



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2026 – 11:54 PM UTC

PDB ID : 4BZ4 / pdb_00004bz4
Title : CorA is a surface-associated copper-binding protein important in *Methylomicrobium album* BG8 copper acquisition
Authors : Johnson, K.A.; Ve, T.; Pedersen, R.B.; Lillehaug, J.R.; Jensen, H.B.; Helland, R.; Karlsen, O.A.
Deposited on : 2013-07-24
Resolution : 1.60 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

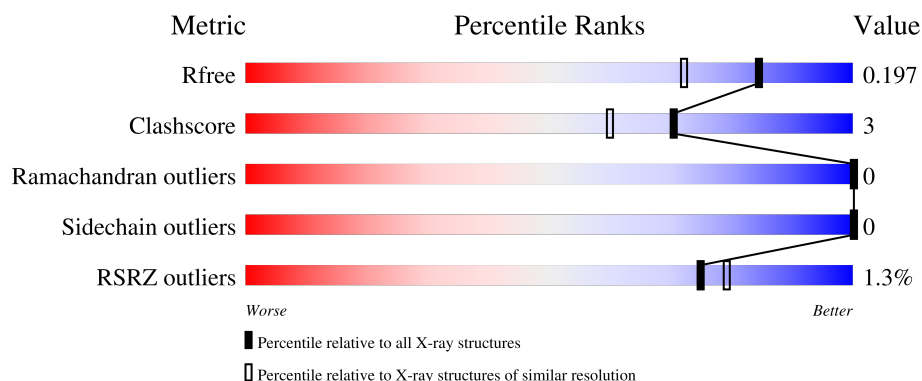
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	231	
1	B	231	
1	C	231	
1	D	231	

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Mol	Chain	Length	Quality of chain
1	E	231	 81% 8% 12%
1	F	231	%  75% 11% 14%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10634 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 COPPER-REPRESSIBLE POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	0	4	0
			1539	986	255	293	5			
1	B	204	Total	C	N	O	S	0	3	0
			1573	1003	263	302	5			
1	C	199	Total	C	N	O	S	0	2	0
			1529	979	255	289	6			
1	D	198	Total	C	N	O	S	0	2	0
			1521	973	253	290	5			
1	E	204	Total	C	N	O	S	0	6	0
			1582	1008	263	306	5			
1	F	199	Total	C	N	O	S	0	6	0
			1542	987	256	294	5			

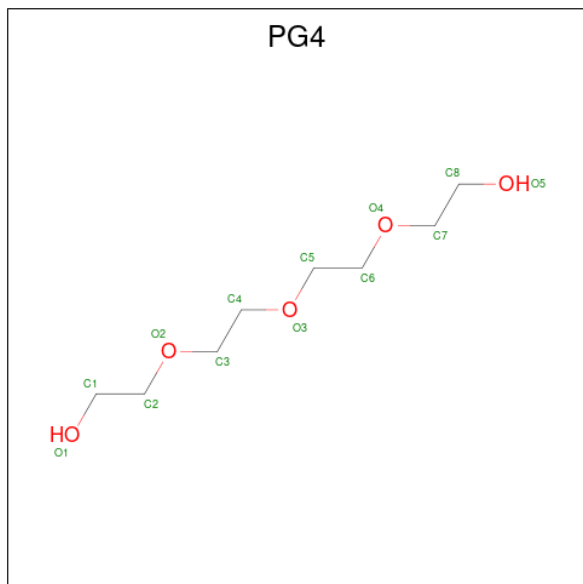
- Molecule 2 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cu	0	0
			1	1		
2	B	1	Total	Cu	0	0
			1	1		
2	C	1	Total	Cu	0	0
			1	1		
2	D	1	Total	Cu	0	0
			1	1		
2	E	1	Total	Cu	0	0
			1	1		
2	F	1	Total	Cu	0	0
			1	1		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

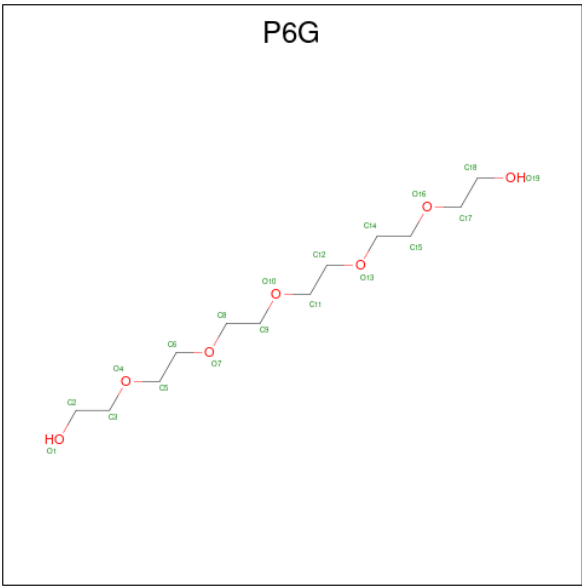
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 6 4 2	0	0
4	C	1	Total C O 6 4 2	0	0
4	D	1	Total C O 7 4 3	0	0
4	E	1	Total C O 6 4 2	0	0
4	F	1	Total C O 8 5 3	0	0

- Molecule 5 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			11	7	4		
5	B	1	Total	C	O	0	0
			8	5	3		
5	C	1	Total	C	O	0	0
			19	12	7		
5	C	1	Total	C	O	0	0
			15	10	5		
5	D	1	Total	C	O	0	0
			8	5	3		
5	E	1	Total	C	O	0	0
			14	9	5		
5	E	1	Total	C	O	0	0
			13	8	5		
5	E	1	Total	C	O	0	0
			8	5	3		
5	F	1	Total	C	O	0	0
			11	7	4		

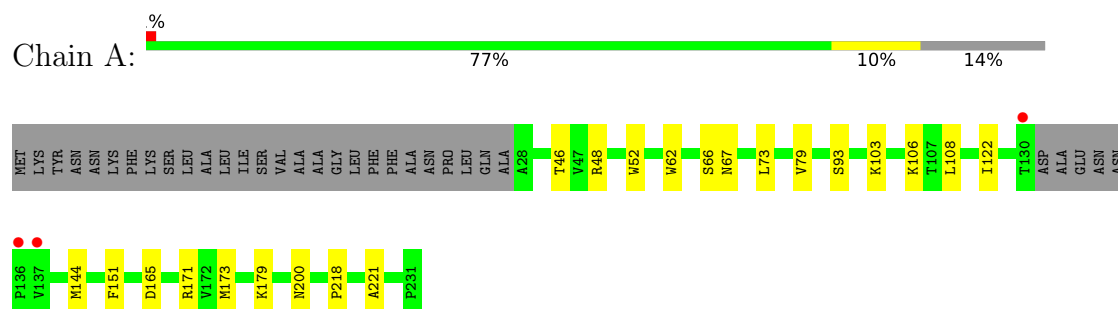
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	206	Total 206	O 206	0	0
6	B	179	Total 179	O 179	0	0
6	C	188	Total 188	O 188	0	0
6	D	200	Total 200	O 200	0	0
6	E	222	Total 222	O 222	0	0
6	F	180	Total 180	O 180	0	0

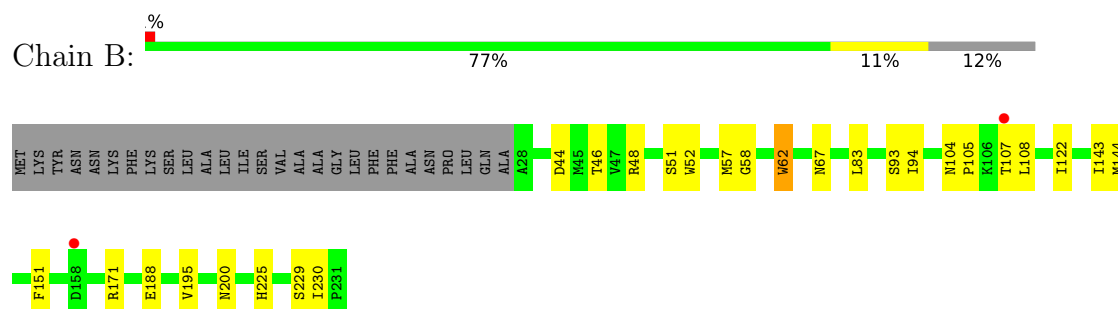
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

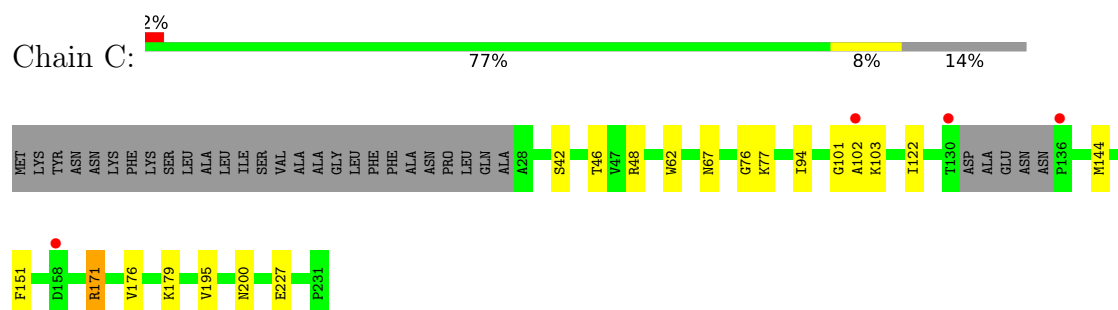
- Molecule 1: COPPER-REPRESSIBLE POLYPEPTIDE



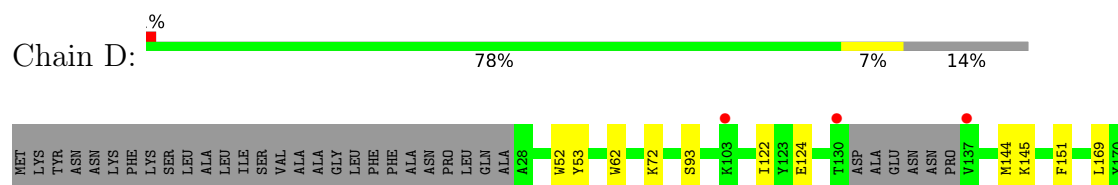
- Molecule 1: COPPER-REPRESSIBLE POLYPEPTIDE



- Molecule 1: COPPER-REPRESSIBLE POLYPEPTIDE

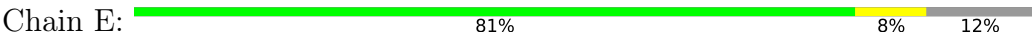


- Molecule 1: COPPER-REPRESSIBLE POLYPEPTIDE

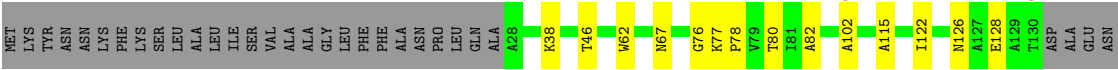
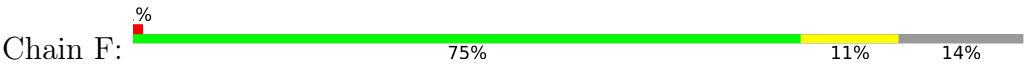




● Molecule 1: COPPER-REPRESSIBLE POLYPEPTIDE



● Molecule 1: COPPER-REPRESSIBLE POLYPEPTIDE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.84Å 113.17Å 81.49Å 90.00° 104.51° 90.00°	Depositor
Resolution (Å)	30.00 – 1.60 30.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (30.00-1.60) 98.7 (30.00-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 1.60Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.158 , 0.188 0.169 , 0.197	Depositor DCC
R_{free} test set	8428 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	12.8	Xtrriage
Anisotropy	0.149	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10634	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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 46.47 % 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 1.1404e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CU1, P6G, PG4, KYN, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.25	3/1585 (0.2%)	1.09	2/2157 (0.1%)
1	B	1.32	3/1616 (0.2%)	1.17	4/2201 (0.2%)
1	C	1.32	4/1567 (0.3%)	1.09	3/2132 (0.1%)
1	D	1.30	4/1558 (0.3%)	1.15	0/2120
1	E	1.32	2/1637 (0.1%)	1.17	1/2230 (0.0%)
1	F	1.36	6/1596 (0.4%)	1.18	3/2171 (0.1%)
All	All	1.31	22/9559 (0.2%)	1.14	13/13011 (0.1%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	220	THR	N-CA	-7.48	1.36	1.46
1	F	199	ILE	C-O	6.64	1.31	1.23
1	F	102	ALA	CA-C	-6.42	1.44	1.52
1	A	165	ASP	N-CA	6.30	1.54	1.46
1	D	203	ILE	C-O	-5.95	1.18	1.24
1	D	224	VAL	CA-CB	5.92	1.61	1.54
1	B	200	ASN	C-O	5.86	1.26	1.23
1	D	124	GLU	C-O	-5.64	1.19	1.24
1	A	108	LEU	C-O	-5.62	1.19	1.24
1	C	171	ARG	N-CA	-5.45	1.39	1.46
1	D	173	MET	SD-CE	-5.36	1.66	1.79
1	F	173	MET	SD-CE	-5.36	1.66	1.79
1	F	82	ALA	C-O	5.33	1.30	1.24
1	C	48	ARG	CZ-NH2	-5.29	1.26	1.33
1	A	66	SER	C-O	5.17	1.30	1.23
1	E	45	MET	N-CA	-5.14	1.39	1.45
1	C	200	ASN	C-O	5.10	1.26	1.23
1	C	77	LYS	C-O	-5.06	1.18	1.24
1	B	229	SER	C-O	5.05	1.29	1.24
1	B	143	ILE	CA-C	-5.04	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	150	GLY	C-O	-5.03	1.18	1.24
1	F	206	THR	C-O	-5.02	1.18	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	48	ARG	CB-CG-CD	8.03	129.77	111.30
1	F	173	MET	CG-SD-CE	-7.49	84.43	100.90
1	A	173	MET	CG-SD-CE	-6.70	86.15	100.90
1	C	76	GLY	N-CA-C	6.57	123.75	115.21
1	B	51	SER	N-CA-C	6.46	119.14	111.71
1	F	102	ALA	N-CA-C	-6.37	98.86	109.24
1	A	200	ASN	CB-CA-C	-6.32	105.50	111.00
1	C	103	LYS	N-CA-C	-5.78	106.87	114.04
1	C	102	ALA	N-CA-C	-5.53	100.17	108.96
1	E	163	GLU	CG-CD-OE2	-5.35	106.09	118.40
1	F	76	GLY	N-CA-C	5.14	121.61	114.92
1	B	230	ILE	O-C-N	5.13	124.60	121.37
1	B	200	ASN	O-C-N	5.05	123.85	121.53

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	1539	0	1468	12	0
1	B	1573	0	1486	14	0
1	C	1529	0	1462	7	0
1	D	1521	0	1450	7	0
1	E	1582	0	1499	10	0
1	F	1542	0	1473	11	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	4	0	5	0	0
4	B	6	0	6	1	0
4	C	6	0	6	0	0
4	D	7	0	9	0	0
4	E	6	0	6	0	0
4	F	8	0	8	2	0
5	A	17	0	22	0	0
5	B	19	0	22	2	0
5	C	34	0	44	0	0
5	D	8	0	9	0	0
5	E	35	0	42	0	0
5	F	11	0	12	0	0
6	A	206	0	0	4	0
6	B	179	0	0	4	0
6	C	188	0	0	1	0
6	D	200	0	0	2	1
6	E	222	0	0	3	0
6	F	180	0	0	4	0
All	All	10634	0	9029	63	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 3.

All (63) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188[B]:GLU:OE2	6:B:2152:HOH:O	1.57	1.20
1:B:57:MET:C	1:B:58:GLY:CA	2.30	1.05
1:B:67[A]:ASN:OD1	6:B:2009:HOH:O	1.80	0.97
5:B:1235:P6G:H31	6:B:2176:HOH:O	1.82	0.79
1:F:80[B]:THR:HG23	6:F:2068:HOH:O	1.86	0.75
1:C:101:GLY:O	6:C:2090:HOH:O	2.04	0.73
1:C:46:THR:H	1:C:67[B]:ASN:ND2	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ASP:OD1	1:B:225[B]:HIS:ND1	2.30	0.64
1:E:128:GLU:CD	1:E:138:LYS:NZ	2.58	0.61
1:D:52:TRP:CG	1:D:93:SER:HG	2.19	0.59
1:F:163:GLU:OE2	6:F:2136:HOH:O	2.17	0.59
1:B:105:PRO:HA	1:B:108:LEU:HD12	1.85	0.58
1:B:104:ASN:O	1:B:107:THR:HG22	2.04	0.57
1:D:176:VAL:HG11	1:D:179:LYS:HD2	1.87	0.57
1:F:115:ALA:HB2	4:F:1234:PG4:H41	1.88	0.55
1:A:67[A]:ASN:OD1	6:A:2008:HOH:O	2.18	0.55
1:D:145:LYS:HE3	6:D:2123:HOH:O	2.06	0.54
1:E:128:GLU:CD	1:E:138:LYS:HZ3	2.16	0.53
1:B:52:TRP:CG	1:B:93:SER:HG	2.26	0.52
4:F:1234:PG4:H42	6:F:2176:HOH:O	2.10	0.52
1:F:38[B]:LYS:NZ	1:F:230:ILE:O	2.43	0.51
1:B:151:PHE:CZ	1:B:171:ARG:HG2	2.46	0.50
5:B:1235:P6G:H32	6:B:2178:HOH:O	2.12	0.50
1:C:42:SER:HB3	1:C:227:GLU:OE1	2.12	0.49
1:B:46:THR:H	1:B:67[B]:ASN:ND2	2.10	0.49
1:A:52:TRP:CG	1:A:93:SER:HG	2.30	0.49
1:E:122:ILE:HB	1:E:144:MET:HB2	1.96	0.48
1:B:83:LEU:HD12	1:B:83:LEU:N	2.28	0.48
1:E:227[A]:GLU:OE2	6:E:2085:HOH:O	2.20	0.48
1:C:151:PHE:CZ	1:C:171:ARG:HG2	2.49	0.48
1:A:122:ILE:HB	1:A:144:MET:HB2	1.96	0.47
1:E:151:PHE:CZ	1:E:171:ARG:HG2	2.49	0.47
1:F:202:ASP:O	1:F:208:TYR:HB2	2.14	0.47
1:D:151:PHE:CZ	1:D:171:ARG:HG2	2.49	0.47
1:B:62:KYN:CE2	4:B:1234:PG4:H31	2.45	0.46
1:A:151:PHE:CZ	1:A:171:ARG:HG2	2.51	0.46
1:F:38[B]:LYS:HD2	6:F:2015:HOH:O	2.15	0.46
1:C:94:ILE:HA	1:C:195:VAL:O	2.16	0.46
1:F:122:ILE:HB	1:F:144:MET:HB2	1.98	0.46
1:D:72:LYS:NZ	6:D:2063:HOH:O	2.49	0.45
1:A:48:ARG:HD3	1:A:218:PRO:O	2.17	0.45
1:C:176:VAL:HG11	1:C:179:LYS:HE3	1.98	0.45
1:F:151:PHE:CZ	1:F:171:ARG:HG2	2.52	0.45
1:F:46:THR:H	1:F:67:ASN:ND2	2.16	0.44
1:D:122:ILE:HB	1:D:144:MET:HB2	2.00	0.44
1:F:128:GLU:HG2	1:F:138:LYS:HD2	1.99	0.44
1:A:103:LYS:HA	1:A:103:LYS:HE2	2.00	0.43
1:F:77:LYS:HA	1:F:78:PRO:HD3	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ILE:HA	1:B:195:VAL:O	2.19	0.43
1:E:105:PRO:HA	1:E:108:LEU:HD12	2.01	0.42
1:B:122:ILE:HB	1:B:144:MET:HB2	2.01	0.42
1:C:122:ILE:HB	1:C:144:MET:HB2	2.00	0.42
1:D:53:TYR:CE1	1:D:169:LEU:HD11	2.56	0.41
1:B:107:THR:HG21	1:E:204:ASP:OD2	2.20	0.41
1:E:46:THR:H	1:E:67[B]:ASN:ND2	2.18	0.41
1:A:46:THR:H	1:A:67[A]:ASN:ND2	2.18	0.41
1:E:77:LYS:NZ	6:E:2077:HOH:O	2.54	0.41
1:E:174[A]:ASP:OD2	6:E:2176:HOH:O	2.20	0.41
1:A:46:THR:HB	1:A:221:ALA:HB1	2.02	0.40
1:A:73:LEU:HD13	1:A:79:VAL:HG21	2.04	0.40
1:A:103:LYS:HB2	6:A:2100:HOH:O	2.20	0.40
1:A:106:LYS:HE3	6:A:2104:HOH:O	2.22	0.40
1:A:179:LYS:HD2	6:A:2164:HOH:O	2.21	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)
1:F:126[B]:ASN:ND2	6:D:2177:HOH:O[2_656]	1.88	0.32

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	198/231 (86%)	194 (98%)	4 (2%)	0	100	100
1	B	202/231 (87%)	198 (98%)	4 (2%)	0	100	100
1	C	196/231 (85%)	191 (97%)	5 (3%)	0	100	100
1	D	195/231 (84%)	190 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	207/231 (90%)	200 (97%)	7 (3%)	0	100	100
1	F	200/231 (87%)	193 (96%)	7 (4%)	0	100	100
All	All	1198/1386 (86%)	1166 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	161/183 (88%)	161 (100%)	0	100	100
1	B	164/183 (90%)	164 (100%)	0	100	100
1	C	159/183 (87%)	159 (100%)	0	100	100
1	D	158/183 (86%)	158 (100%)	0	100	100
1	E	167/183 (91%)	167 (100%)	0	100	100
1	F	163/183 (89%)	163 (100%)	0	100	100
All	All	972/1098 (88%)	972 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	40	ASN
1	D	67	ASN
1	F	40	ASN
1	F	67	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	KYN	C	62	1	13,14,15	1.48	2 (15%)	13,18,20	2.65	6 (46%)
1	KYN	D	62	1	13,14,15	1.58	2 (15%)	13,18,20	2.12	4 (30%)
1	KYN	E	62	1	13,14,15	1.27	2 (15%)	13,18,20	1.54	3 (23%)
1	KYN	F	62	1	13,14,15	1.35	1 (7%)	13,18,20	2.67	5 (38%)
1	KYN	A	62	1	13,14,15	1.29	2 (15%)	13,18,20	1.96	4 (30%)
1	KYN	B	62	1	13,14,15	1.54	3 (23%)	13,18,20	2.27	4 (30%)

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	KYN	C	62	1	-	2/9/10/12	0/1/1/1
1	KYN	D	62	1	-	2/9/10/12	0/1/1/1
1	KYN	E	62	1	-	2/9/10/12	0/1/1/1
1	KYN	F	62	1	-	2/9/10/12	0/1/1/1
1	KYN	A	62	1	-	2/9/10/12	0/1/1/1
1	KYN	B	62	1	-	2/9/10/12	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	62	KYN	CG-N1	3.29	1.48	1.38
1	A	62	KYN	CD2-C1	3.05	1.54	1.48
1	F	62	KYN	CD2-C1	2.83	1.54	1.48
1	D	62	KYN	CB-CA	-2.57	1.48	1.53
1	C	62	KYN	O2-C1	2.54	1.26	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	62	KYN	CD2-CG	2.54	1.45	1.41
1	C	62	KYN	CB-C1	2.41	1.54	1.51
1	D	62	KYN	CD2-CG	2.37	1.45	1.41
1	B	62	KYN	CE2-CD2	2.28	1.43	1.39
1	E	62	KYN	CG-N1	2.15	1.45	1.38
1	B	62	KYN	O2-C1	2.12	1.26	1.22
1	A	62	KYN	CG-N1	2.08	1.44	1.38

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	62	KYN	CD1-CG-CD2	-5.38	112.40	118.16
1	C	62	KYN	CA-CB-C1	-5.30	106.83	113.10
1	B	62	KYN	CA-CB-C1	-4.97	107.22	113.10
1	F	62	KYN	CE2-CD2-CG	4.60	123.62	118.96
1	A	62	KYN	CA-CB-C1	-4.48	107.80	113.10
1	C	62	KYN	CE2-CD2-CG	4.44	123.45	118.96
1	F	62	KYN	CE1-CZ-CE2	-4.00	115.31	120.24
1	C	62	KYN	O2-C1-CB	-3.97	115.98	120.70
1	B	62	KYN	CE2-CD2-CG	3.94	122.95	118.96
1	D	62	KYN	CA-CB-C1	-3.87	108.52	113.10
1	D	62	KYN	O2-C1-CB	-3.76	116.23	120.70
1	C	62	KYN	CD1-CG-CD2	-3.33	114.60	118.16
1	E	62	KYN	O2-C1-CB	-3.23	116.86	120.70
1	B	62	KYN	CB-C1-CD2	-3.02	116.31	119.82
1	B	62	KYN	CD1-CG-CD2	-2.92	115.03	118.16
1	F	62	KYN	O2-C1-CB	-2.90	117.25	120.70
1	D	62	KYN	CE2-CD2-CG	2.77	121.76	118.96
1	D	62	KYN	CD1-CG-CD2	-2.68	115.29	118.16
1	A	62	KYN	CD1-CG-CD2	-2.56	115.42	118.16
1	C	62	KYN	CE1-CZ-CE2	-2.54	117.11	120.24
1	E	62	KYN	CB-C1-CD2	2.52	122.75	119.82
1	F	62	KYN	CD1-CG-N1	2.51	125.03	120.11
1	E	62	KYN	CA-CB-C1	-2.40	110.26	113.10
1	A	62	KYN	O2-C1-CB	-2.31	117.96	120.70
1	A	62	KYN	CE1-CD1-CG	2.11	123.89	121.03
1	C	62	KYN	CD2-CG-N1	2.07	125.58	122.68

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	62	KYN	O2-C1-CB-CA
1	B	62	KYN	O2-C1-CB-CA
1	C	62	KYN	O2-C1-CB-CA
1	B	62	KYN	CD2-C1-CB-CA
1	E	62	KYN	O2-C1-CB-CA
1	F	62	KYN	O2-C1-CB-CA
1	A	62	KYN	CD2-C1-CB-CA
1	C	62	KYN	CD2-C1-CB-CA
1	D	62	KYN	CD2-C1-CB-CA
1	E	62	KYN	CD2-C1-CB-CA
1	F	62	KYN	CD2-C1-CB-CA
1	D	62	KYN	O2-C1-CB-CA

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	62	KYN	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 12 are monoatomic - leaving 17 for Mogul analysis.

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	$\# Z > 2$
5	P6G	C	1236	-	14,14,18	0.54	0	13,13,17	0.39	0
5	P6G	E	1237	-	7,7,18	0.65	0	6,6,17	0.91	0
5	P6G	A	1236	-	6,6,18	0.60	0	5,5,17	0.52	0
5	P6G	B	1236	-	7,7,18	0.67	0	6,6,17	0.88	0
4	PG4	F	1234	-	7,7,12	0.70	0	6,6,11	0.45	0
5	P6G	D	1235	-	7,7,18	0.74	0	6,6,17	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	P6G	A	1235	-	9,9,18	0.63	0	8,8,17	1.01	0
4	PG4	E	1234	-	5,5,12	0.63	0	4,4,11	0.60	0
4	PG4	D	1234	-	6,6,12	0.39	0	5,5,11	0.95	0
5	P6G	B	1235	-	10,10,18	0.54	0	9,9,17	0.85	0
5	P6G	E	1235	-	13,13,18	0.57	0	12,12,17	0.92	0
5	P6G	F	1235	-	10,10,18	0.73	0	9,9,17	1.34	1 (11%)
4	PG4	B	1234	-	5,5,12	0.68	0	4,4,11	0.70	0
4	PG4	A	1234	-	3,3,12	0.50	0	2,2,11	0.15	0
5	P6G	C	1235	-	18,18,18	0.64	0	17,17,17	0.69	0
4	PG4	C	1234	-	5,5,12	0.82	0	4,4,11	0.58	0
5	P6G	E	1236	-	12,12,18	0.35	0	11,11,17	0.81	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
5	P6G	C	1236	-	-	2/12/12/16	-
5	P6G	E	1237	-	-	2/5/5/16	-
5	P6G	A	1236	-	-	2/4/4/16	-
5	P6G	B	1236	-	-	3/5/5/16	-
4	PG4	F	1234	-	-	3/5/5/10	-
5	P6G	D	1235	-	-	2/5/5/16	-
5	P6G	A	1235	-	-	2/7/7/16	-
4	PG4	E	1234	-	-	1/3/3/10	-
4	PG4	D	1234	-	-	0/4/4/10	-
5	P6G	B	1235	-	-	4/8/8/16	-
5	P6G	E	1235	-	-	2/11/11/16	-
5	P6G	F	1235	-	-	2/8/8/16	-
4	PG4	B	1234	-	-	2/3/3/10	-
4	PG4	A	1234	-	-	1/1/1/10	-
5	P6G	C	1235	-	-	2/16/16/16	-
4	PG4	C	1234	-	-	1/3/3/10	-
5	P6G	E	1236	-	-	2/10/10/16	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1235	P6G	C11-O10-C9	2.57	124.50	113.26

There are no chirality outliers.

All (33) torsion outliers are listed below:

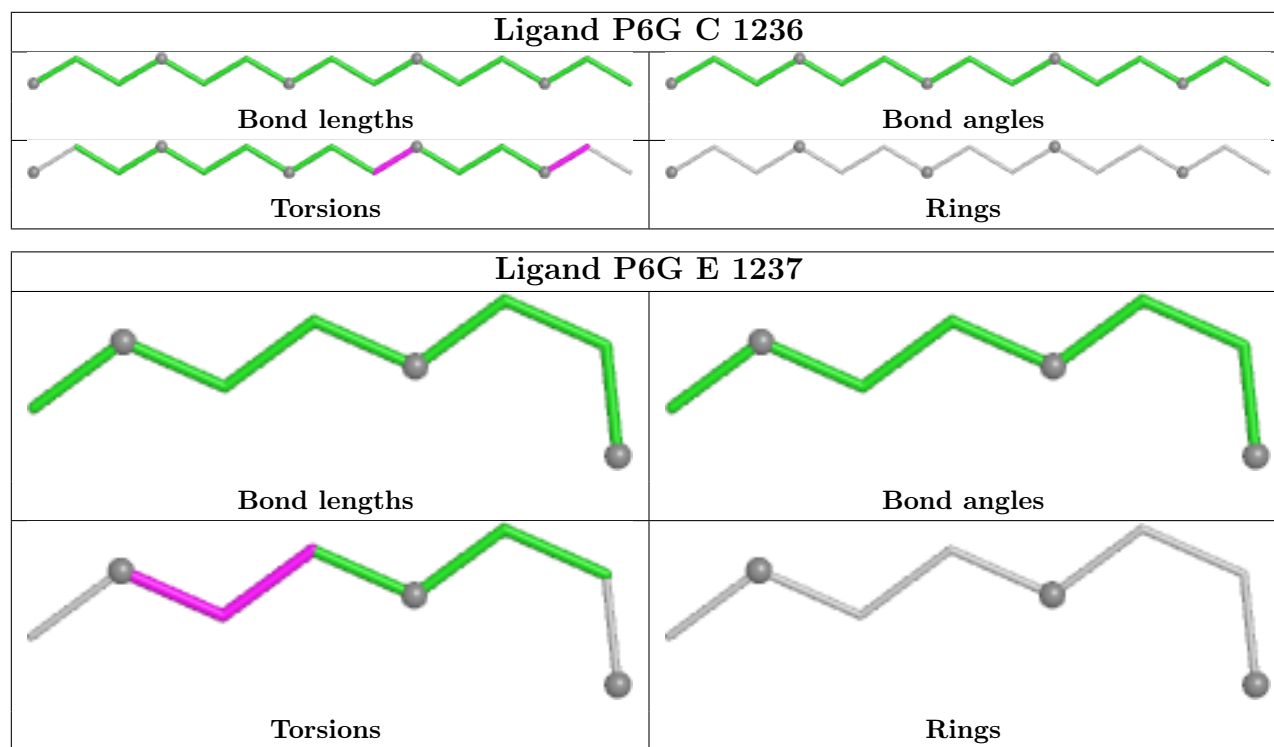
Mol	Chain	Res	Type	Atoms
5	E	1237	P6G	O4-C5-C6-O7
5	B	1236	P6G	O4-C5-C6-O7
5	D	1235	P6G	O4-C5-C6-O7
5	C	1235	P6G	O13-C14-C15-O16
5	A	1235	P6G	O1-C2-C3-O4
5	B	1235	P6G	O1-C2-C3-O4
5	C	1235	P6G	O16-C17-C18-O19
5	E	1236	P6G	O10-C11-C12-O13
5	F	1235	P6G	O10-C11-C12-O13
5	B	1235	P6G	O4-C5-C6-O7
4	C	1234	PG4	O2-C3-C4-O3
5	A	1236	P6G	O1-C2-C3-O4
5	A	1236	P6G	O4-C5-C6-O7
5	B	1236	P6G	O1-C2-C3-O4
4	F	1234	PG4	C4-C3-O2-C2
4	F	1234	PG4	C6-C5-O3-C4
5	D	1235	P6G	C5-C6-O7-C8
5	F	1235	P6G	C12-C11-O10-C9
4	F	1234	PG4	O3-C5-C6-O4
4	E	1234	PG4	C1-C2-O2-C3
5	B	1235	P6G	C9-C8-O7-C6
4	B	1234	PG4	O2-C3-C4-O3
5	E	1235	P6G	O7-C8-C9-O10
5	C	1236	P6G	C2-C3-O4-C5
5	B	1236	P6G	C5-C6-O7-C8
5	E	1235	P6G	C6-C5-O4-C3
5	A	1235	P6G	C2-C3-O4-C5
5	B	1235	P6G	O7-C8-C9-O10
4	A	1234	PG4	O1-C1-C2-O2
5	C	1236	P6G	C9-C8-O7-C6
5	E	1236	P6G	O4-C5-C6-O7
5	E	1237	P6G	C5-C6-O7-C8
4	B	1234	PG4	C1-C2-O2-C3

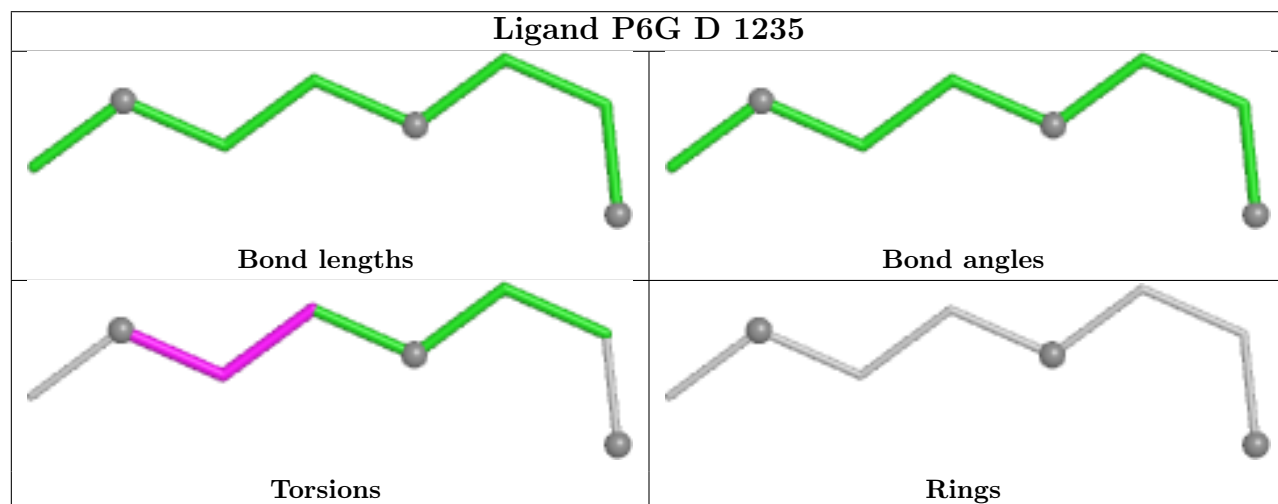
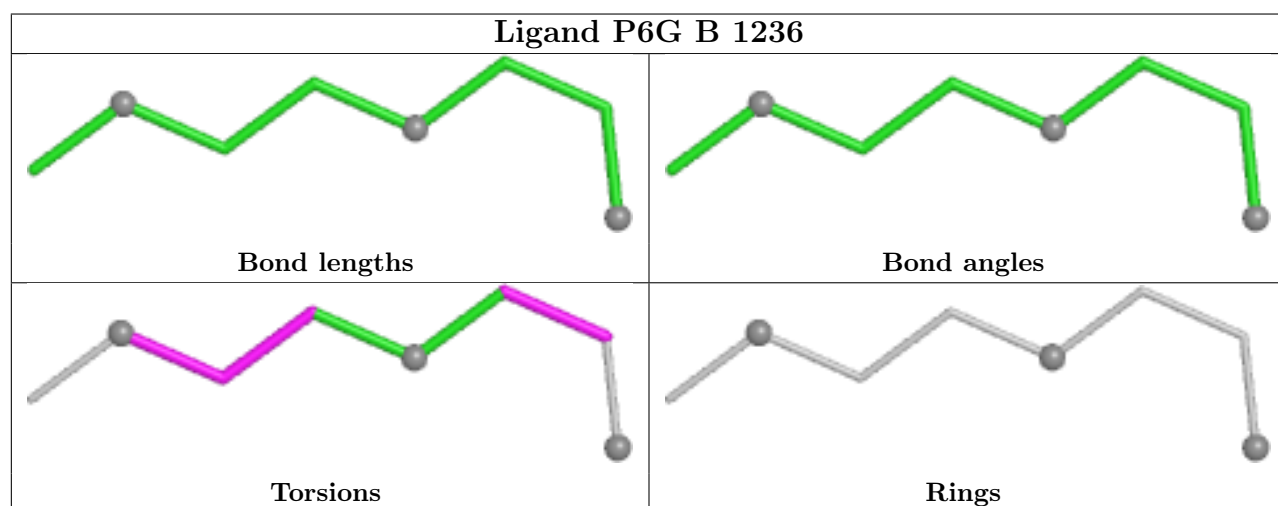
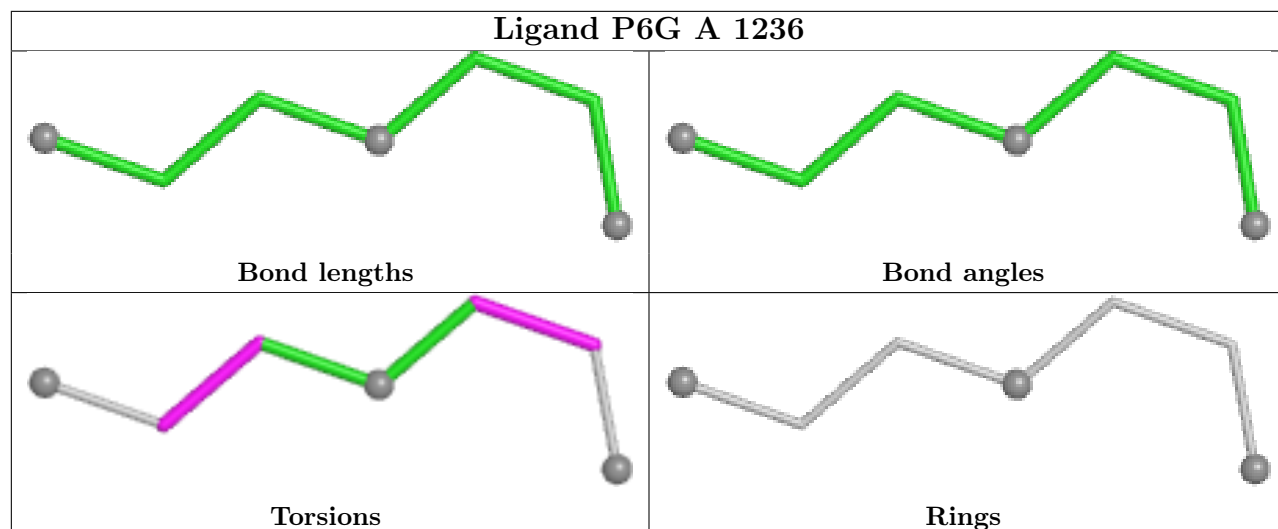
There are no ring outliers.

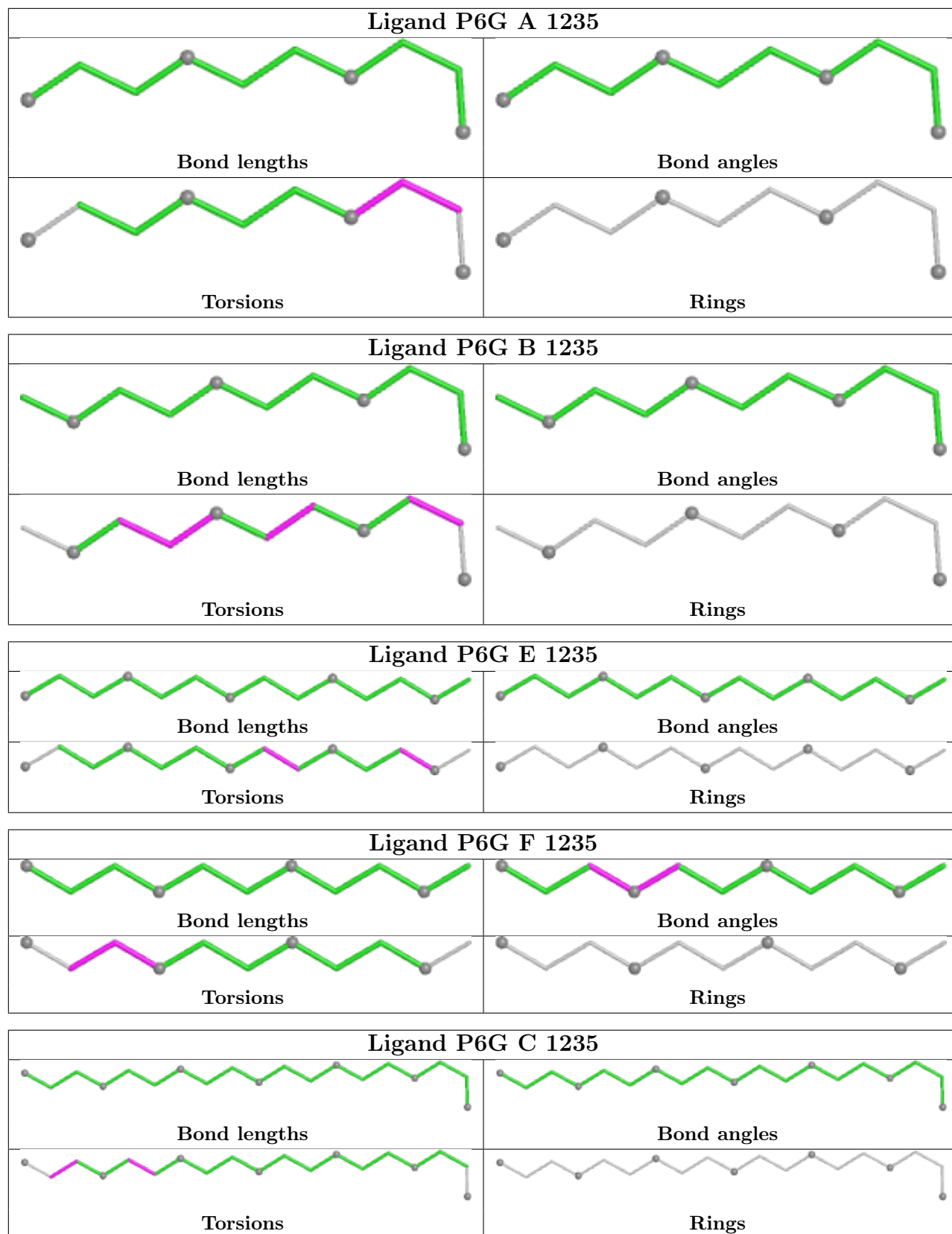
3 monomers are involved in 5 short contacts:

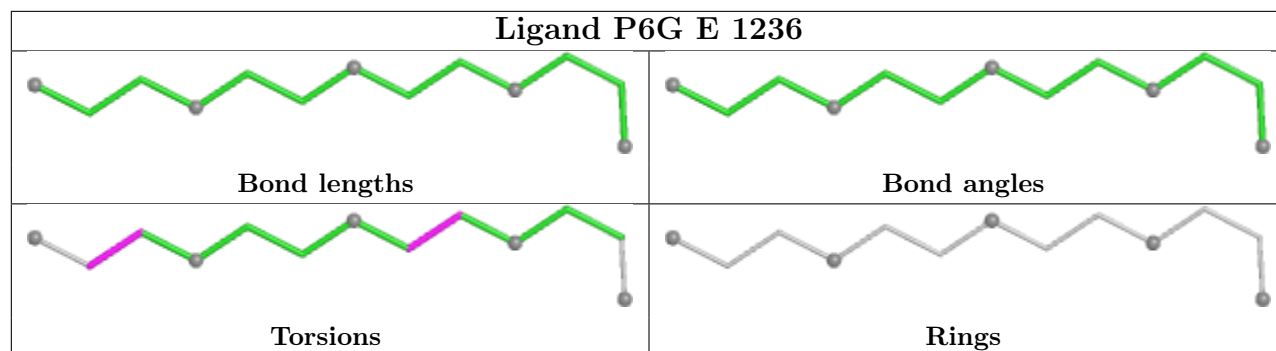
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1234	PG4	2	0
5	B	1235	P6G	2	0
4	B	1234	PG4	1	0

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 [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	198/231 (85%)	-0.14	3 (1%) 72 76	7, 15, 28, 63	4 (2%)
1	B	203/231 (87%)	-0.29	2 (0%) 79 83	7, 14, 25, 31	3 (1%)
1	C	198/231 (85%)	-0.23	4 (2%) 65 69	7, 13, 29, 52	2 (1%)
1	D	197/231 (85%)	-0.16	3 (1%) 72 76	7, 14, 31, 53	2 (1%)
1	E	203/231 (87%)	-0.43	1 (0%) 87 90	6, 11, 22, 33	6 (2%)
1	F	198/231 (85%)	-0.38	3 (1%) 72 76	6, 11, 26, 52	6 (3%)
All	All	1197/1386 (86%)	-0.27	16 (1%) 75 79	6, 13, 28, 63	23 (1%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	136	PRO	4.8
1	F	136	PRO	4.0
1	C	102	ALA	4.0
1	C	136	PRO	3.9
1	D	130	THR	3.8
1	F	130	THR	3.7
1	B	107	THR	3.6
1	E	107	THR	3.1
1	C	130	THR	2.9
1	D	137	VAL	2.8
1	C	158	ASP	2.7
1	A	130	THR	2.4
1	B	158	ASP	2.1
1	A	137	VAL	2.1
1	D	103	LYS	2.1
1	F	102	ALA	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, 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
1	KYN	A	62	14/15	0.95	0.07	11,13,17,17	0
1	KYN	D	62	14/15	0.95	0.06	9,11,15,15	0
1	KYN	C	62	14/15	0.96	0.06	10,12,17,17	0
1	KYN	B	62	14/15	0.96	0.06	8,12,15,16	0
1	KYN	E	62	14/15	0.97	0.06	8,11,18,18	0
1	KYN	F	62	14/15	0.97	0.06	8,10,16,16	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.

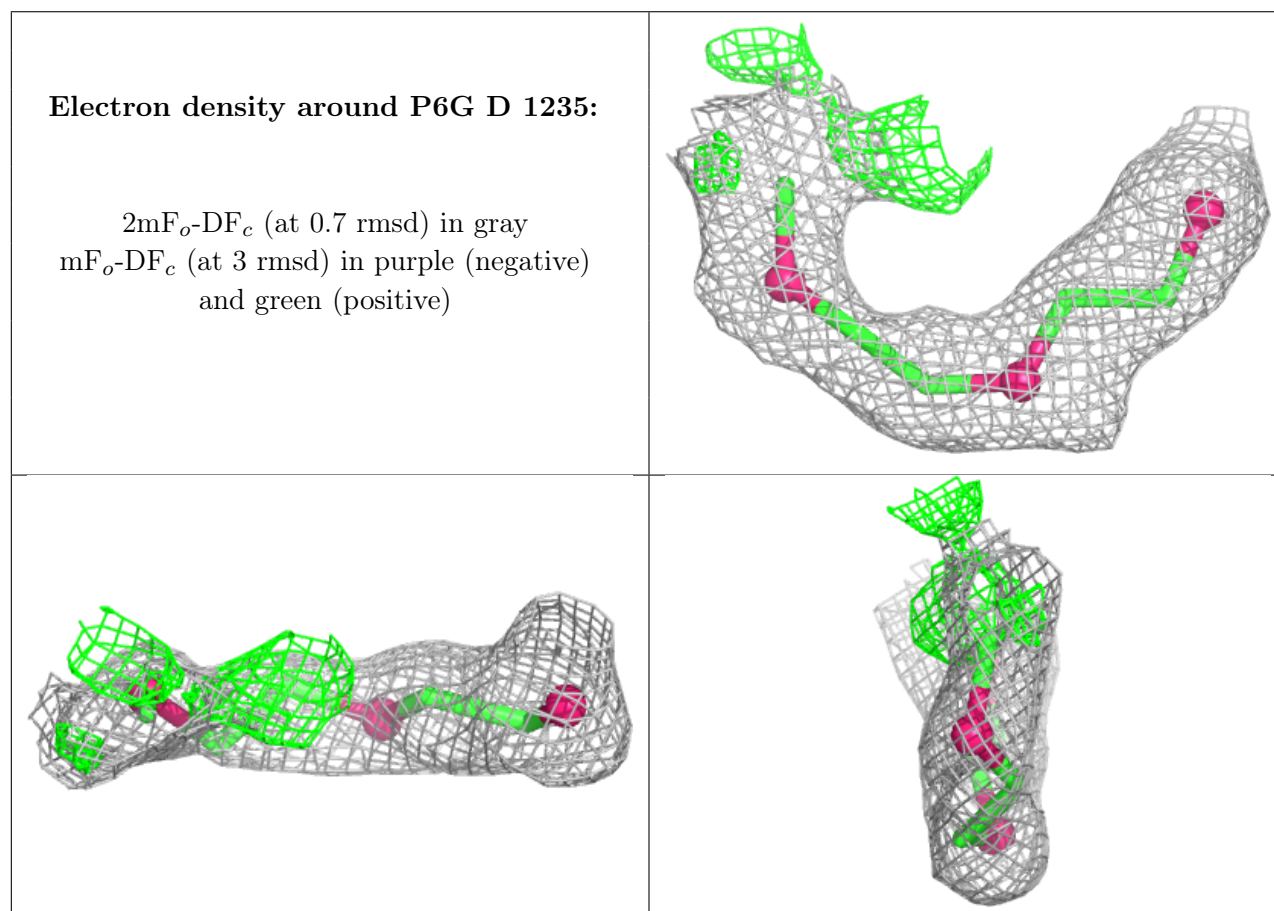
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	P6G	D	1235	8/19	0.77	0.18	31,37,41,43	0
5	P6G	B	1235	11/19	0.79	0.17	30,32,40,40	0
5	P6G	A	1236	7/19	0.79	0.15	41,45,46,52	0
5	P6G	E	1237	8/19	0.83	0.14	35,39,40,44	0
4	PG4	C	1234	6/13	0.84	0.14	27,28,29,32	0
4	PG4	F	1234	8/13	0.84	0.14	22,30,35,36	0
5	P6G	B	1236	8/19	0.85	0.14	35,37,44,49	0
4	PG4	E	1234	6/13	0.85	0.14	21,23,25,25	0
4	PG4	B	1234	6/13	0.85	0.14	28,30,33,34	0
5	P6G	E	1235	14/19	0.86	0.15	24,29,45,48	0
5	P6G	C	1236	15/19	0.86	0.13	28,31,37,38	0
5	P6G	F	1235	11/19	0.86	0.15	27,30,35,42	0
4	PG4	A	1234	4/13	0.88	0.13	30,31,32,33	0
5	P6G	A	1235	10/19	0.89	0.12	29,33,36,37	0
5	P6G	E	1236	13/19	0.89	0.11	25,28,41,47	0
4	PG4	D	1234	7/13	0.90	0.10	23,27,31,41	0

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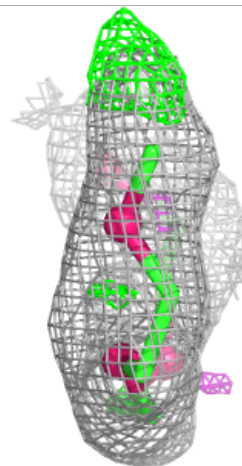
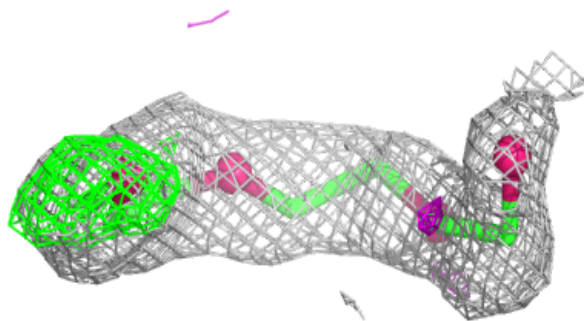
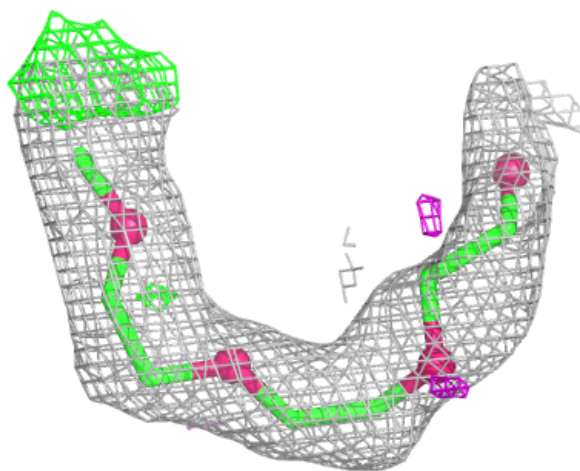
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	P6G	C	1235	19/19	0.90	0.11	20,25,43,44	0
3	CA	B	1233	1/1	0.99	0.08	16,16,16,16	0
2	CU1	A	1232	1/1	0.99	0.06	20,20,20,20	0
2	CU1	B	1232	1/1	0.99	0.04	13,13,13,13	0
2	CU1	D	1232	1/1	0.99	0.04	18,18,18,18	0
2	CU1	E	1232	1/1	0.99	0.03	14,14,14,14	0
2	CU1	F	1232	1/1	0.99	0.03	18,18,18,18	0
3	CA	F	1233	1/1	1.00	0.07	11,11,11,11	0
3	CA	A	1233	1/1	1.00	0.07	14,14,14,14	0
2	CU1	C	1232	1/1	1.00	0.04	19,19,19,19	0
3	CA	C	1233	1/1	1.00	0.08	14,14,14,14	0
3	CA	D	1233	1/1	1.00	0.06	13,13,13,13	0
3	CA	E	1233	1/1	1.00	0.10	13,13,13,13	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.



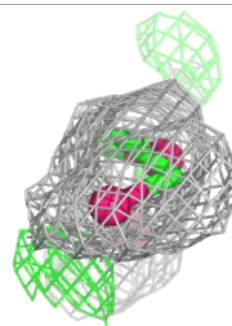
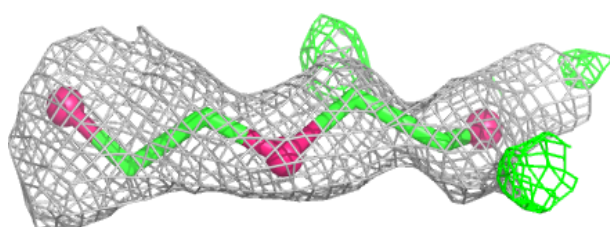
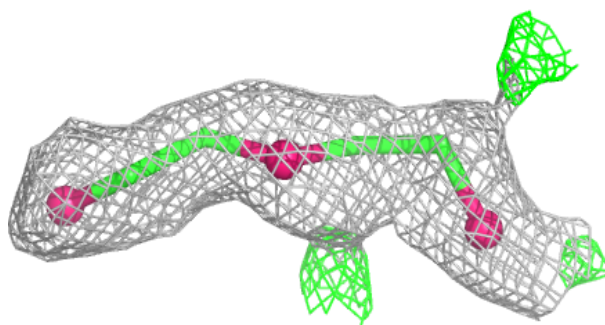
Electron density around P6G B 1235:

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

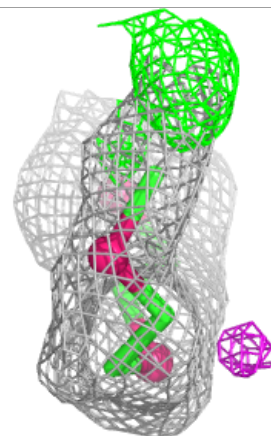
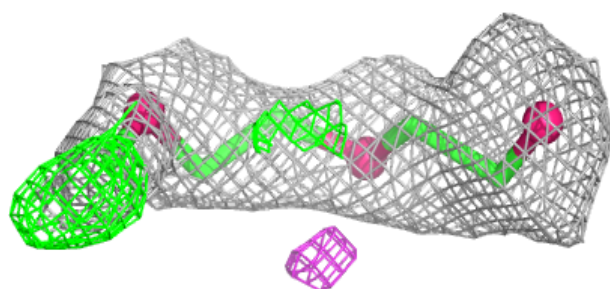
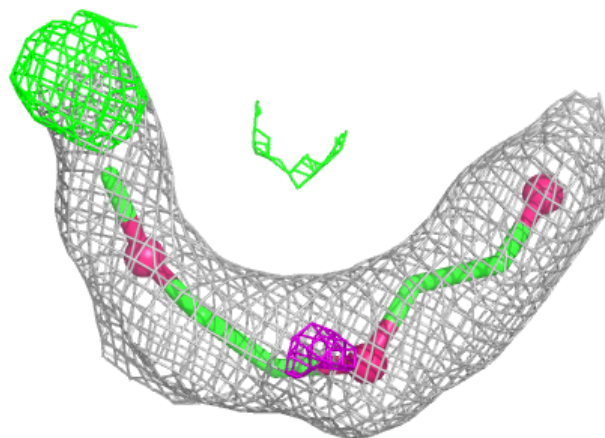


Electron density around P6G A 1236:

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

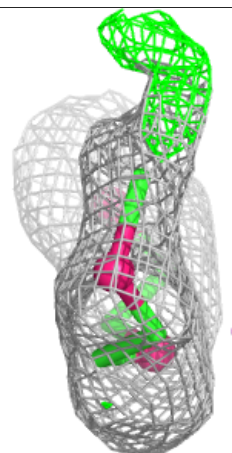
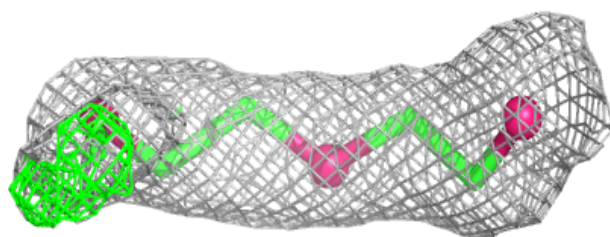
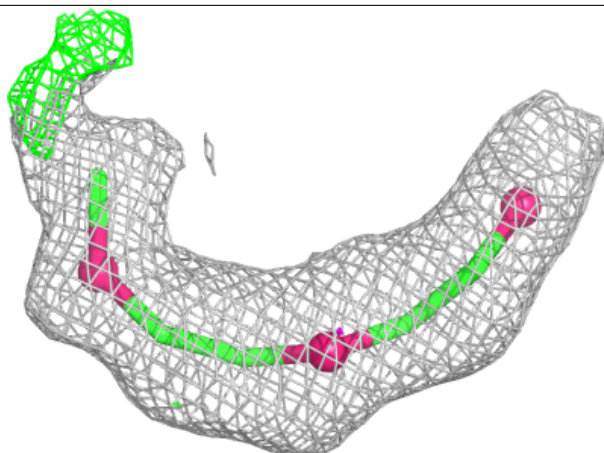
**Electron density around P6G E 1237:**

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



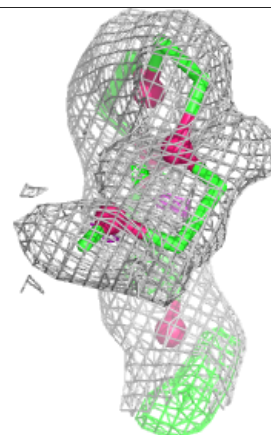
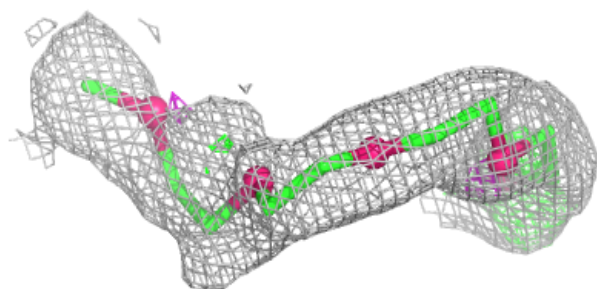
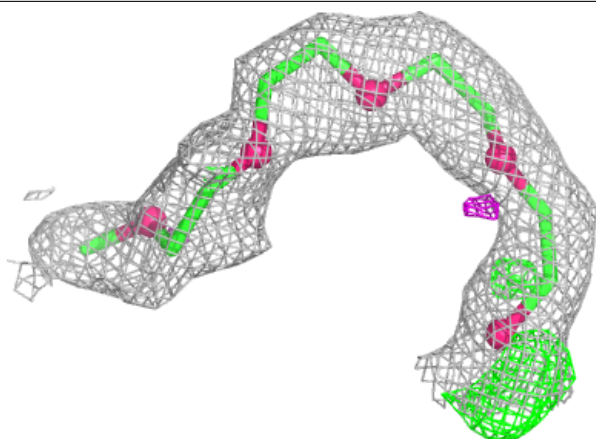
Electron density around P6G B 1236:

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



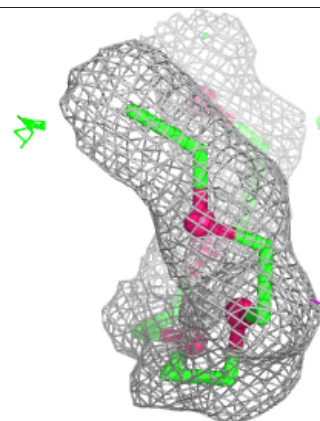
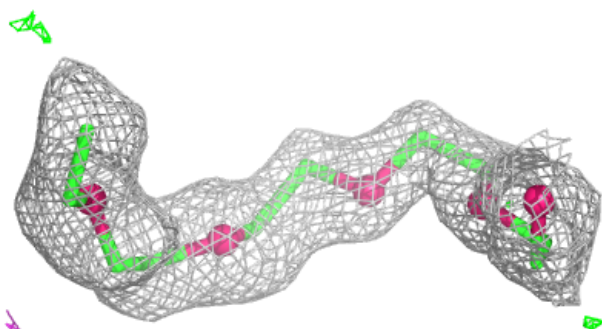
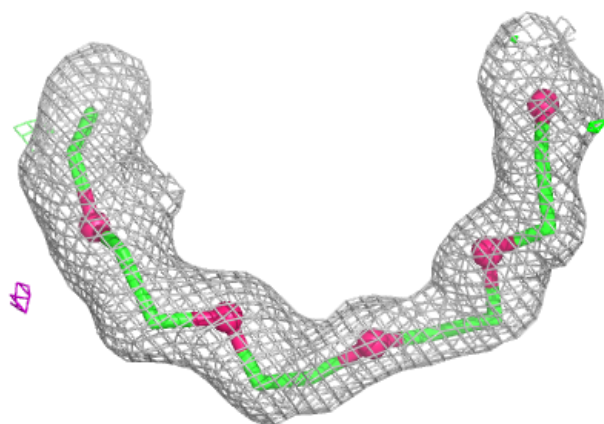
Electron density around P6G E 1235:

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

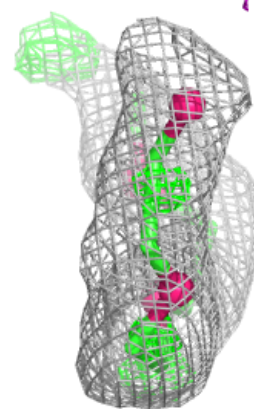
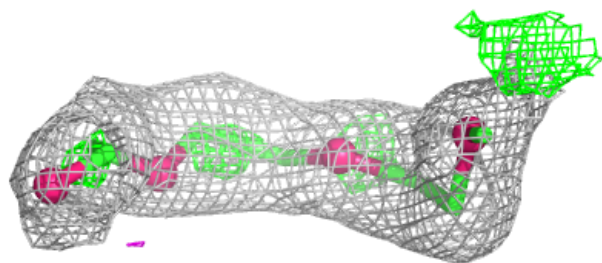
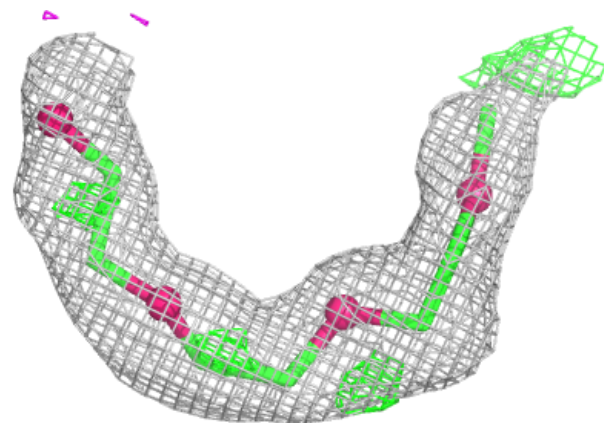


Electron density around P6G C 1236:

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

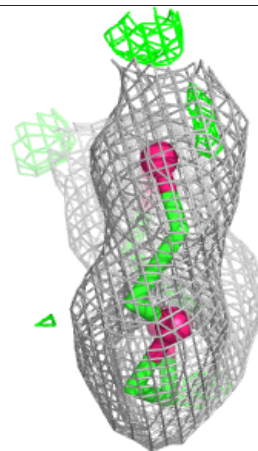
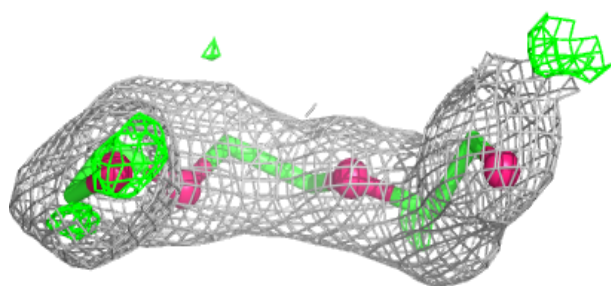
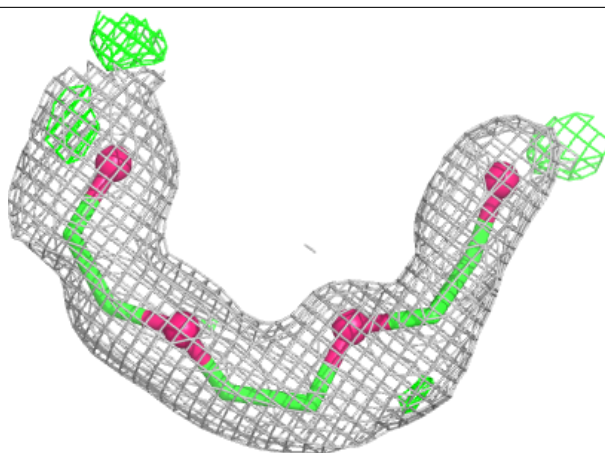
**Electron density around P6G F 1235:**

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



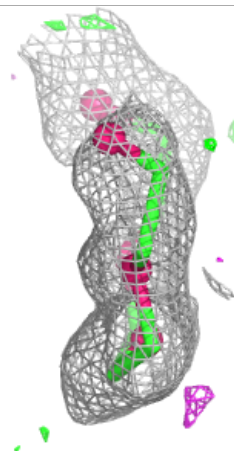
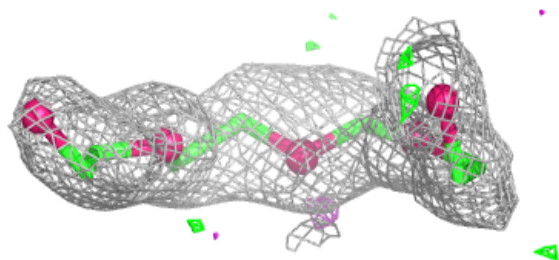
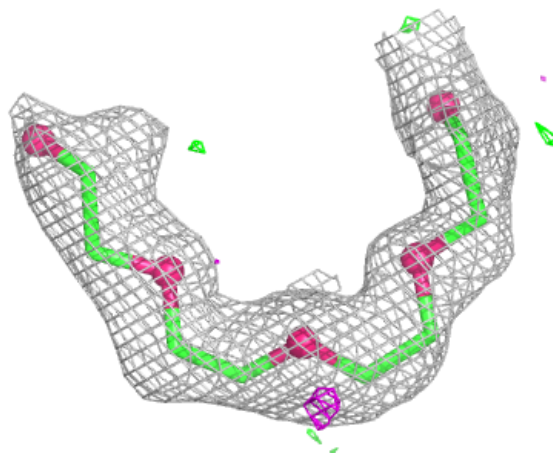
Electron density around P6G A 1235:

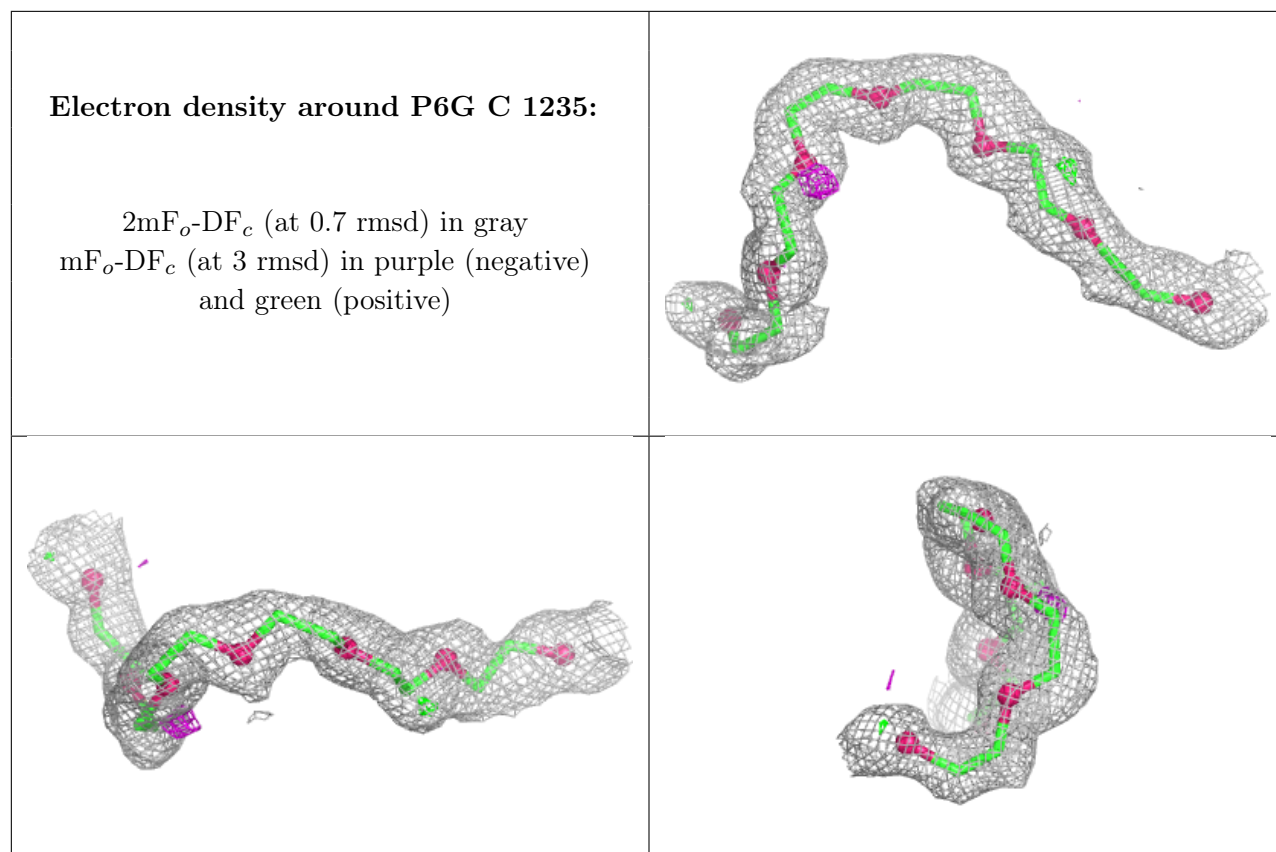
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around P6G E 1236:

$2mF_o-DF_c$ (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.