (5%)
4	EDO	A	503	-	3,3,3	0.48	0	2,2,2	0.34	0
4	EDO	B	501	-	3,3,3	0.47	0	2,2,2	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	LPD	E	102	2	8,8,8	0.29	0	10,10,10	0.28	0
5	DXE	A	504	-	5,5,5	0.44	0	4,4,4	0.22	0
10	ACE	H	101	2	1,2,2	0.79	0	1,1,1	0.28	0
9	LPD	H	103	2	8,8,8	0.29	0	10,10,10	0.41	0
3	SO4	A	501	-	4,4,4	0.14	0	6,6,6	0.07	0
4	EDO	A	502	-	3,3,3	0.47	0	2,2,2	0.33	0
8	QVR	H	102	2	19,22,22	0.62	0	19,32,32	0.72	1 (5%)

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
9	LPD	G	101	2	-	1/4/11/11	0/1/1/1
4	EDO	C	501	-	-	0/1/1/1	-
8	QVR	E	101	2	-	0/3/23/23	0/3/3/3
9	LPD	F	103	2	-	0/4/11/11	0/1/1/1
6	PG6	B	502	-	-	7/15/15/15	-
4	EDO	D	501	-	-	0/1/1/1	-
4	EDO	E	103	-	-	0/1/1/1	-
7	PEG	C	502	-	-	2/4/4/4	-
8	QVR	G	102	2	-	0/3/23/23	0/3/3/3
4	EDO	A	503	-	-	0/1/1/1	-
8	QVR	F	102	2	-	0/3/23/23	0/3/3/3
4	EDO	B	501	-	-	0/1/1/1	-
9	LPD	E	102	2	-	2/4/11/11	0/1/1/1
5	DXE	A	504	-	-	1/3/3/3	-
9	LPD	H	103	2	-	0/4/11/11	0/1/1/1
4	EDO	A	502	-	-	0/1/1/1	-
8	QVR	H	102	2	-	0/3/23/23	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	102	QVR	C50-C55-N57	2.37	123.96	120.35
8	F	102	QVR	C50-C55-N57	2.35	123.93	120.35
8	H	102	QVR	C50-C55-N57	2.33	123.89	120.35
8	E	101	QVR	C50-C55-N57	2.28	123.82	120.35

There are no chirality outliers.

All (13) torsion outliers are listed below:

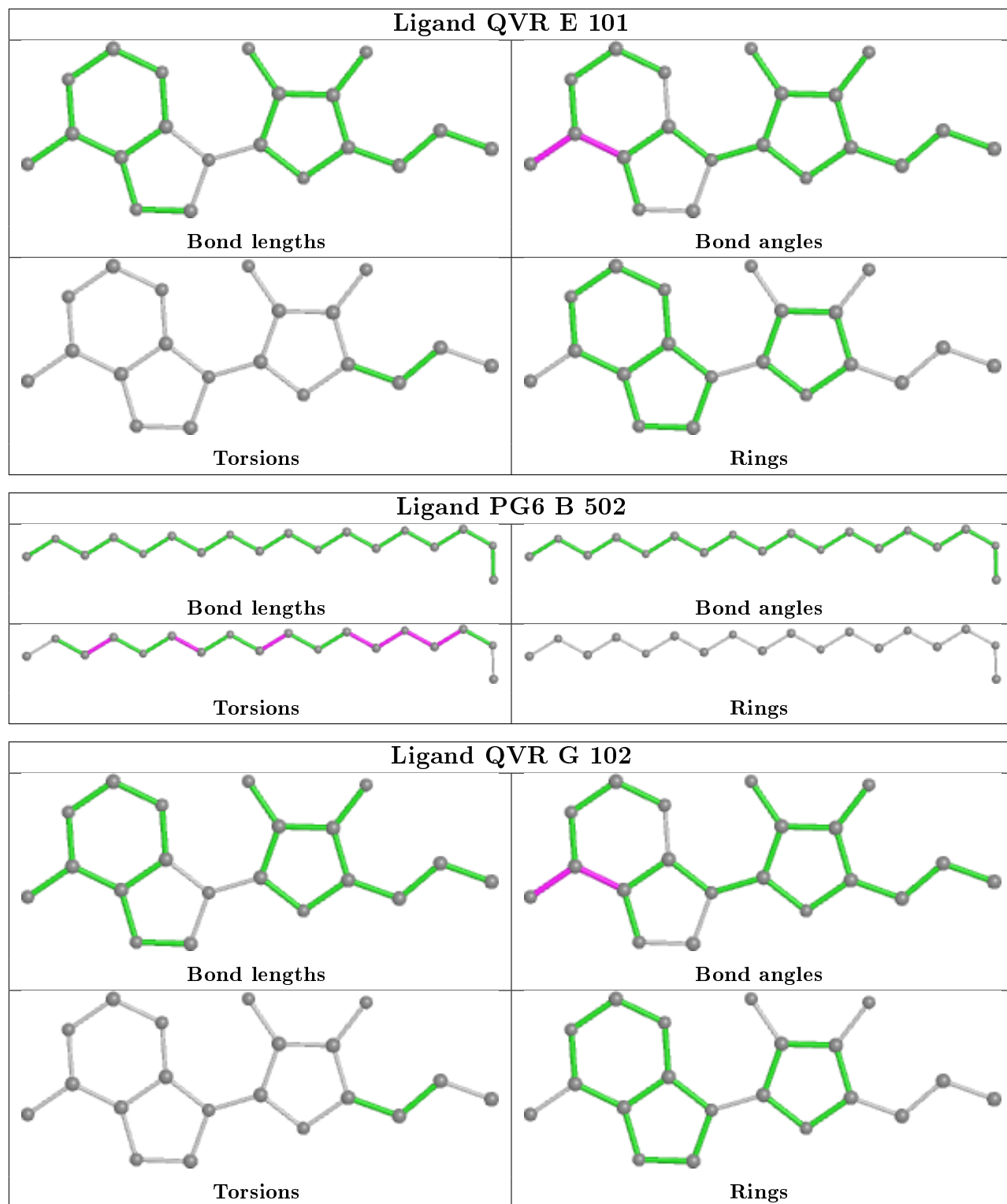
Mol	Chain	Res	Type	Atoms
6	B	502	PG6	O4-C8-C9-O5
7	C	502	PEG	O2-C3-C4-O4
7	C	502	PEG	O1-C1-C2-O2
6	B	502	PG6	C2-C3-O2-C4
6	B	502	PG6	O1-C2-C3-O2
6	B	502	PG6	O3-C6-C7-O4
5	A	504	DXE	O1-C2-C3-O2
6	B	502	PG6	O5-C10-C11-O6
6	B	502	PG6	C5-C4-O2-C3
6	B	502	PG6	O2-C4-C5-O3
9	G	101	LPD	O-C-CA-CB
9	E	102	LPD	O-C-CA-CB
9	E	102	LPD	N2-C-CA-CB

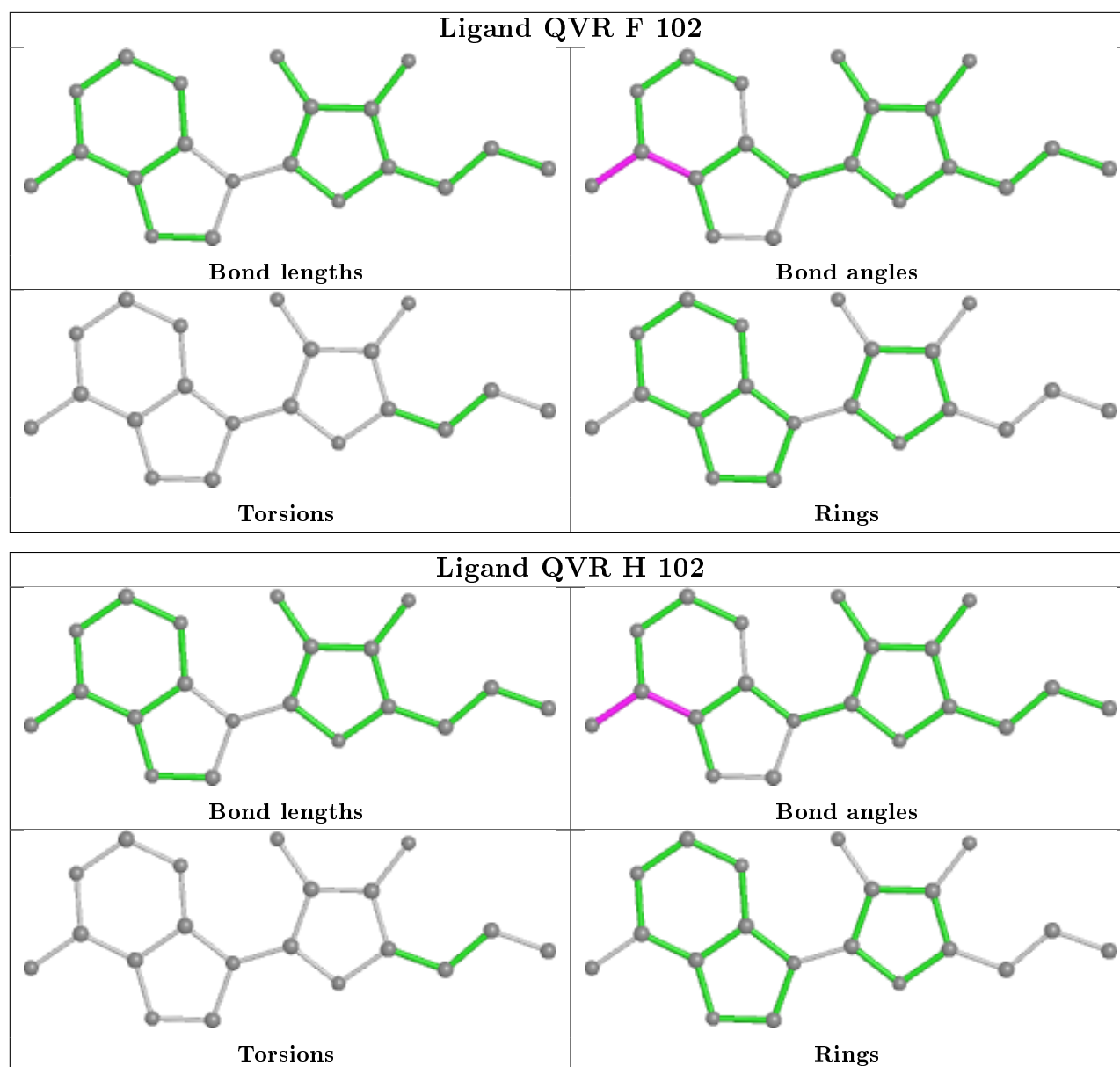
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	EDO	1	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	344/361 (95%)	-0.37	1 (0%) 94 93	17, 29, 48, 84	1 (0%)
1	B	343/361 (95%)	-0.34	2 (0%) 89 88	19, 31, 51, 90	0
1	C	344/361 (95%)	-0.21	3 (0%) 84 83	26, 43, 65, 96	0
1	D	343/361 (95%)	-0.21	4 (1%) 79 78	33, 41, 58, 80	0
2	E	11/12 (91%)	0.41	1 (9%) 9 8	27, 31, 65, 85	0
2	F	12/12 (100%)	0.22	0 100 100	28, 36, 49, 58	0
2	G	8/12 (66%)	0.80	1 (12%) 3 3	34, 43, 60, 67	0
2	H	12/12 (100%)	0.48	1 (8%) 11 10	36, 50, 84, 97	0
All	All	1417/1492 (94%)	-0.26	13 (0%) 84 83	17, 37, 59, 97	1 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	477[A]	TYR	3.8
2	G	-3	PRO	3.6
1	D	347	ARG	3.4
1	D	346	ILE	3.3
1	C	135	ARG	3.2
1	B	135	ARG	3.1
1	B	346	ILE	3.1
2	H	-4	MET	3.0
2	E	-6	GLN	3.0
1	D	477[A]	TYR	2.9
1	D	135	ARG	2.9
1	A	135	ARG	2.8
1	C	283	SER	2.6

## 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 [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [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.

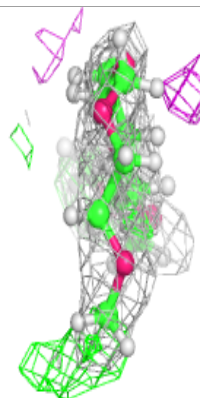
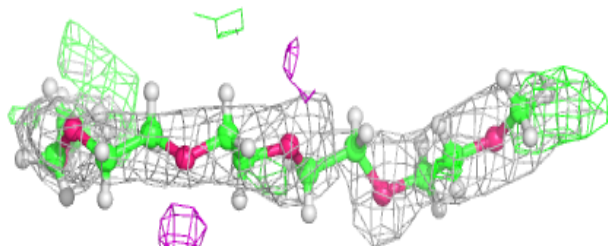
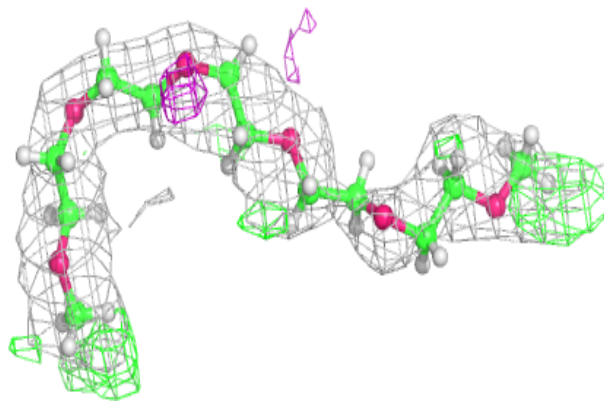
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	PG6	B	502	18/18	0.65	0.19	55,71,93,95	0
7	PEG	C	502	7/7	0.66	0.15	52,63,73,73	0
4	EDO	D	501	4/4	0.80	0.11	42,50,51,51	0
9	LPD	H	103	8/8	0.84	0.19	23,29,37,37	0
9	LPD	F	103	8/8	0.84	0.14	23,28,37,37	0
5	DXE	A	504	6/6	0.85	0.13	45,54,65,65	0
4	EDO	A	502	4/4	0.86	0.16	40,48,52,53	0
9	LPD	G	101	8/8	0.86	0.19	25,30,38,38	0
4	EDO	C	501	4/4	0.87	0.18	68,81,83,84	0
4	EDO	E	103	4/4	0.89	0.16	60,72,73,74	0
3	SO4	A	501	5/5	0.89	0.16	106,106,107,107	0
9	LPD	E	102	8/8	0.91	0.12	24,27,33,33	0
4	EDO	B	501	4/4	0.92	0.08	44,53,56,58	0
4	EDO	A	503	4/4	0.93	0.10	52,62,63,64	0
8	QVR	H	102	20/20	0.95	0.09	28,36,45,46	0
10	ACE	H	101	3/3	0.95	0.13	61,61,61,62	0
8	QVR	E	101	20/20	0.95	0.10	22,25,31,31	0
8	QVR	F	102	20/20	0.96	0.13	20,26,32,32	0
8	QVR	G	102	20/20	0.96	0.07	28,33,40,41	0
10	ACE	F	101	3/3	0.96	0.11	41,41,42,42	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.

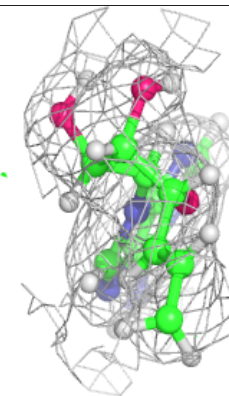
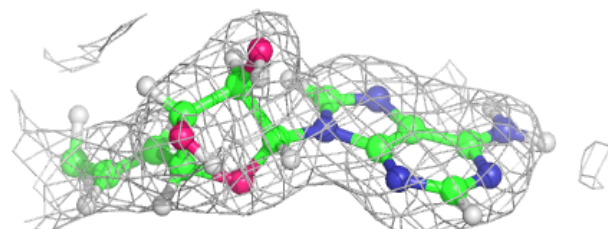
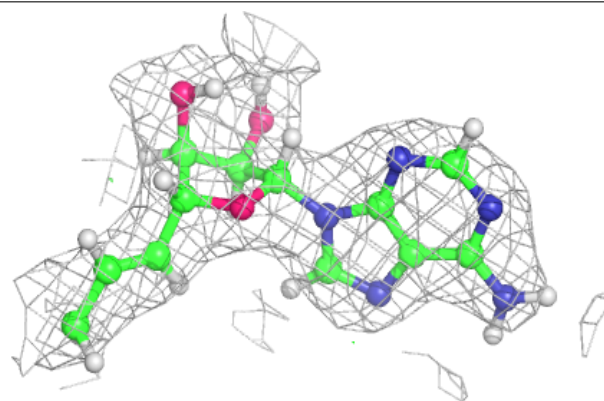


**Electron density around PG6 B 502:**

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

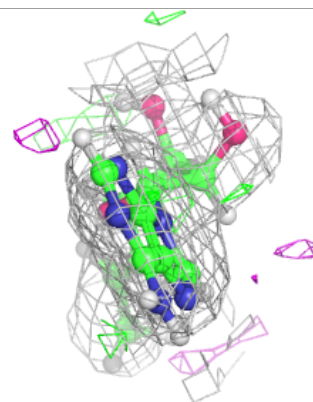
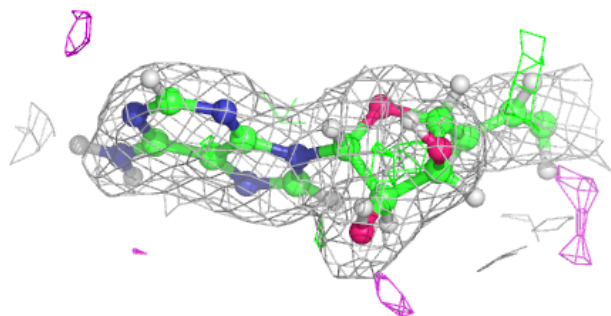
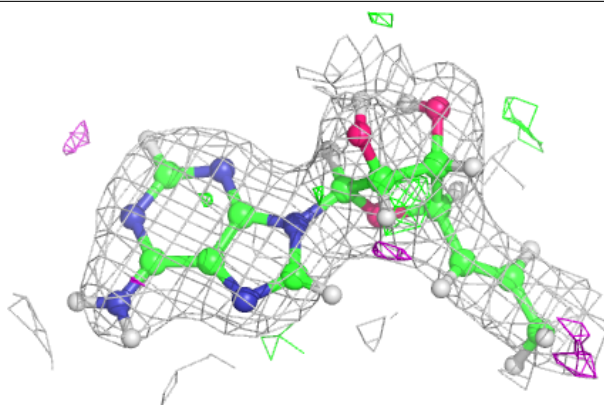
**Electron density around QVR H 102:**

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

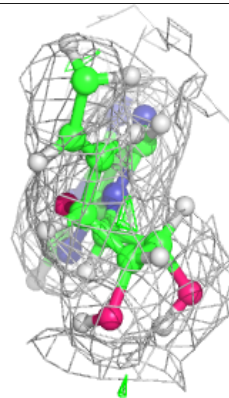
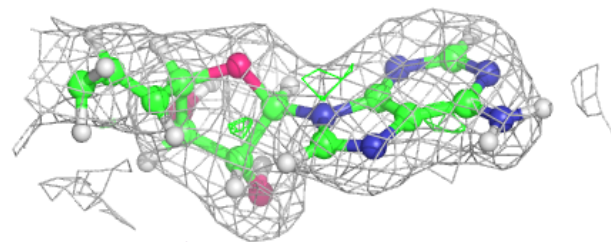
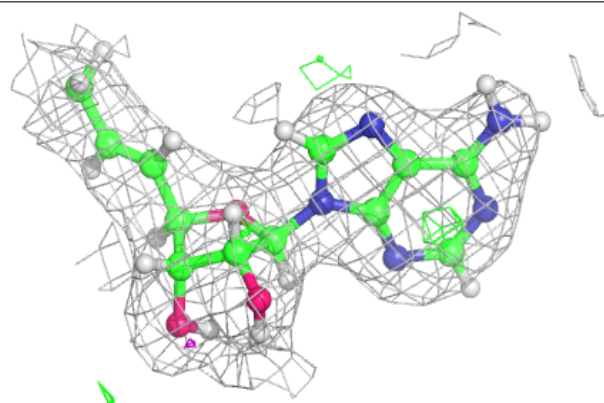


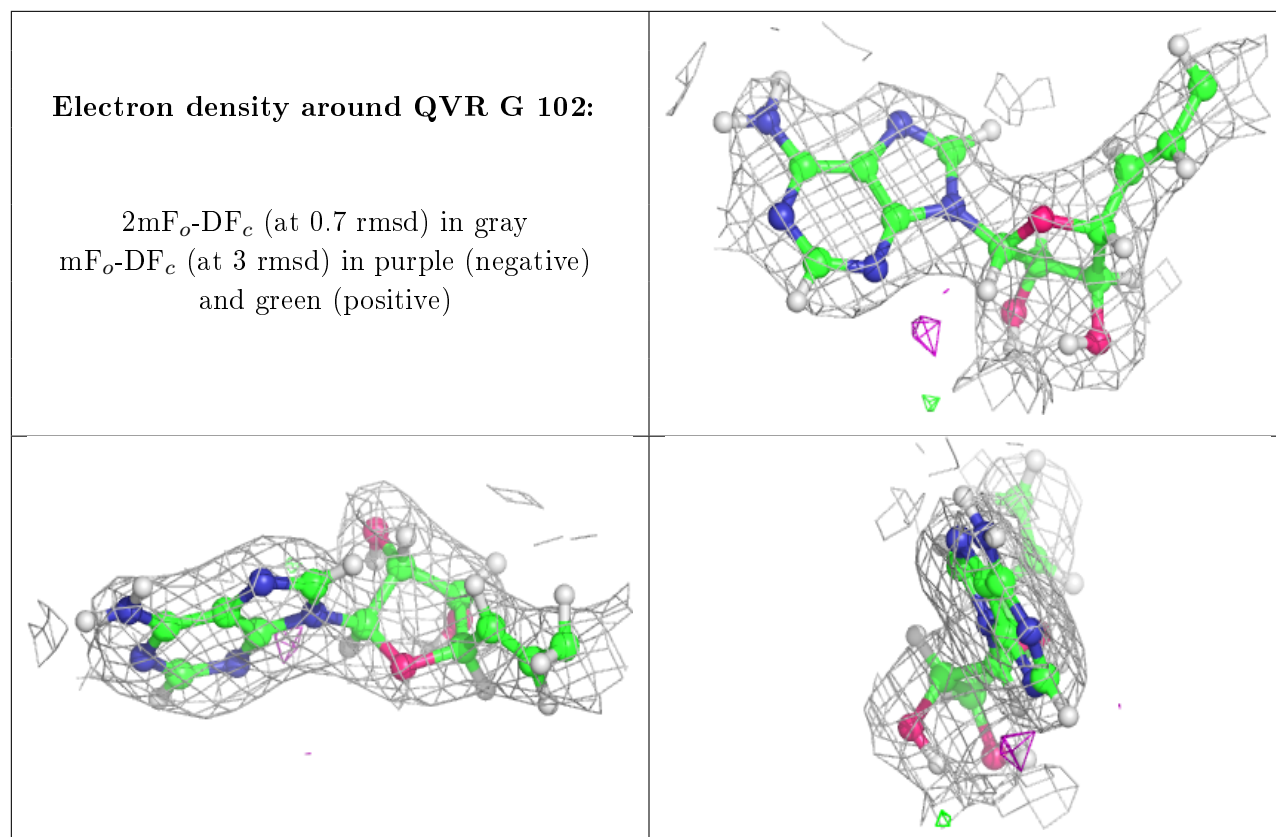
**Electron density around QVR E 101:**

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

**Electron density around QVR F 102:**

$2mF_o-DF_c$  (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.