W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

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)

The following versions of software and data (see references (i)) 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 2.00 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.
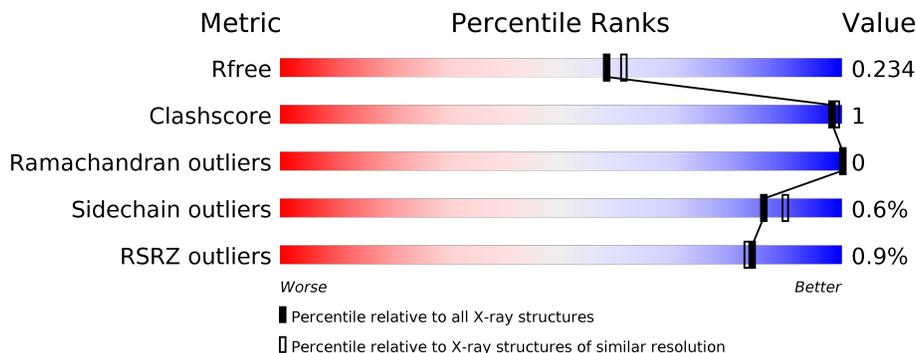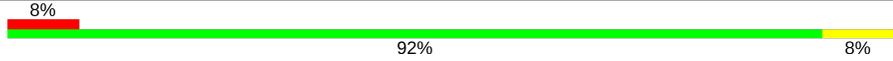

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	361	94% · 5%
1	B	361	% 93% · 5%
1	C	361	% 94% · 5%
1	D	361	% 92% · 5%
2	E	12	8% 92% 8%
2	F	12	100%

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Mol	Chain	Length	Quality of chain
2	G	12	8% ▬▬▬ 67% ░░░░ 33%
2	H	12	8% ▬▬▬ 92% ▬ 8%

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

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
2	E	11	Total 155	C 47	H 78	N 16	O 13	S 1	0	0	0
2	F	12	Total 175	C 56	H 87	N 17	O 14	S 1	0	0	0

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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	0
			175	56	87	17	14	1			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
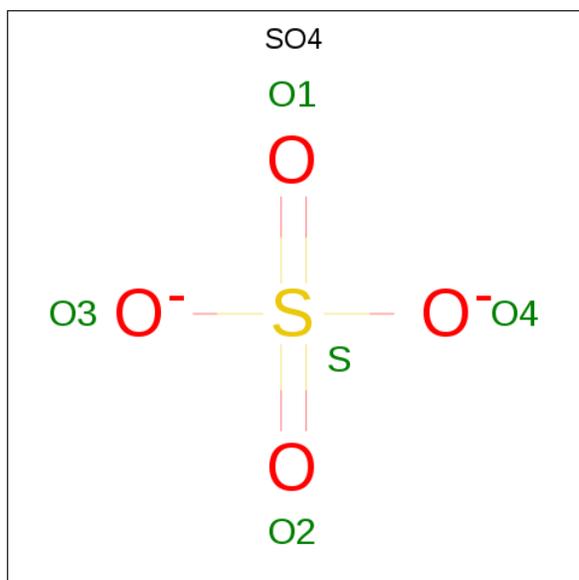
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
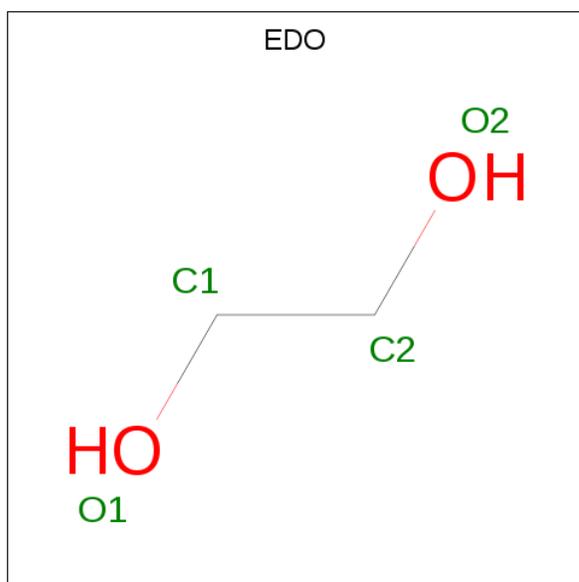
EDO

O2

OH

C1

C2

HO

O1

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

- Molecule 5 is 1,2-DIMETHOXYETHANE (three-letter code: DXE) (formula: $C_4H_{10}O_2$).
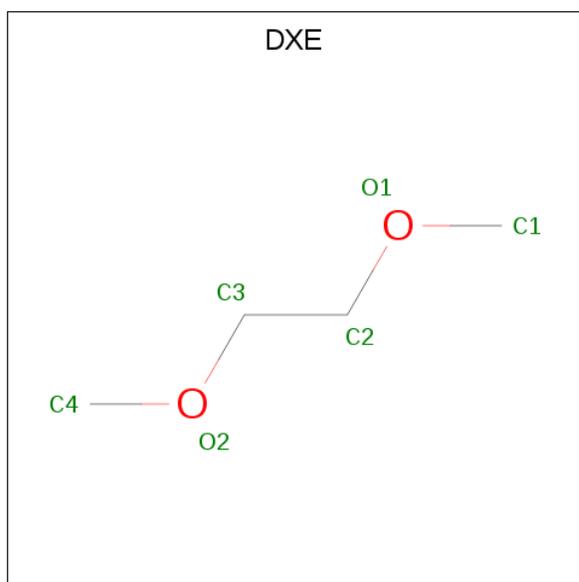
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	A	1	16	4	10	2	0	0

- Molecule 6 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY]-ETHOXY}-ETHANE (three-letter code: PG6) (formula: $C_{12}H_{26}O_6$).
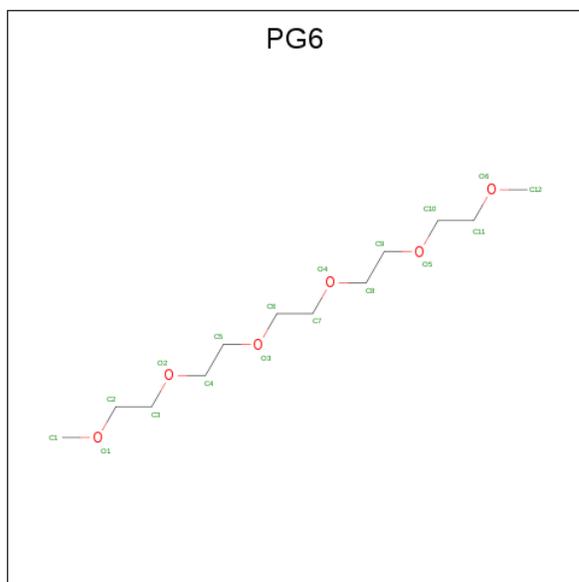
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
6	B	1	44	12	26	6	0	0

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

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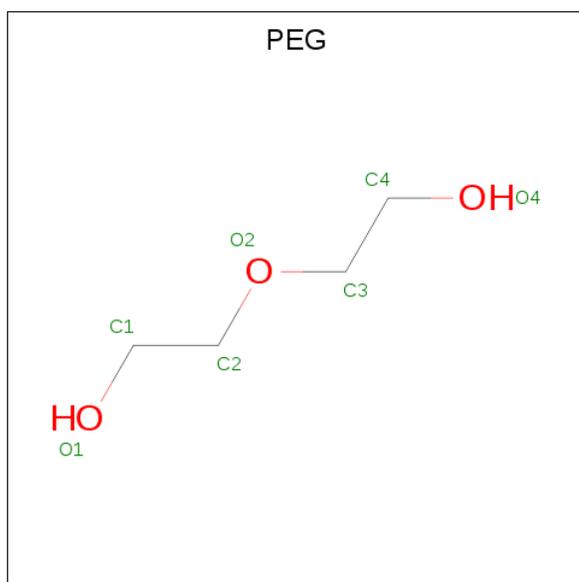
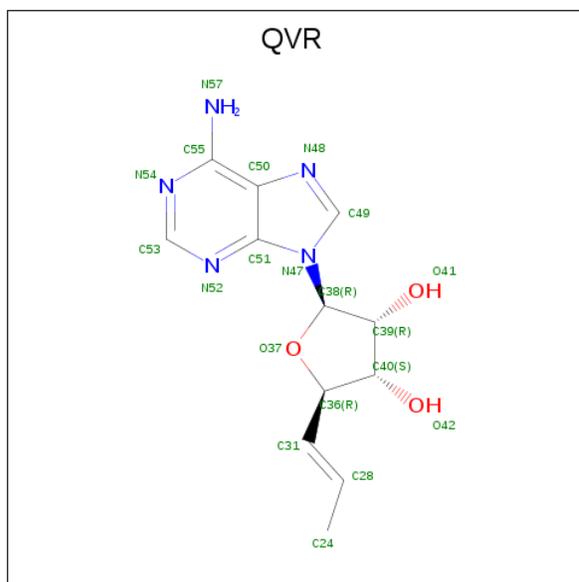| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 8 is (2 {R},3 {R},4 {S},5 {R})-2-(6-aminopurin-9-yl)-5-[({E})-prop-1-enyl]oxolane-3,4-diol (three-letter code: QVR) (formula: $C_{12}H_{15}N_5O_3$).

QVR

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

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

- Molecule 9 is L-PROLINAMIDE (three-letter code: LPD) (formula: $C_5H_{10}N_2O$).
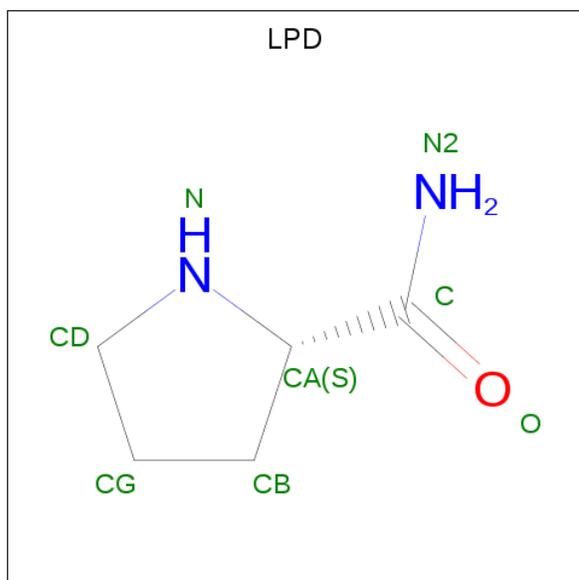
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	E	1	Total 17	C 5	H 9	N 2	O 1	0	0
9	F	1	Total 17	C 5	H 9	N 2	O 1	0	0
9	G	1	Total 17	C 5	H 9	N 2	O 1	0	0
9	H	1	Total 17	C 5	H 9	N 2	O 1	0	0

- Molecule 10 is ACETYL GROUP (three-letter code: ACE) (formula: C_2H_4O).

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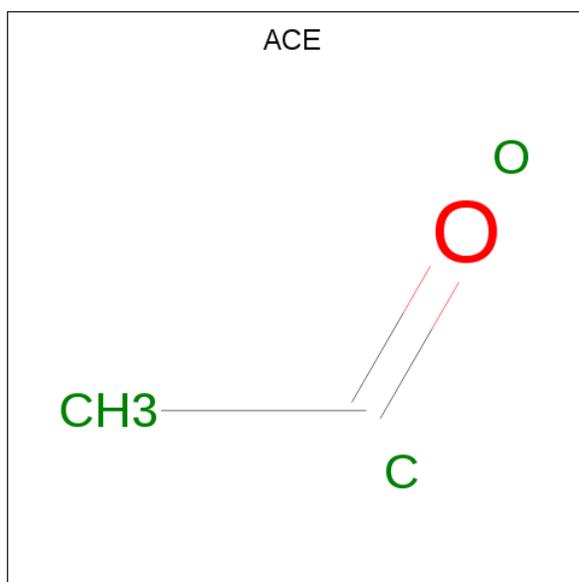
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	F	1	Total 3	C 2	O 1	0	0
10	H	1	Total 3	C 2	O 1	0	0

• Molecule 11 is water.

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

3 Residue-property plots ⓘ

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
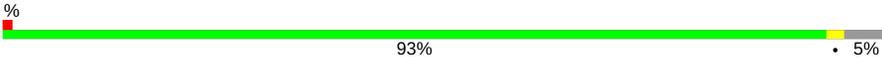
- Molecule 1: Histone-arginine methyltransferase CARM1

- Molecule 1: Histone-arginine methyltransferase CARM1
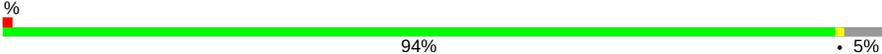
- Molecule 1: Histone-arginine methyltransferase CARM1

- Molecule 2: Polyadenylate-binding protein 1

- 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 (i)

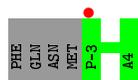| Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	74.83Å　98.54Å　208.34Å 90.00°　90.00°　90.00°	Depositor
Resolution (Å)	46.05　–　2.00 46.05　–　2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.05-2.00) 99.9 (46.05-2.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.42 (at 2.00Å)	Xtriage
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^2)	29.7	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 44.7	EDS
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	23651	wwPDB-VP
Average B, all atoms (Å^2)	42.0	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 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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (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(^{o})	Ideal(^{o})
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.

The worst 5 of 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

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
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

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	328	ARG
2	H	1	ARG
1	C	467	LEU
1	B	169	ARG
1	D	441	LEU

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
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(^{o})	Ideal(^{o})
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.
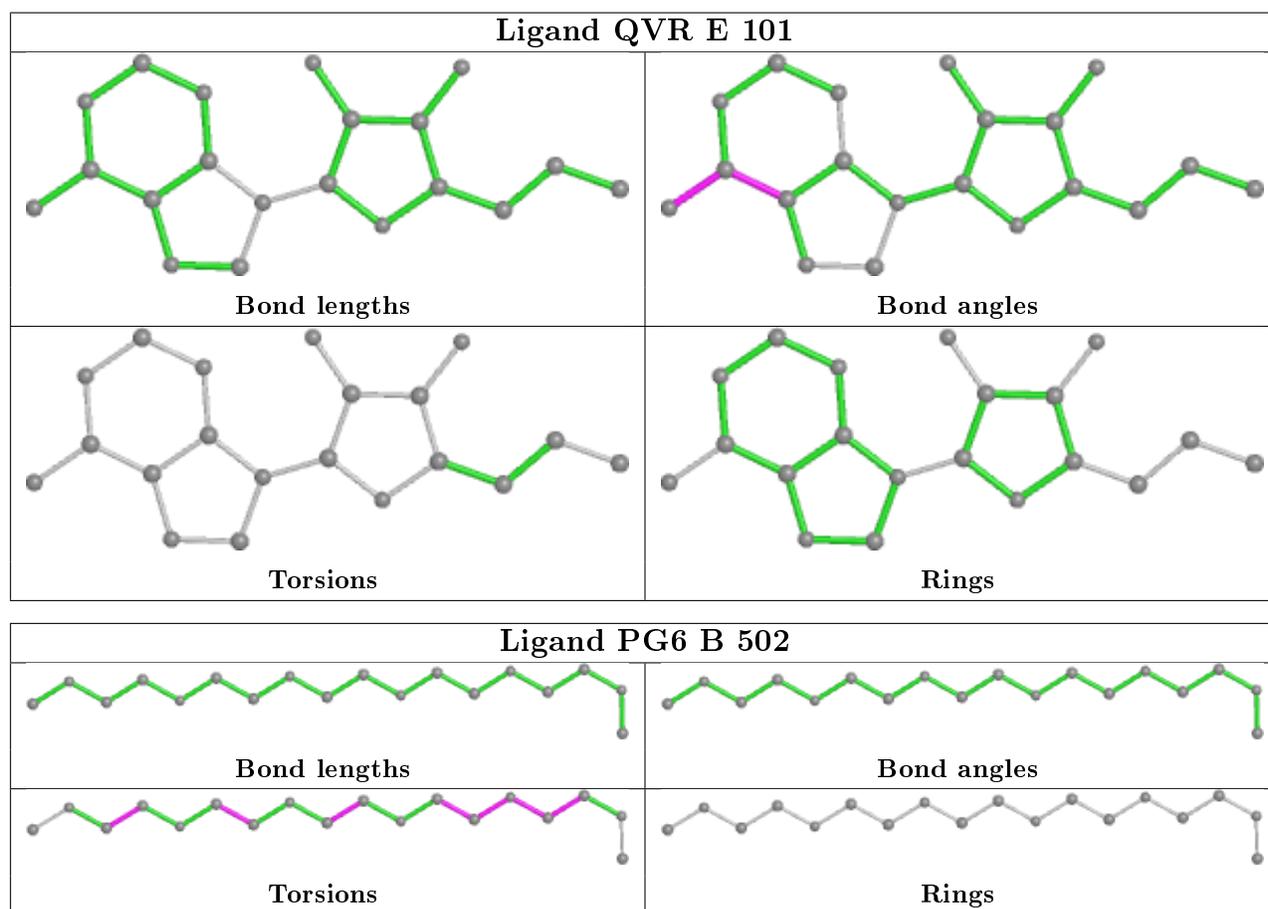
5 of 13 torsion outliers are listed below:

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

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand QVR E 101

Ligand PG6 B 502

Ligand QVR G 102

Bond lengths

Bond angles

Torsions

Rings

Ligand QVR F 102

Bond lengths

Bond angles

Torsions

Rings

Ligand QVR H 102

Bond lengths

Bond angles

Torsions

Rings
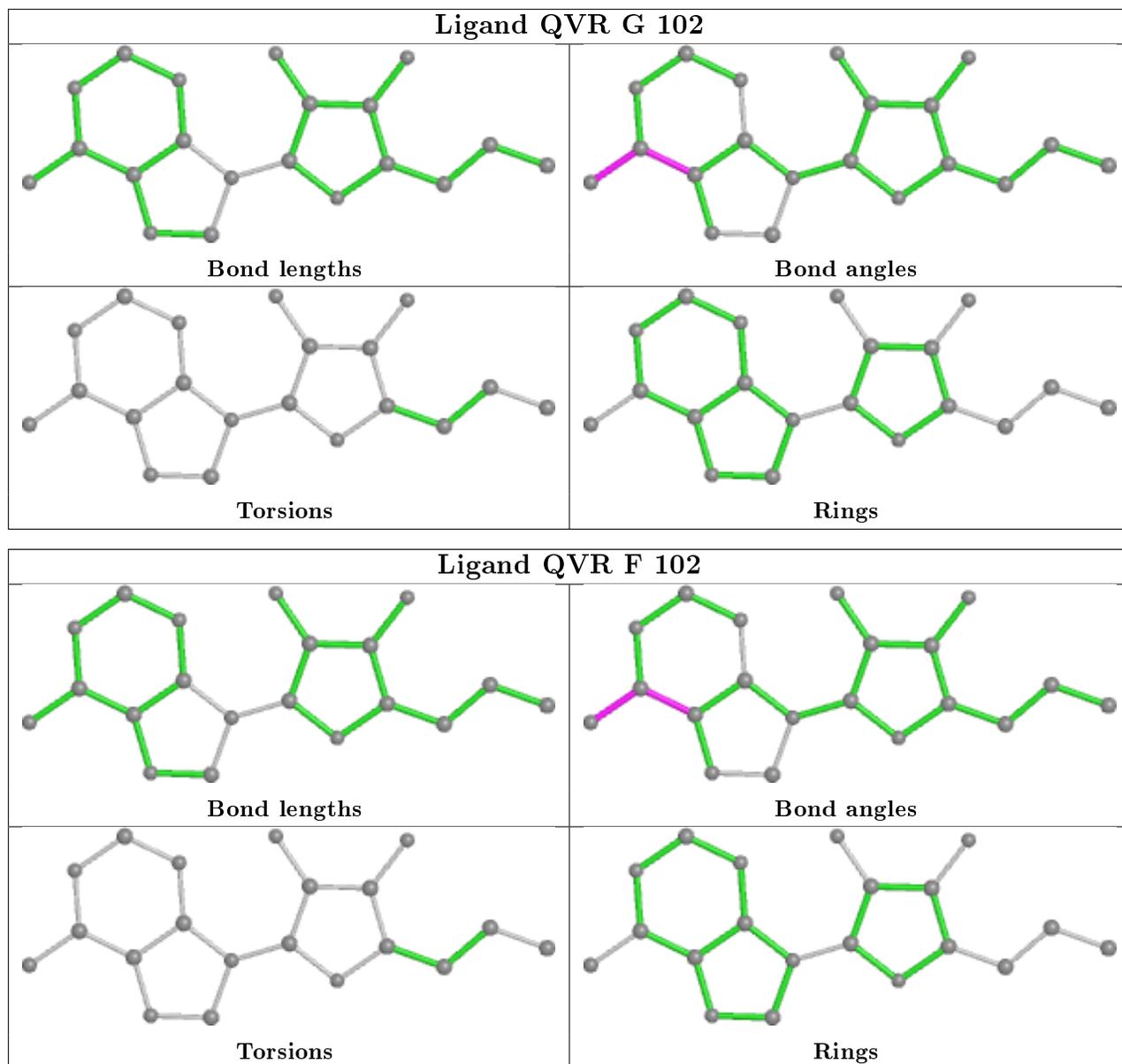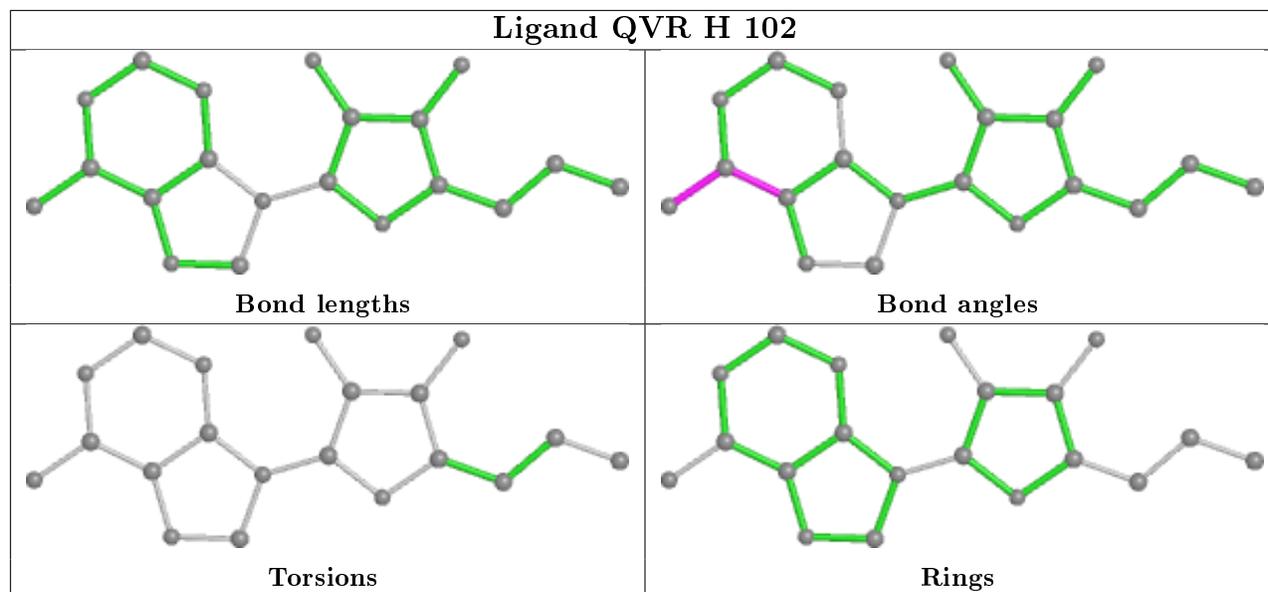
5.7 Other polymers (i)

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 (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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	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%)

The worst 5 of 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

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

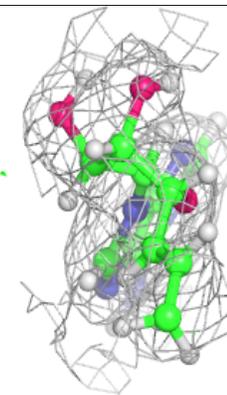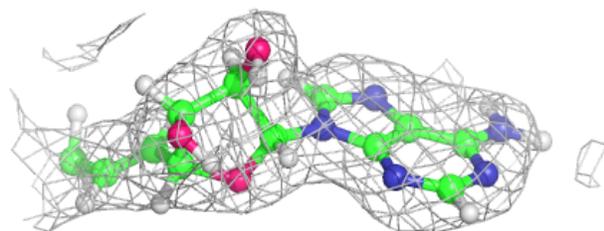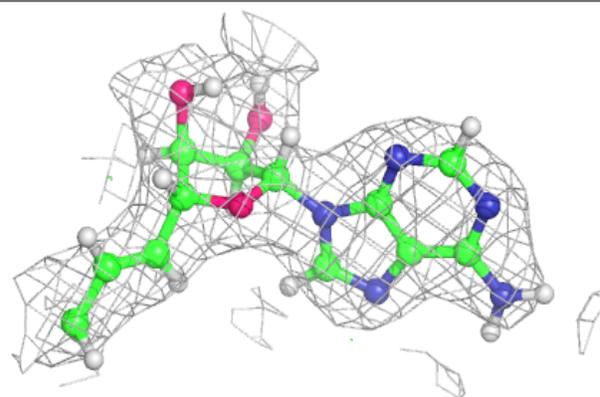| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	PG6	B	502	18/18	0.65	0.19	55,71,93,95	0
7	PEG	C	502	7/7	0.66	0.15	52,63,73,73	0
4	EDO	D	501	4/4	0.80	0.11	42,50,51,51	0
9	LPD	H	103	8/8	0.84	0.19	23,29,37,37	0
9	LPD	F	103	8/8	0.84	0.14	23,28,37,37	0
5	DXE	A	504	6/6	0.85	0.13	45,54,65,65	0
4	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.
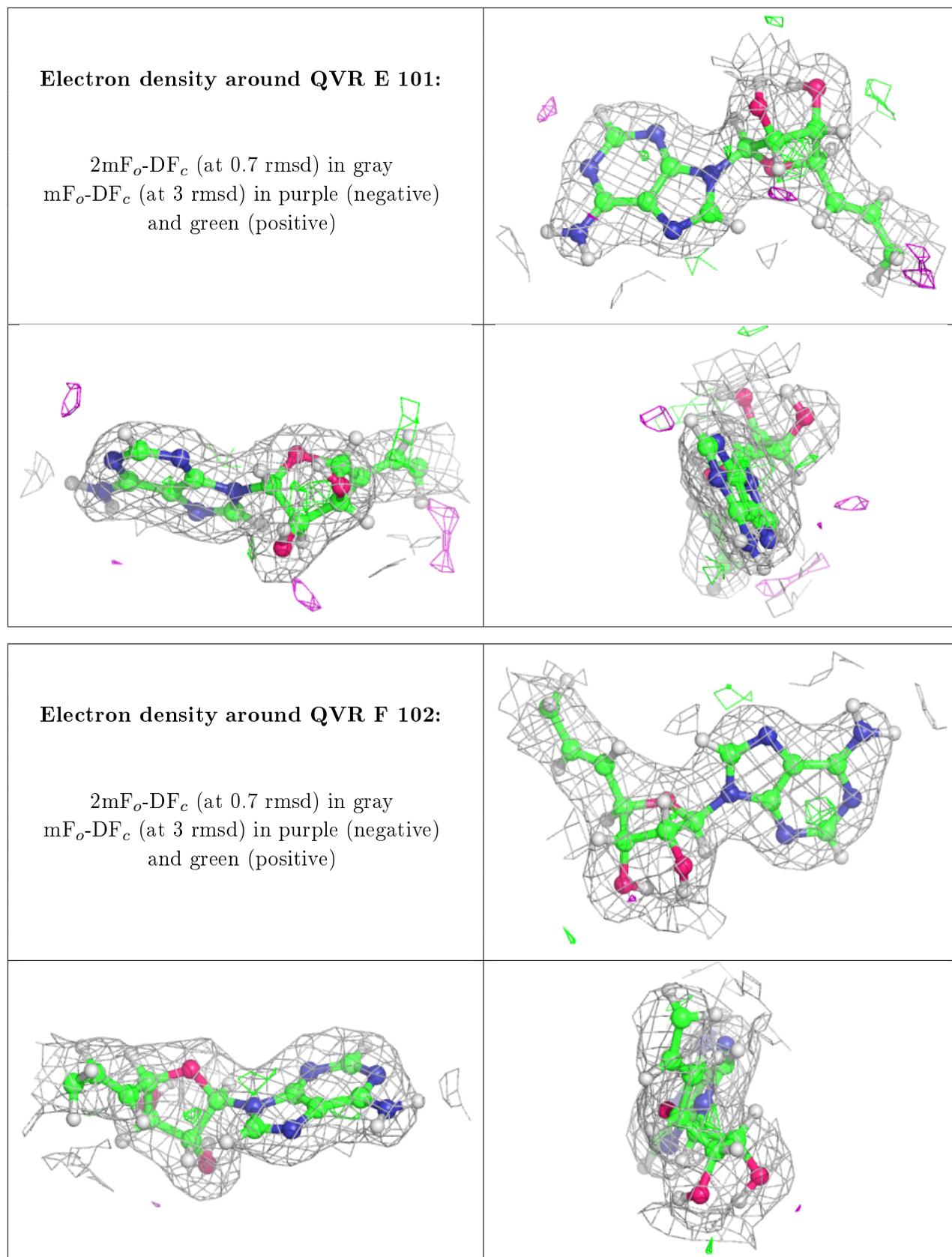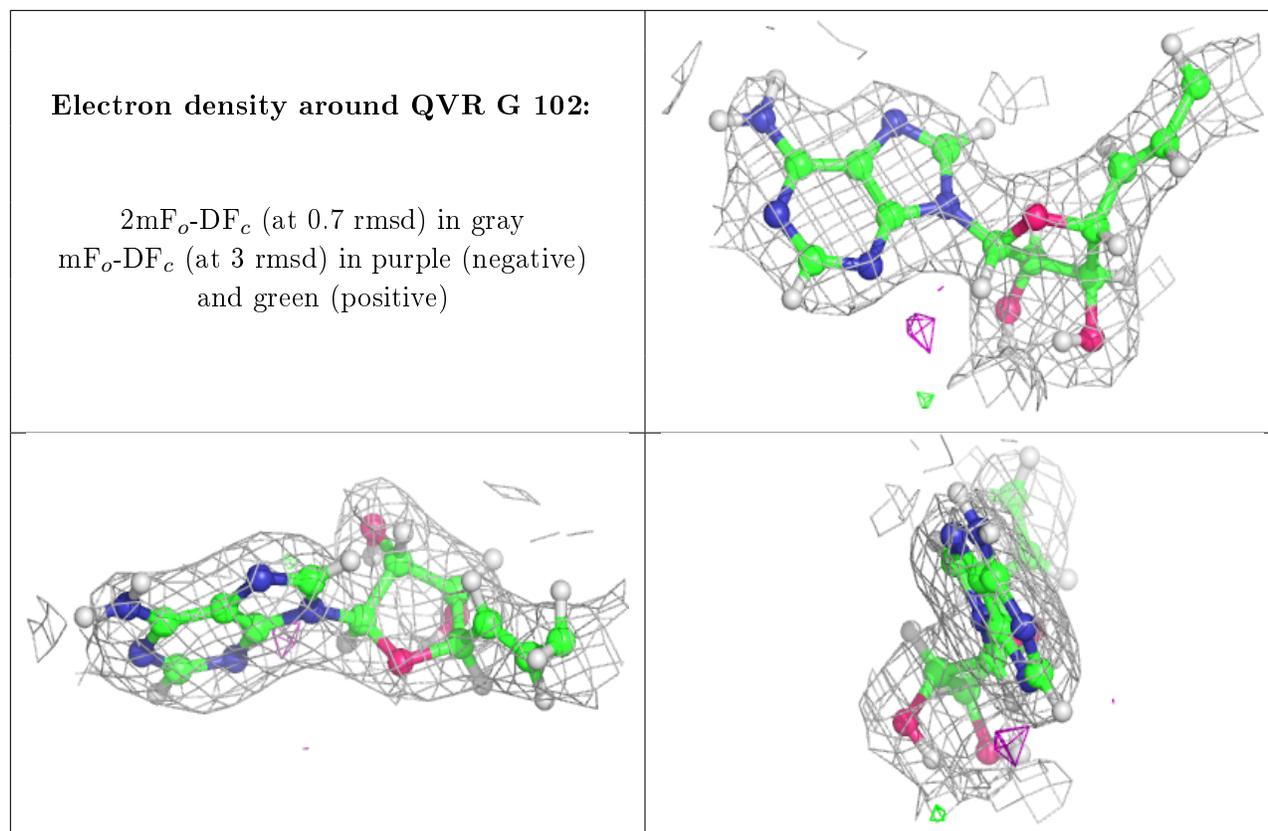
Electron density around PG6 B 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
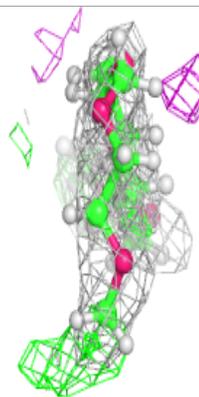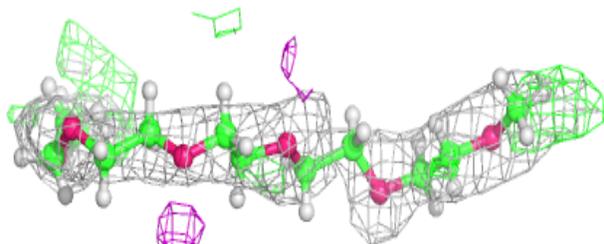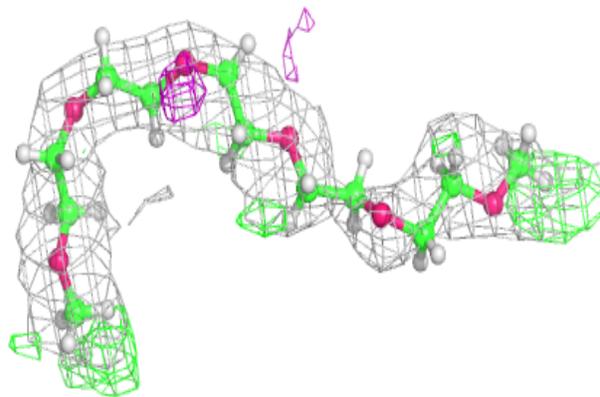
Electron density around QVR H 102:

$2mF_o-DF_c$ (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)

Electron density around QVR G 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 ⓘ

There are no such residues in this entry.