



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 12:04 pm BST

PDB ID : 3KZQ  
Title : The crystal structure of the protein with unknown function from *Vibrio parahaemolyticus* RIMD 2210633  
Authors : Zhang, R.; Weger, A.; Shackelford, G.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2009-12-08  
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

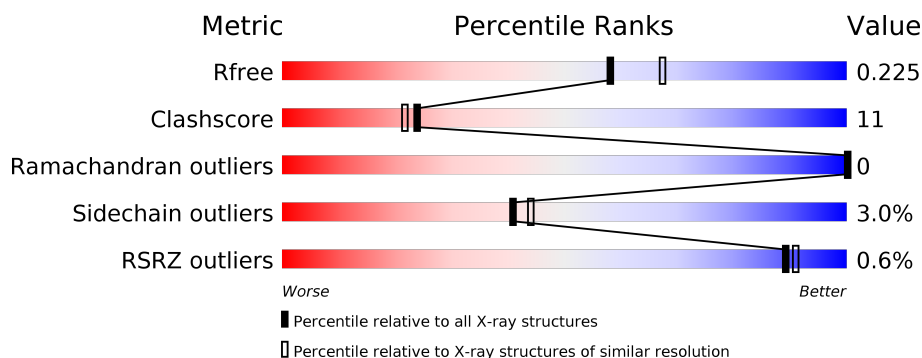
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	208	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>..</div> </div> </div>
1	B	208	<div> <div>80%</div> <div>17%</div> <div>..</div> </div>
1	C	208	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>..</div> </div> </div>
1	D	208	<div> <div>87%</div> <div>11%</div> <div>..</div> </div>
1	E	208	<div> <div>82%</div> <div>14%</div> <div>..</div> </div>
1	F	208	<div> <div>80%</div> <div>17%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PG6	A	209	-	-	X	-
2	PG6	B	212	-	-	X	-
2	PG6	C	209	-	-	X	-
2	PG6	E	209	-	-	X	-
2	PG6	E	210	-	-	X	-
2	PG6	E	211	-	-	X	-
4	GOL	C	210	-	-	X	-
4	GOL	D	209	-	-	X	-
4	GOL	F	209	-	-	X	-

## 2 Entry composition [i](#)

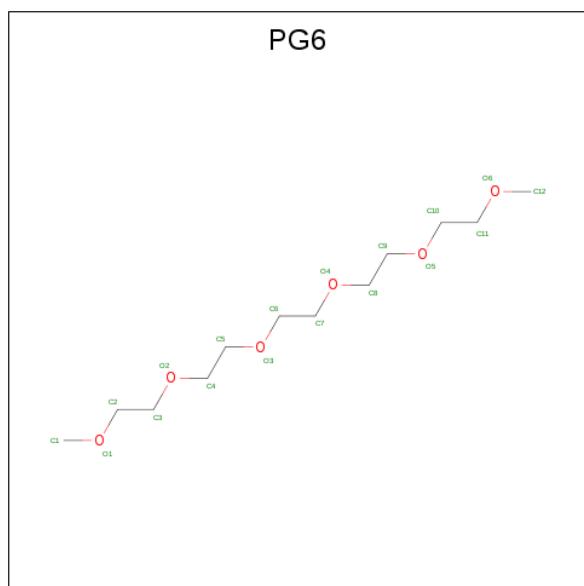
There are 5 unique types of molecules in this entry. The entry contains 11141 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Putative uncharacterized protein VP2116.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1671	1079	270	310	12			
1	B	206	Total	C	N	O	S	0	0	0
			1671	1079	270	310	12			
1	C	206	Total	C	N	O	S	0	0	0
			1671	1079	270	310	12			
1	D	206	Total	C	N	O	S	0	0	0
			1671	1079	270	310	12			
1	E	206	Total	C	N	O	S	0	0	0
			1671	1079	270	310	12			
1	F	206	Total	C	N	O	S	0	0	0
			1671	1079	270	310	12			

- Molecule 2 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANE (three-letter code: PG6) (formula: C<sub>12</sub>H<sub>26</sub>O<sub>6</sub>).

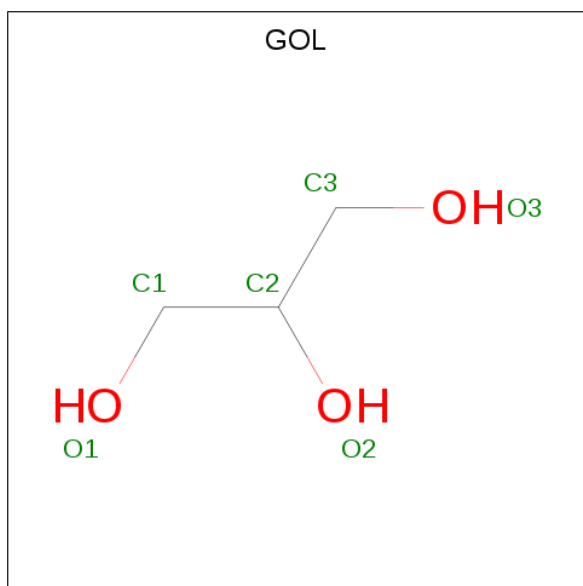


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			18	12	6		
2	B	1	Total	C	O	0	0
			18	12	6		
2	C	1	Total	C	O	0	0
			15	10	5		
2	E	1	Total	C	O	0	0
			12	8	4		
2	E	1	Total	C	O	0	0
			18	12	6		
2	E	1	Total	C	O	0	0
			18	12	6		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Mg	0	0
			3	3		
3	E	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		

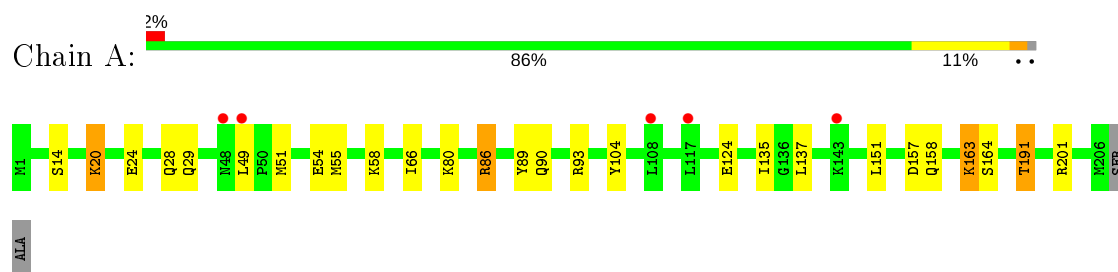
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	140	Total	O	0	0
			140	140		
5	B	176	Total	O	0	0
			176	176		
5	C	172	Total	O	0	0
			172	172		
5	D	133	Total	O	0	0
			133	133		
5	E	179	Total	O	0	0
			179	179		
5	F	164	Total	O	0	0
			164	164		

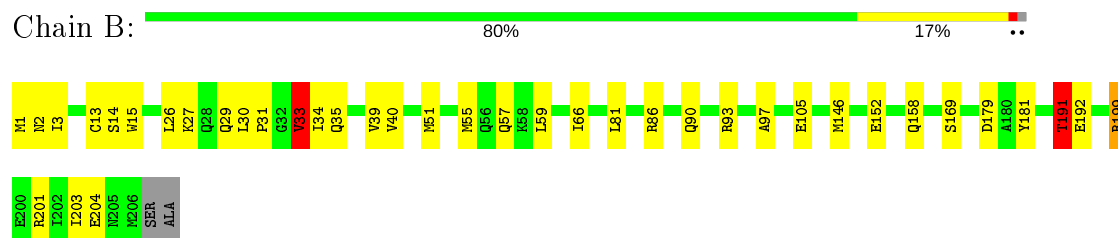
### 3 Residue-property plots [i](#)

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.

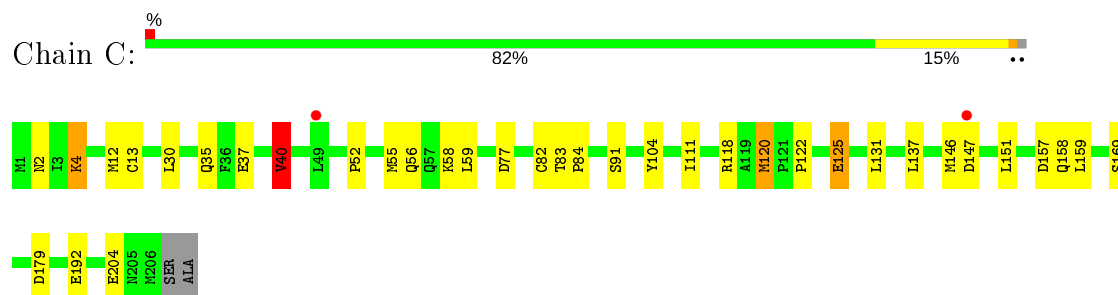
- Molecule 1: Putative uncharacterized protein VP2116



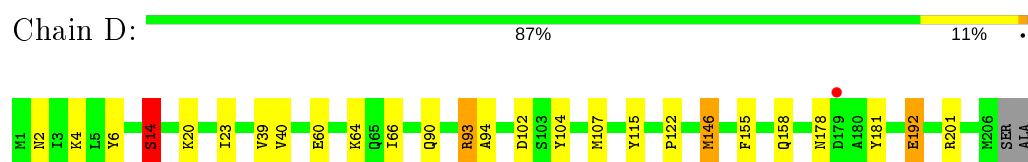
- Molecule 1: Putative uncharacterized protein VP2116



- Molecule 1: Putative uncharacterized protein VP2116



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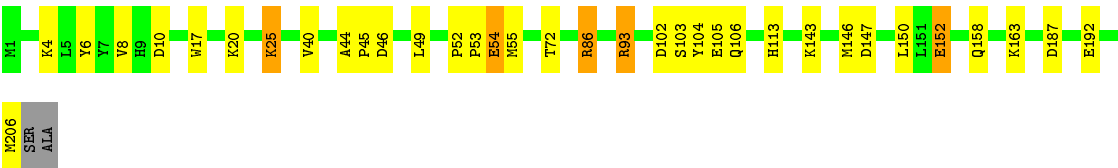
- Molecule 1: Putative uncharacterized protein VP2116

Chain E: 

82%

14%

..



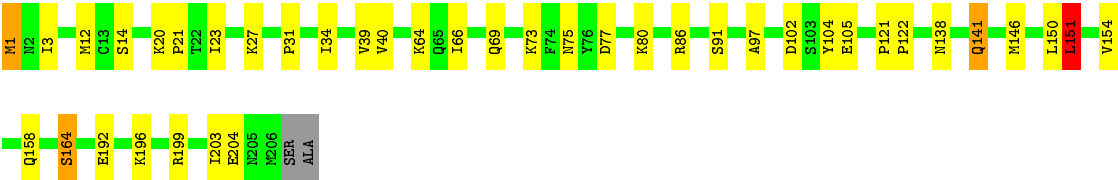
● Molecule 1: Putative uncharacterized protein VP2116

Chain F: 

80%

17%

..





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.30Å 118.11Å 206.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.78 – 2.10 31.78 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.4 (31.78-2.10) 98.4 (31.78-2.10)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.179 , 0.218 0.189 , 0.225	Depositor DCC
$R_{free}$ test set	6103 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.8	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 38.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11141	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PG6, GOL, MG

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	1.10	3/1714 (0.2%)	0.97	3/2328 (0.1%)
1	B	1.25	3/1714 (0.2%)	1.03	6/2328 (0.3%)
1	C	1.19	3/1714 (0.2%)	1.04	7/2328 (0.3%)
1	D	1.08	3/1714 (0.2%)	0.89	1/2328 (0.0%)
1	E	1.25	5/1714 (0.3%)	1.12	8/2328 (0.3%)
1	F	1.16	1/1714 (0.1%)	1.00	4/2328 (0.2%)
All	All	1.17	18/10284 (0.2%)	1.01	29/13968 (0.2%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	204	GLU	CG-CD	8.17	1.64	1.51
1	B	192	GLU	CG-CD	6.83	1.62	1.51
1	C	169	SER	CB-OG	-6.00	1.34	1.42
1	E	152	GLU	CG-CD	5.82	1.60	1.51
1	D	192	GLU	CG-CD	5.63	1.60	1.51
1	F	204	GLU	CG-CD	5.61	1.60	1.51
1	E	192	GLU	CG-CD	5.59	1.60	1.51
1	A	163	LYS	CE-NZ	5.56	1.62	1.49
1	C	125	GLU	CG-CD	5.43	1.60	1.51
1	E	8	VAL	CB-CG2	5.42	1.64	1.52
1	E	25	LYS	CD-CE	5.39	1.64	1.51
1	D	14	SER	CB-OG	-5.30	1.35	1.42
1	C	204	GLU	CG-CD	5.29	1.59	1.51
1	A	28	GLN	CG-CD	5.16	1.62	1.51
1	B	152	GLU	CG-CD	5.15	1.59	1.51
1	E	54	GLU	CB-CG	5.09	1.61	1.52
1	D	146	MET	CG-SD	5.09	1.94	1.81
1	A	89	TYR	CD2-CE2	5.03	1.46	1.39

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	93	ARG	NE-CZ-NH2	-17.37	111.62	120.30
1	E	93	ARG	NE-CZ-NH1	13.84	127.22	120.30
1	E	146	MET	CG-SD-CE	-9.70	84.69	100.20
1	C	40	VAL	CG1-CB-CG2	8.97	125.26	110.90
1	A	20	LYS	CD-CE-NZ	-8.94	91.13	111.70
1	F	146	MET	CG-SD-CE	-8.84	86.06	100.20
1	C	120	MET	CG-SD-CE	-8.51	86.58	100.20
1	B	199	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	E	93	ARG	CG-CD-NE	-6.86	97.40	111.80
1	C	146	MET	CG-SD-CE	-6.80	89.33	100.20
1	E	93	ARG	CD-NE-CZ	6.73	133.02	123.60
1	C	169	SER	N-CA-CB	-6.06	101.41	110.50
1	E	86	ARG	NE-CZ-NH1	-6.05	117.27	120.30
1	B	191	THR	N-CA-CB	-5.83	99.22	110.30
1	C	157	ASP	CB-CG-OD1	5.83	123.55	118.30
1	C	58	LYS	CD-CE-NZ	5.75	124.93	111.70
1	B	201	ARG	CG-CD-NE	-5.67	99.90	111.80
1	B	33	VAL	CB-CA-C	-5.64	100.69	111.40
1	E	10	ASP	CB-CG-OD1	5.62	123.36	118.30
1	F	73	LYS	CD-CE-NZ	-5.60	98.81	111.70
1	F	164	SER	CA-CB-OG	-5.54	96.23	111.20
1	A	157	ASP	CB-CG-OD1	5.30	123.07	118.30
1	B	30	LEU	CA-CB-CG	5.15	127.15	115.30
1	E	187	ASP	CB-CG-OD1	5.12	122.91	118.30
1	B	26	LEU	CB-CG-CD1	-5.08	102.36	111.00
1	A	163	LYS	CD-CE-NZ	5.04	123.28	111.70
1	D	93	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	F	151	LEU	CA-CB-CG	-5.01	103.78	115.30
1	C	30	LEU	CB-CG-CD2	-5.00	102.50	111.00

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	1671	0	1653	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1671	0	1653	35	0
1	C	1671	0	1653	39	0
1	D	1671	0	1653	23	0
1	E	1671	0	1653	54	0
1	F	1671	0	1653	33	0
2	A	18	0	26	9	0
2	B	18	0	26	9	0
2	C	15	0	19	10	0
2	E	48	0	67	55	0
3	B	3	0	0	0	0
3	E	1	0	0	0	0
4	C	18	0	24	9	0
4	D	12	0	16	6	0
4	F	18	0	24	7	0
5	A	140	0	0	2	0
5	B	176	0	0	7	0
5	C	172	0	0	4	0
5	D	133	0	0	0	0
5	E	179	0	0	8	0
5	F	164	0	0	4	0
All	All	11141	0	10120	225	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (225) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:GLN:HE22	2:A:209:PG6:H111	1.21	1.05
1:F:12:MET:CE	1:F:91:SER:HB3	1.87	1.05
1:B:2:ASN:HB3	5:B:1030:HOH:O	1.58	1.03
1:B:29:GLN:OE1	1:B:191:THR:HG21	1.56	1.02
4:C:211:GOL:H32	5:C:216:HOH:O	1.62	1.00
1:F:12:MET:HE3	1:F:91:SER:HB3	1.42	1.00
1:E:158:GLN:NE2	2:E:211:PG6:H12	1.78	0.97
1:F:104:TYR:H	4:F:209:GOL:H32	1.28	0.96
1:A:158:GLN:OE1	2:A:209:PG6:H122	1.66	0.95
1:C:12:MET:CE	1:C:91:SER:HB3	1.96	0.95
1:E:20:LYS:HD3	2:E:209:PG6:H22	1.49	0.94
1:E:17:TRP:O	2:E:209:PG6:H41	1.67	0.93
1:E:113:HIS:HE1	2:E:209:PG6:H12	1.35	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:MET:HB2	2:C:209:PG6:H71	1.51	0.90
1:A:29:GLN:OE1	1:A:191:THR:HG21	1.71	0.89
1:B:15:TRP:HD1	2:B:212:PG6:H41	1.37	0.89
1:E:52:PRO:HD3	2:E:210:PG6:H51	1.53	0.89
2:E:209:PG6:H13	5:E:1092:HOH:O	1.72	0.89
1:C:82:CYS:O	4:C:210:GOL:H31	1.72	0.88
1:A:158:GLN:HE22	2:A:209:PG6:C11	1.87	0.86
1:E:52:PRO:CD	2:E:210:PG6:H51	2.09	0.83
1:E:106:GLN:HG3	2:E:211:PG6:O6	1.77	0.83
1:B:181:TYR:O	2:E:210:PG6:H72	1.80	0.79
1:E:104:TYR:H	2:E:211:PG6:H81	1.48	0.78
1:F:12:MET:CE	1:F:91:SER:CB	2.62	0.77
1:C:12:MET:HE3	1:C:91:SER:HB3	1.66	0.77
1:E:49:LEU:HD21	2:E:210:PG6:H41	1.68	0.76
2:E:211:PG6:H91	5:E:764:HOH:O	1.86	0.75
1:C:12:MET:CE	1:C:91:SER:CB	2.65	0.74
1:E:113:HIS:HE1	2:E:209:PG6:C1	2.00	0.74
1:B:93:ARG:O	1:B:146:MET:HE3	1.88	0.74
1:D:104:TYR:HB3	4:D:209:GOL:H31	1.70	0.73
1:C:118:ARG:HB2	1:C:120:MET:CE	2.18	0.72
1:E:106:GLN:HG3	2:E:211:PG6:C12	2.20	0.72
1:F:104:TYR:N	4:F:209:GOL:H32	2.05	0.71
1:A:90:GLN:NE2	1:A:93:ARG:HH11	1.89	0.71
1:E:49:LEU:HD21	2:E:210:PG6:C4	2.20	0.71
1:C:55:MET:HB2	2:C:209:PG6:C7	2.21	0.70
1:C:12:MET:HE3	1:C:91:SER:CB	2.20	0.70
1:E:17:TRP:O	2:E:209:PG6:C4	2.38	0.70
1:F:12:MET:HE2	1:F:91:SER:HB3	1.73	0.70
1:F:12:MET:HE2	1:F:91:SER:CB	2.21	0.70
1:A:104:TYR:OH	2:A:209:PG6:H123	1.93	0.69
1:A:158:GLN:NE2	2:A:209:PG6:H111	2.04	0.69
1:A:51:MET:HE2	1:A:55:MET:HG2	1.74	0.69
1:C:118:ARG:CB	1:C:120:MET:HE2	2.23	0.69
1:F:12:MET:HE3	1:F:91:SER:CB	2.20	0.69
1:D:14:SER:H	4:D:210:GOL:H31	1.56	0.68
1:C:77:ASP:OD2	1:E:113:HIS:HD2	1.77	0.67
1:B:97:ALA:HB2	1:B:146:MET:CE	2.25	0.66
1:F:105:GLU:H	4:F:209:GOL:H11	1.61	0.66
1:E:158:GLN:HE22	2:E:211:PG6:H12	1.60	0.65
1:B:90:GLN:NE2	1:B:93:ARG:HH11	1.95	0.65
1:C:52:PRO:HG3	2:C:209:PG6:H41	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:GLN:HE21	1:A:93:ARG:NH1	1.96	0.64
1:E:4:LYS:HD2	1:E:6:TYR:CZ	2.33	0.64
1:B:27:LYS:HE2	1:B:105:GLU:OE2	1.99	0.63
1:E:103:SER:HA	2:E:211:PG6:C11	2.28	0.63
1:E:113:HIS:CE1	2:E:209:PG6:C1	2.82	0.62
1:C:2:ASN:ND2	1:C:35:GLN:HE22	1.98	0.62
1:A:20:LYS:HE2	1:A:24:GLU:OE2	1.99	0.62
1:D:102:ASP:HA	4:D:209:GOL:H11	1.82	0.61
1:E:55:MET:CE	2:E:210:PG6:H112	2.29	0.61
1:C:52:PRO:HG3	2:C:209:PG6:H32	1.83	0.61
1:A:90:GLN:HE21	1:A:93:ARG:HH11	1.47	0.61
1:C:55:MET:HE2	2:C:209:PG6:H91	1.83	0.60
1:D:90:GLN:NE2	1:D:93:ARG:HH11	1.99	0.60
1:A:104:TYR:CE1	2:A:209:PG6:H123	2.36	0.60
1:D:94:ALA:HB1	1:D:107:MET:HE2	1.84	0.60
1:B:97:ALA:HB2	1:B:146:MET:HE2	1.84	0.59
1:B:181:TYR:O	2:E:210:PG6:C7	2.51	0.59
1:A:51:MET:CE	1:A:55:MET:HG2	2.31	0.59
1:D:14:SER:HB3	1:D:66:ILE:CD1	2.32	0.59
1:F:14:SER:H	4:F:211:GOL:H31	1.67	0.59
1:E:158:GLN:HE21	2:E:211:PG6:H12	1.67	0.59
1:B:14:SER:HB3	1:B:66:ILE:CD1	2.33	0.59
1:B:29:GLN:OE1	1:B:191:THR:CG2	2.44	0.59
1:E:113:HIS:CE1	2:E:209:PG6:H12	2.27	0.59
1:E:106:GLN:HG3	2:E:211:PG6:H121	1.84	0.59
1:C:179:ASP:HB2	5:C:253:HOH:O	2.02	0.58
1:B:15:TRP:CD1	2:B:212:PG6:H41	2.29	0.58
1:E:103:SER:HA	2:E:211:PG6:H112	1.85	0.58
1:D:155:PHE:O	1:D:158:GLN:HB2	2.02	0.58
1:E:104:TYR:CB	2:E:211:PG6:H81	2.33	0.58
1:B:51:MET:CE	1:B:59:LEU:HD22	2.34	0.58
1:D:39:VAL:HA	1:D:158:GLN:HE22	1.68	0.58
1:E:104:TYR:CE1	2:E:211:PG6:H13	2.39	0.58
1:C:118:ARG:CB	1:C:120:MET:CE	2.80	0.57
1:F:69:GLN:HB2	5:F:227:HOH:O	2.04	0.57
1:E:104:TYR:OH	2:E:211:PG6:H13	2.05	0.57
1:E:104:TYR:H	2:E:211:PG6:C8	2.16	0.57
1:E:86:ARG:NH1	5:E:229:HOH:O	2.38	0.57
1:C:118:ARG:HB3	1:C:120:MET:HE2	1.85	0.56
1:A:90:GLN:NE2	1:A:93:ARG:NH1	2.54	0.56
1:E:104:TYR:HB2	2:E:211:PG6:H81	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:31:PRO:HD2	1:F:34:ILE:HD12	1.87	0.56
1:E:20:LYS:CD	2:E:209:PG6:H22	2.30	0.55
1:F:86:ARG:HH12	4:F:211:GOL:H11	1.71	0.55
1:C:118:ARG:HB2	1:C:120:MET:HE3	1.86	0.55
1:D:40:VAL:H	1:D:158:GLN:HE21	1.55	0.55
1:A:104:TYR:CZ	2:A:209:PG6:H123	2.42	0.55
1:B:35:GLN:HG3	5:B:370:HOH:O	2.07	0.55
1:B:179:ASP:O	2:E:210:PG6:H12	2.06	0.55
1:C:12:MET:HE3	1:C:91:SER:OG	2.07	0.55
1:C:55:MET:CB	2:C:209:PG6:H71	2.31	0.54
1:C:12:MET:HE2	1:C:91:SER:CB	2.37	0.54
1:D:2:ASN:H	1:D:178:ASN:ND2	2.06	0.54
1:B:97:ALA:HB2	1:B:146:MET:HE3	1.90	0.53
1:C:2:ASN:HD21	1:C:35:GLN:HE22	1.56	0.53
1:E:72:THR:HG23	2:E:209:PG6:H42	1.90	0.53
1:D:4:LYS:HD2	1:D:6:TYR:CZ	2.44	0.53
1:A:124:GLU:HG3	5:A:529:HOH:O	2.08	0.53
1:F:39:VAL:HA	1:F:158:GLN:HE22	1.74	0.52
1:E:102:ASP:C	2:E:211:PG6:H82	2.30	0.52
1:E:105:GLU:HB2	2:E:211:PG6:H102	1.92	0.52
2:E:211:PG6:H51	5:E:231:HOH:O	2.10	0.51
1:B:39:VAL:HA	1:B:158:GLN:HE22	1.74	0.51
1:C:52:PRO:HB3	2:C:209:PG6:H32	1.93	0.51
1:B:13:CYS:SG	2:B:212:PG6:H42	2.50	0.51
1:E:206:MET:N	5:E:291:HOH:O	2.43	0.51
1:B:33:VAL:HG22	5:B:265:HOH:O	2.11	0.50
1:F:40:VAL:H	1:F:158:GLN:HE21	1.59	0.50
1:E:55:MET:HE2	2:E:210:PG6:H112	1.92	0.50
1:C:55:MET:CE	2:C:209:PG6:H91	2.41	0.50
2:B:212:PG6:C1	5:B:646:HOH:O	2.59	0.50
1:C:84:PRO:CD	4:C:210:GOL:H12	2.42	0.50
1:B:90:GLN:HE21	1:B:93:ARG:HH11	1.58	0.49
1:F:12:MET:HE1	1:F:122:PRO:C	2.32	0.49
1:F:196:LYS:HE3	5:F:337:HOH:O	2.12	0.49
1:C:13:CYS:HA	4:C:212:GOL:H31	1.94	0.49
1:E:103:SER:HA	2:E:211:PG6:H111	1.92	0.49
1:E:158:GLN:NE2	2:E:211:PG6:C1	2.65	0.49
1:A:20:LYS:HD2	5:A:210:HOH:O	2.11	0.49
1:E:55:MET:HG3	2:E:210:PG6:H61	1.95	0.49
2:B:212:PG6:H11	5:B:646:HOH:O	2.13	0.49
1:C:111:ILE:HD13	1:C:131:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:ASN:H	1:D:178:ASN:HD21	1.59	0.49
1:C:12:MET:HE1	1:C:122:PRO:O	2.14	0.48
1:D:102:ASP:HA	4:D:209:GOL:C1	2.43	0.48
1:B:31:PRO:HD2	1:B:34:ILE:HD12	1.95	0.48
1:E:143:LYS:HE3	1:E:147:ASP:OD2	2.14	0.48
1:E:49:LEU:CD2	2:E:210:PG6:H41	2.41	0.48
1:D:90:GLN:HE21	1:D:93:ARG:HH11	1.62	0.48
1:A:14:SER:HB3	1:A:66:ILE:CD1	2.44	0.47
1:C:40:VAL:H	1:C:158:GLN:NE2	2.12	0.47
1:E:104:TYR:CZ	2:E:211:PG6:H13	2.49	0.47
1:E:54:GLU:HB2	2:E:210:PG6:H91	1.96	0.47
1:B:51:MET:HE2	1:B:55:MET:CB	2.45	0.47
1:B:1:MET:HG2	1:B:3:ILE:HD11	1.97	0.47
1:C:4:LYS:HE3	1:C:37:GLU:OE1	2.15	0.47
1:E:104:TYR:OH	2:E:211:PG6:C1	2.63	0.47
1:B:169:SER:HB2	2:B:212:PG6:H71	1.96	0.47
1:E:152:GLU:HA	1:E:152:GLU:OE1	2.13	0.47
1:F:199:ARG:O	1:F:203:ILE:HG12	2.15	0.47
1:B:51:MET:HE2	1:B:55:MET:C	2.35	0.47
1:D:40:VAL:H	1:D:158:GLN:NE2	2.12	0.47
1:A:54:GLU:CD	1:A:54:GLU:H	2.19	0.47
2:B:212:PG6:H61	5:B:239:HOH:O	2.14	0.47
1:D:60:GLU:O	1:D:64:LYS:HG3	2.15	0.47
1:F:20:LYS:HB3	1:F:21:PRO:HD3	1.96	0.47
1:B:27:LYS:CE	1:B:105:GLU:OE2	2.63	0.46
1:E:158:GLN:HE22	2:E:211:PG6:C1	2.27	0.46
1:F:151:LEU:HG	1:F:151:LEU:O	2.13	0.46
1:B:51:MET:HE2	1:B:55:MET:CG	2.46	0.46
1:A:55:MET:SD	1:A:86:ARG:HG2	2.55	0.46
1:E:46:ASP:CG	1:E:93:ARG:HH22	2.19	0.46
1:C:56:GLN:OE1	4:C:210:GOL:O2	2.31	0.46
1:F:40:VAL:H	1:F:158:GLN:NE2	2.14	0.46
1:E:102:ASP:HA	2:E:211:PG6:H82	1.98	0.46
2:E:209:PG6:H52	2:E:209:PG6:H32	1.49	0.46
1:E:72:THR:HA	2:E:209:PG6:H62	1.96	0.45
1:B:51:MET:HE3	1:B:59:LEU:HD22	1.99	0.45
1:C:111:ILE:HD13	1:C:131:LEU:CD1	2.45	0.45
1:D:181:TYR:CD2	1:D:181:TYR:N	2.84	0.45
1:F:27:LYS:HE2	5:F:254:HOH:O	2.15	0.45
1:C:84:PRO:HD2	4:C:210:GOL:H12	1.98	0.45
1:C:118:ARG:HD3	1:C:120:MET:HE1	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:GLN:NE2	1:D:93:ARG:NH1	2.65	0.45
1:A:90:GLN:NE2	1:A:93:ARG:HD2	2.32	0.44
1:A:29:GLN:OE1	1:A:191:THR:CG2	2.55	0.44
2:E:209:PG6:H11	5:E:789:HOH:O	2.17	0.44
1:A:104:TYR:CE1	2:A:209:PG6:H112	2.53	0.44
1:D:102:ASP:CA	4:D:209:GOL:H11	2.47	0.44
1:E:104:TYR:N	2:E:211:PG6:H81	2.26	0.44
1:E:44:ALA:HA	1:E:45:PRO:HD3	1.86	0.44
1:A:93:ARG:HB3	1:A:151:LEU:HD21	2.01	0.43
1:D:102:ASP:C	4:D:209:GOL:H11	2.39	0.43
1:F:14:SER:HB3	1:F:66:ILE:CD1	2.48	0.43
1:F:192:GLU:HG3	5:F:1084:HOH:O	2.17	0.43
1:D:201:ARG:HD3	1:D:201:ARG:HA	1.76	0.43
2:E:209:PG6:H31	5:E:221:HOH:O	2.18	0.43
1:F:102:ASP:C	4:F:209:GOL:H31	2.39	0.43
1:C:120:MET:HE3	1:C:120:MET:HB2	1.84	0.43
1:B:86:ARG:HH12	2:B:212:PG6:H12	1.83	0.43
1:C:104:TYR:HB3	4:C:211:GOL:H12	2.00	0.43
1:B:90:GLN:NE2	1:B:93:ARG:NH1	2.63	0.42
1:C:52:PRO:CG	2:C:209:PG6:H32	2.47	0.42
1:A:135:ILE:HG22	1:A:137:LEU:HG	2.01	0.42
1:B:199:ARG:O	1:B:203:ILE:HG12	2.18	0.42
1:E:40:VAL:HG22	1:E:158:GLN:HE21	1.85	0.42
1:F:138:ASN:HB3	1:F:141:GLN:HG2	2.00	0.42
1:B:51:MET:HE1	1:B:59:LEU:HD22	2.02	0.42
4:C:210:GOL:H11	5:C:350:HOH:O	2.19	0.42
1:A:104:TYR:OH	2:A:209:PG6:C12	2.65	0.42
1:C:83:THR:HA	4:C:210:GOL:H12	2.01	0.42
1:D:115:TYR:HB2	1:D:122:PRO:HB3	2.02	0.42
1:E:49:LEU:HG	2:E:210:PG6:H22	2.01	0.42
1:F:97:ALA:HB2	1:F:151:LEU:HD13	2.02	0.42
1:F:121:PRO:HA	1:F:122:PRO:HD2	1.94	0.41
1:B:40:VAL:H	1:B:158:GLN:HE21	1.68	0.41
1:F:20:LYS:HA	1:F:23:ILE:HG22	2.02	0.41
1:F:75:ASN:OD1	1:F:77:ASP:HB2	2.20	0.41
1:A:201:ARG:HA	1:A:201:ARG:HD3	1.84	0.41
1:F:105:GLU:H	4:F:209:GOL:C1	2.29	0.41
1:A:51:MET:HE2	1:A:55:MET:C	2.40	0.41
1:F:1:MET:HG2	1:F:3:ILE:HD11	2.02	0.41
1:D:20:LYS:HA	1:D:23:ILE:HG22	2.03	0.41
2:C:209:PG6:H41	2:C:209:PG6:H61	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:150:LEU:O	1:F:154:VAL:HG23	2.21	0.40
1:E:55:MET:CE	2:E:210:PG6:C11	2.96	0.40
1:B:51:MET:HE2	1:B:55:MET:HG2	2.03	0.40
1:E:55:MET:HE3	2:E:210:PG6:C11	2.51	0.40
2:B:212:PG6:C5	5:B:239:HOH:O	2.69	0.40
1:C:158:GLN:NE2	5:C:229:HOH:O	2.53	0.40
2:E:211:PG6:H101	5:E:223:HOH:O	2.20	0.40

There are no symmetry-related clashes.

## 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	204/208 (98%)	201 (98%)	3 (2%)	0	100	100
1	B	204/208 (98%)	201 (98%)	3 (2%)	0	100	100
1	C	204/208 (98%)	201 (98%)	3 (2%)	0	100	100
1	D	204/208 (98%)	199 (98%)	5 (2%)	0	100	100
1	E	204/208 (98%)	201 (98%)	3 (2%)	0	100	100
1	F	204/208 (98%)	200 (98%)	4 (2%)	0	100	100
All	All	1224/1248 (98%)	1203 (98%)	21 (2%)	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	184/185 (100%)	177 (96%)	7 (4%)	33	34
1	B	184/185 (100%)	180 (98%)	4 (2%)	52	57
1	C	184/185 (100%)	175 (95%)	9 (5%)	25	23
1	D	184/185 (100%)	181 (98%)	3 (2%)	62	69
1	E	184/185 (100%)	180 (98%)	4 (2%)	52	57
1	F	184/185 (100%)	178 (97%)	6 (3%)	38	40
All	All	1104/1110 (100%)	1071 (97%)	33 (3%)	41	44

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LEU
1	A	58	LYS
1	A	80	LYS
1	A	86	ARG
1	A	163	LYS
1	A	164	SER
1	A	191	THR
1	B	33	VAL
1	B	57	GLN
1	B	81	LEU
1	B	191	THR
1	C	4	LYS
1	C	40	VAL
1	C	59	LEU
1	C	125	GLU
1	C	137	LEU
1	C	147	ASP
1	C	151	LEU
1	C	159	LEU
1	C	192	GLU
1	D	14	SER
1	D	146	MET
1	D	192	GLU
1	E	25	LYS
1	E	53	PRO
1	E	150	LEU
1	E	163	LYS
1	F	1	MET

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Mol	Chain	Res	Type
1	F	64	LYS
1	F	80	LYS
1	F	141	GLN
1	F	151	LEU
1	F	164	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	90	GLN
1	A	123	HIS
1	A	130	GLN
1	B	48	ASN
1	B	90	GLN
1	B	158	GLN
1	B	205	ASN
1	C	2	ASN
1	C	48	ASN
1	C	156	GLN
1	C	158	GLN
1	D	57	GLN
1	D	90	GLN
1	D	158	GLN
1	D	178	ASN
1	E	35	GLN
1	E	69	GLN
1	E	113	HIS
1	E	158	GLN
1	F	130	GLN
1	F	158	GLN
1	F	176	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	$\# Z  > 2$
4	GOL	C	212	-	5,5,5	0.45	0	5,5,5	0.86	0
2	PG6	A	209	-	17,17,17	1.05	0	16,16,16	0.90	0
2	PG6	C	209	-	14,14,17	1.08	0	13,13,16	1.55	3 (23%)
2	PG6	E	211	-	17,17,17	1.24	0	16,16,16	1.14	1 (6%)
2	PG6	B	212	-	17,17,17	0.65	0	16,16,16	0.52	0
2	PG6	E	210	3	17,17,17	1.04	0	16,16,16	1.82	5 (31%)
4	GOL	C	210	-	5,5,5	0.44	0	5,5,5	1.02	0
4	GOL	F	210	-	5,5,5	0.70	0	5,5,5	1.47	1 (20%)
4	GOL	D	210	-	5,5,5	0.56	0	5,5,5	0.72	0
4	GOL	C	211	-	5,5,5	0.33	0	5,5,5	1.52	1 (20%)
4	GOL	D	209	-	5,5,5	0.73	0	5,5,5	1.18	1 (20%)
4	GOL	F	209	-	5,5,5	0.51	0	5,5,5	1.05	0
4	GOL	F	211	-	5,5,5	0.32	0	5,5,5	0.68	0
2	PG6	E	209	-	11,11,17	1.16	0	10,10,16	1.71	3 (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
4	GOL	C	212	-	-	4/4/4/4	-
2	PG6	A	209	-	-	10/15/15/15	-
2	PG6	C	209	-	-	8/12/12/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PG6	E	211	-	-	10/15/15/15	-
2	PG6	B	212	-	-	10/15/15/15	-
2	PG6	E	210	3	-	9/15/15/15	-
4	GOL	C	210	-	-	0/4/4/4	-
4	GOL	F	210	-	-	3/4/4/4	-
4	GOL	D	210	-	-	3/4/4/4	-
4	GOL	C	211	-	-	4/4/4/4	-
4	GOL	D	209	-	-	2/4/4/4	-
4	GOL	F	209	-	-	2/4/4/4	-
4	GOL	F	211	-	-	2/4/4/4	-
2	PG6	E	209	-	-	6/9/9/15	-

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	210	PG6	O2-C3-C2	4.08	128.80	110.39
2	E	209	PG6	O3-C6-C7	3.44	125.92	110.39
2	C	209	PG6	O2-C3-C2	3.20	124.83	110.39
4	F	210	GOL	C3-C2-C1	3.01	123.39	111.70
2	E	210	PG6	C1-O1-C2	2.61	129.19	112.96
2	C	209	PG6	O2-C4-C5	2.43	121.36	110.39
2	E	210	PG6	C8-O4-C7	2.43	123.82	113.29
4	D	209	GOL	O2-C2-C1	-2.28	99.09	109.12
2	E	210	PG6	O5-C9-C8	2.25	120.53	110.39
2	E	211	PG6	C8-O4-C7	2.23	122.93	113.29
2	E	209	PG6	C1-O1-C2	2.23	126.81	112.96
2	E	209	PG6	O2-C3-C2	2.09	119.83	110.39
2	E	210	PG6	C6-O3-C5	2.08	122.32	113.29
4	C	211	GOL	O2-C2-C3	2.06	118.19	109.12
2	C	209	PG6	O4-C7-C6	2.04	119.61	110.39

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	212	GOL	O1-C1-C2-C3
4	C	212	GOL	C1-C2-C3-O3
4	D	210	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	D	210	GOL	O1-C1-C2-C3
4	F	211	GOL	O1-C1-C2-O2
4	F	209	GOL	C1-C2-C3-O3
2	E	210	PG6	C2-C3-O2-C4
2	A	209	PG6	C5-C4-O2-C3
2	C	209	PG6	C4-C5-O3-C6
2	E	209	PG6	C5-C4-O2-C3
2	E	211	PG6	C4-C5-O3-C6
2	E	210	PG6	O1-C2-C3-O2
2	E	211	PG6	O5-C10-C11-O6
2	B	212	PG6	C10-C11-O6-C12
2	A	209	PG6	O2-C4-C5-O3
2	C	209	PG6	O1-C2-C3-O2
2	A	209	PG6	C3-C2-O1-C1
2	E	211	PG6	C10-C11-O6-C12
2	B	212	PG6	O2-C4-C5-O3
4	C	212	GOL	O1-C1-C2-O2
2	C	209	PG6	C9-C8-O4-C7
2	E	210	PG6	O4-C8-C9-O5
2	E	210	PG6	O5-C10-C11-O6
2	E	211	PG6	O3-C6-C7-O4
2	E	210	PG6	O3-C6-C7-O4
2	C	209	PG6	O2-C4-C5-O3
2	E	211	PG6	O1-C2-C3-O2
4	F	211	GOL	O1-C1-C2-C3
4	F	210	GOL	O1-C1-C2-C3
4	F	210	GOL	C1-C2-C3-O3
4	D	209	GOL	O1-C1-C2-C3
4	C	211	GOL	O1-C1-C2-C3
4	C	211	GOL	C1-C2-C3-O3
2	B	212	PG6	O3-C6-C7-O4
2	A	209	PG6	C8-C9-O5-C10
4	C	212	GOL	O2-C2-C3-O3
4	D	209	GOL	O2-C2-C3-O3
4	C	211	GOL	O1-C1-C2-O2
4	C	211	GOL	O2-C2-C3-O3
2	B	212	PG6	O5-C10-C11-O6
2	E	210	PG6	O2-C4-C5-O3
2	A	209	PG6	O5-C10-C11-O6
2	E	211	PG6	O4-C8-C9-O5
2	A	209	PG6	O4-C8-C9-O5
4	D	210	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	F	210	GOL	O2-C2-C3-O3
2	A	209	PG6	C6-C7-O4-C8
2	A	209	PG6	C11-C10-O5-C9
2	E	209	PG6	O1-C2-C3-O2
2	A	209	PG6	C7-C6-O3-C5
2	C	209	PG6	C5-C4-O2-C3
2	E	210	PG6	C4-C5-O3-C6
2	E	209	PG6	C6-C7-O4-C8
2	E	209	PG6	C3-C2-O1-C1
2	E	211	PG6	C11-C10-O5-C9
2	A	209	PG6	C9-C8-O4-C7
2	E	211	PG6	C8-C9-O5-C10
2	E	211	PG6	C2-C3-O2-C4
2	E	209	PG6	C2-C3-O2-C4
2	C	209	PG6	C3-C2-O1-C1
4	F	209	GOL	O2-C2-C3-O3
2	C	209	PG6	C8-C9-O5-C10
2	B	212	PG6	C7-C6-O3-C5
2	E	210	PG6	C11-C10-O5-C9
2	E	210	PG6	C8-C9-O5-C10
2	E	209	PG6	O2-C4-C5-O3
2	B	212	PG6	C5-C4-O2-C3
2	B	212	PG6	C3-C2-O1-C1
2	B	212	PG6	O4-C8-C9-O5
2	B	212	PG6	C8-C9-O5-C10
2	B	212	PG6	C11-C10-O5-C9
2	E	211	PG6	O2-C4-C5-O3
2	C	209	PG6	O4-C8-C9-O5

There are no ring outliers.

13 monomers are involved in 105 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	212	GOL	1	0
2	A	209	PG6	9	0
2	C	209	PG6	10	0
2	E	211	PG6	26	0
2	B	212	PG6	9	0
2	E	210	PG6	15	0
4	C	210	GOL	6	0
4	D	210	GOL	1	0
4	C	211	GOL	2	0

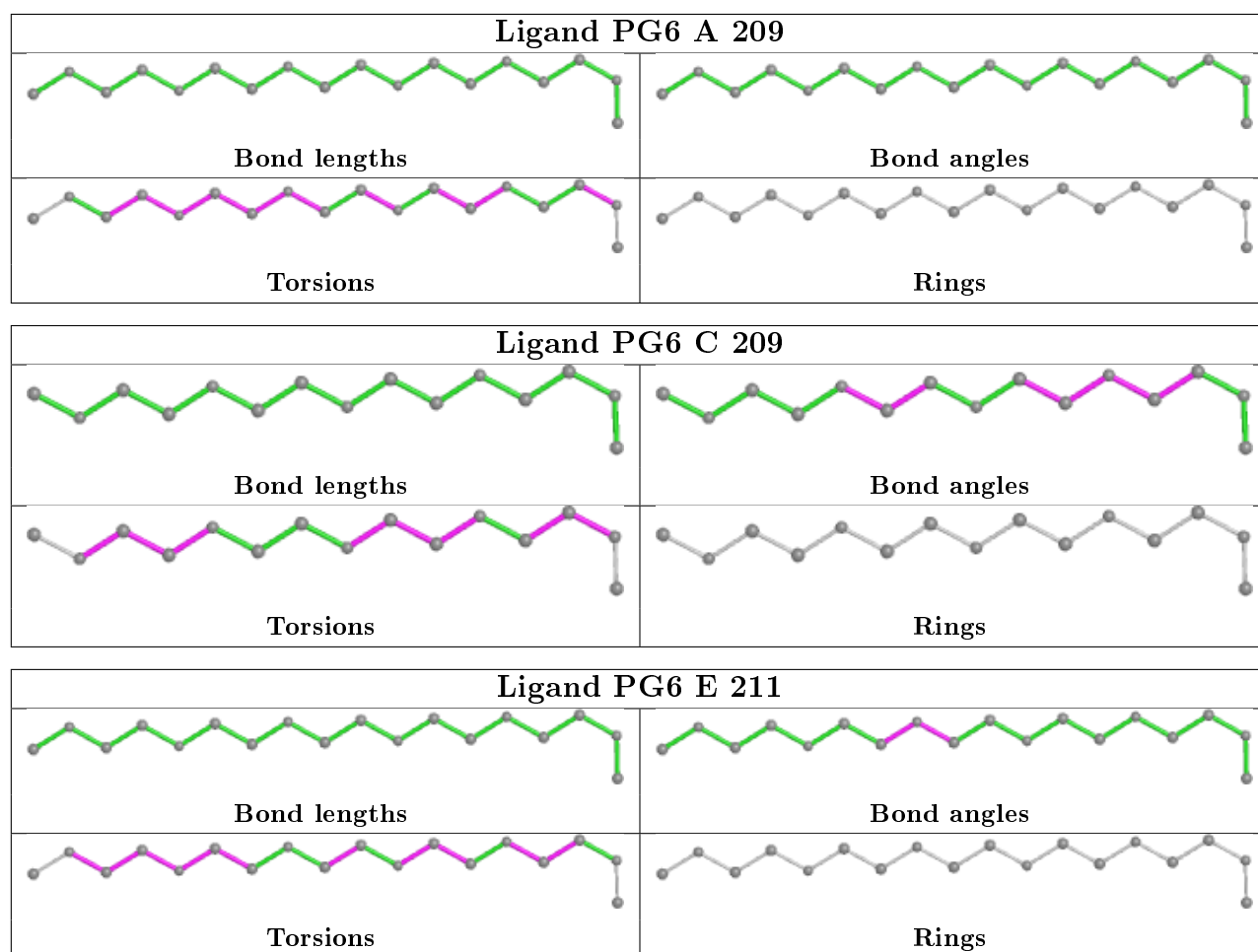
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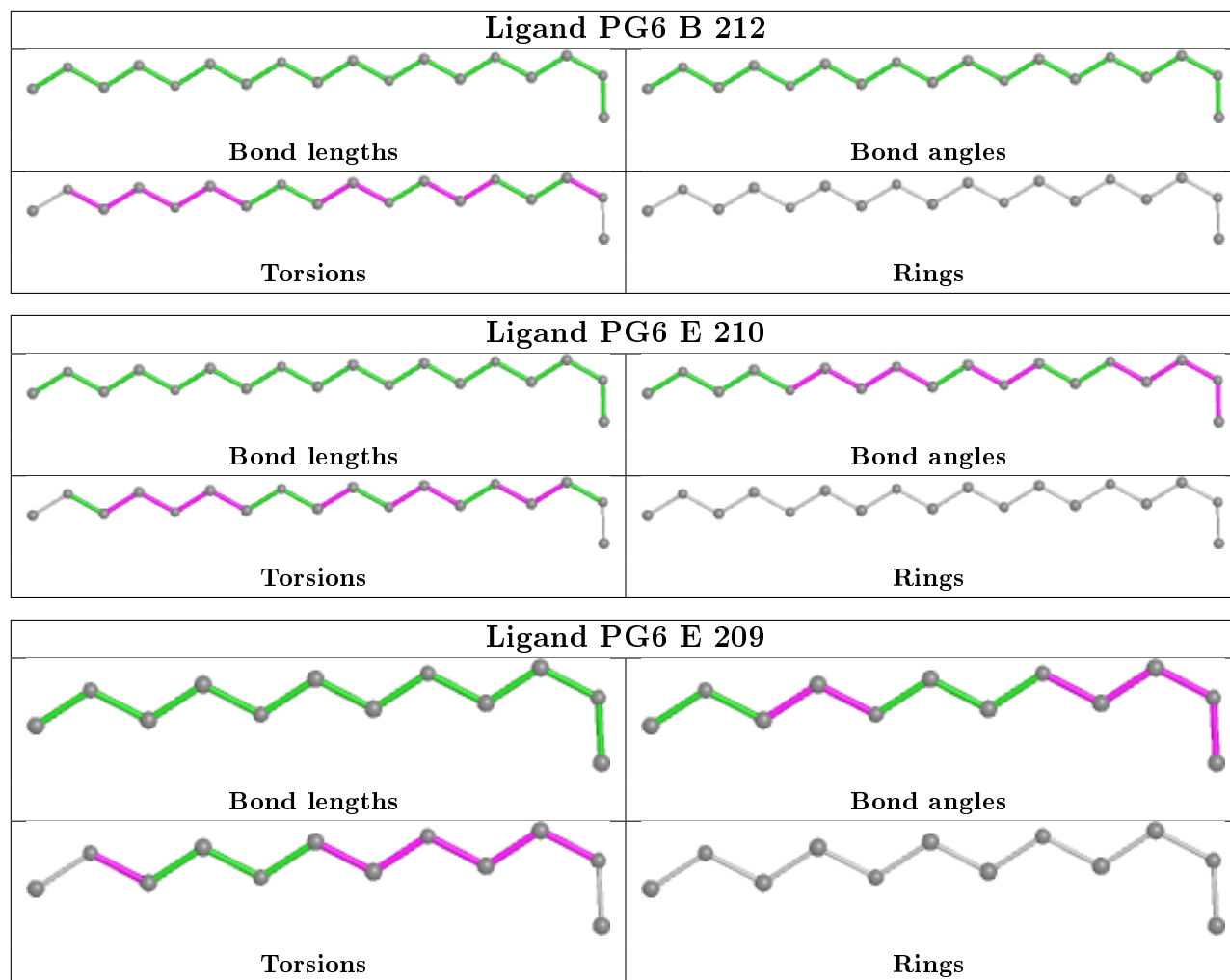


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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	209	GOL	5	0
4	F	209	GOL	5	0
4	F	211	GOL	2	0
2	E	209	PG6	14	0

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, 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	206/208 (99%)	-0.13	5 (2%) 59 64	8, 16, 28, 35	0
1	B	206/208 (99%)	-0.34	0 100 100	6, 14, 26, 31	0
1	C	206/208 (99%)	-0.28	2 (0%) 82 85	8, 15, 27, 33	0
1	D	206/208 (99%)	-0.27	1 (0%) 91 92	10, 18, 30, 34	0
1	E	206/208 (99%)	-0.30	0 100 100	6, 13, 25, 35	0
1	F	206/208 (99%)	-0.36	0 100 100	7, 14, 26, 32	0
All	All	1236/1248 (99%)	-0.28	8 (0%) 89 91	6, 15, 27, 35	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	49	LEU	2.8
1	C	147	ASP	2.7
1	A	48	ASN	2.5
1	A	117	LEU	2.4
1	A	143	LYS	2.3
1	A	108	LEU	2.2
1	C	49	LEU	2.1
1	D	179	ASP	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

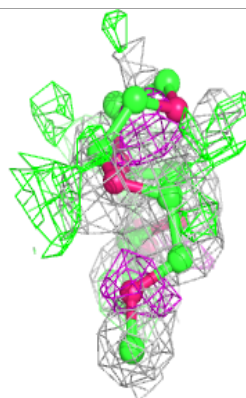
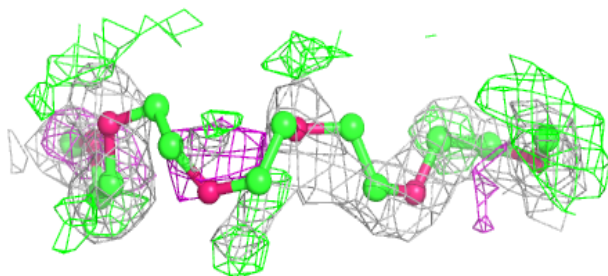
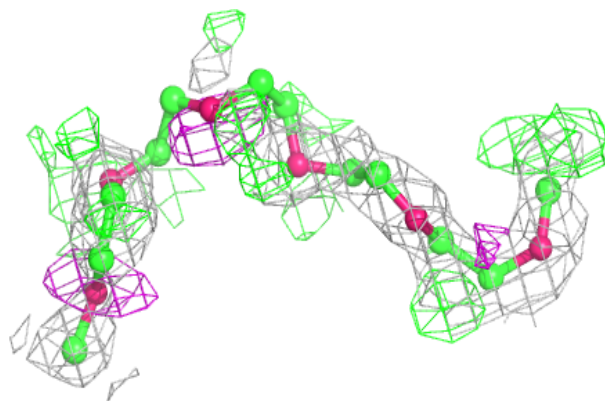
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	PG6	A	209	18/18	0.59	0.36	21,62,82,83	0
2	PG6	B	212	18/18	0.73	0.21	58,72,77,78	0
4	GOL	C	211	6/6	0.75	0.27	47,52,54,56	0
4	GOL	F	210	6/6	0.77	0.21	50,55,57,58	0
2	PG6	E	211	18/18	0.77	0.35	21,48,63,65	0
2	PG6	C	209	15/18	0.78	0.30	38,54,73,73	0
4	GOL	D	209	6/6	0.79	0.31	47,57,59,63	0
4	GOL	D	210	6/6	0.80	0.21	48,57,59,64	0
4	GOL	F	209	6/6	0.81	0.21	40,46,49,50	0
4	GOL	F	211	6/6	0.82	0.15	58,62,63,64	0
4	GOL	C	210	6/6	0.85	0.24	43,45,48,52	0
4	GOL	C	212	6/6	0.85	0.13	55,56,57,57	0
2	PG6	E	210	18/18	0.85	0.35	23,44,66,67	0
2	PG6	E	209	12/18	0.87	0.32	16,31,51,53	0
3	MG	E	212	1/1	0.96	0.08	34,34,34,34	0
3	MG	B	209	1/1	0.98	0.11	33,33,33,33	0
3	MG	B	211	1/1	0.98	0.07	34,34,34,34	0
3	MG	B	210	1/1	0.99	0.08	30,30,30,30	0

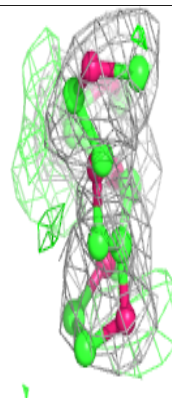
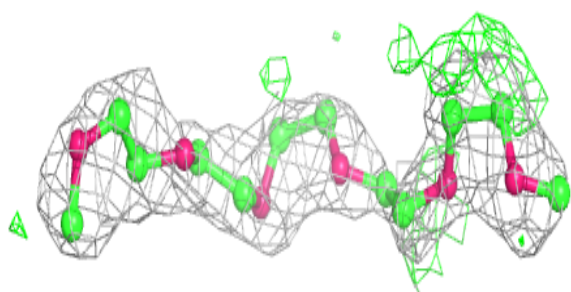
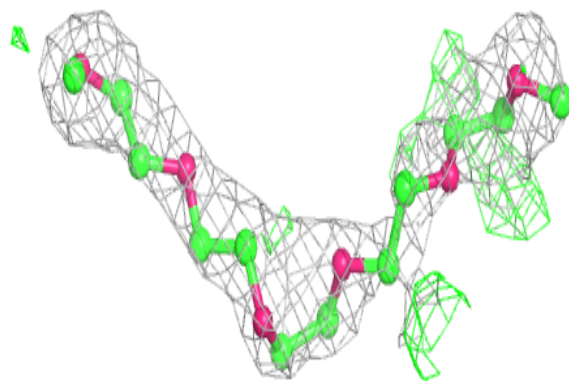
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around PG6 A 209:**

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

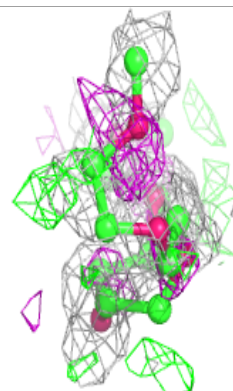
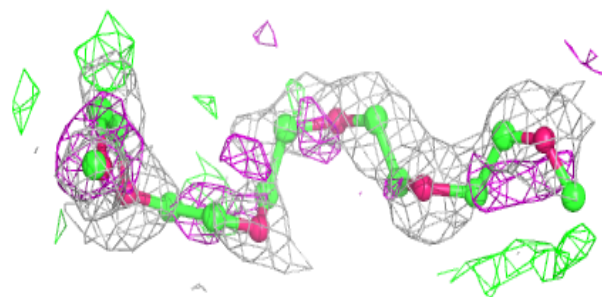
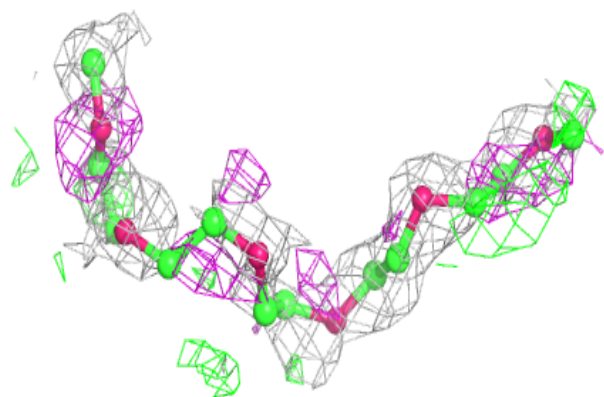
**Electron density around PG6 B 212:**

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

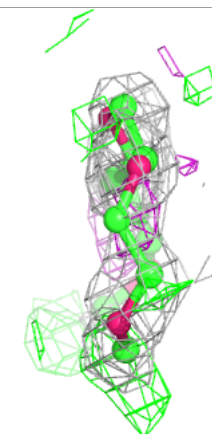
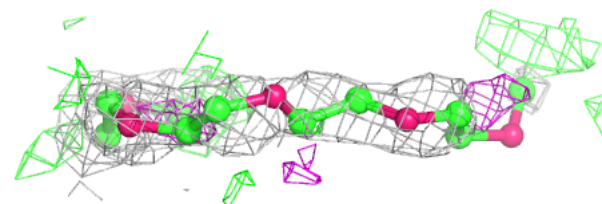
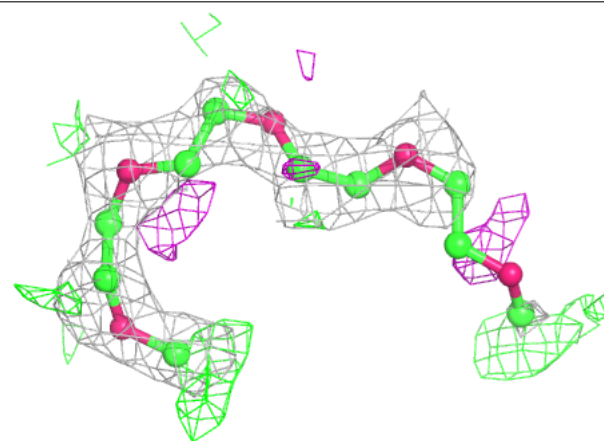


**Electron density around PG6 E 211:**

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

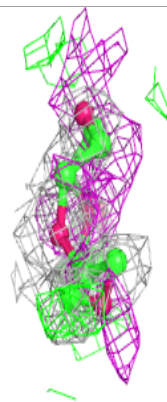
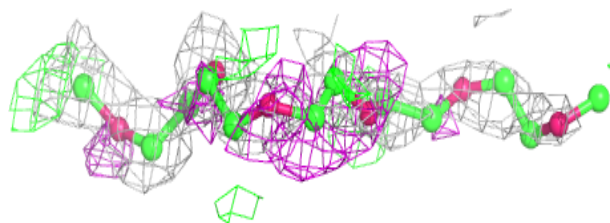
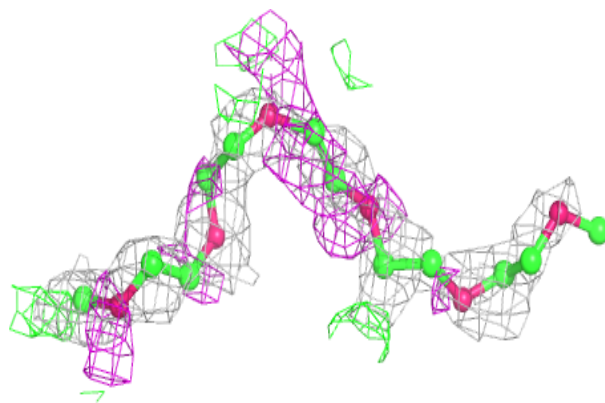
**Electron density around PG6 C 209:**

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

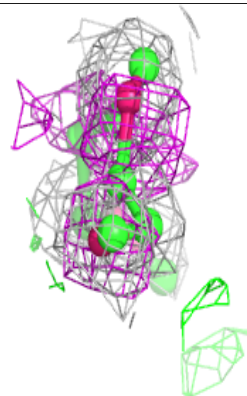
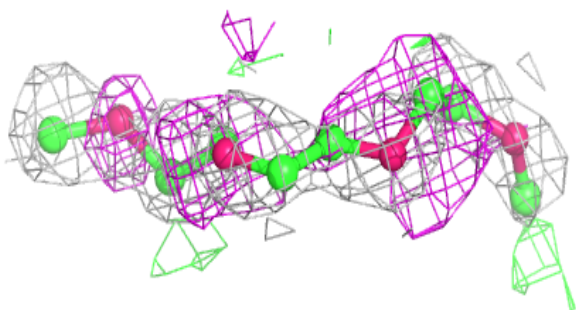
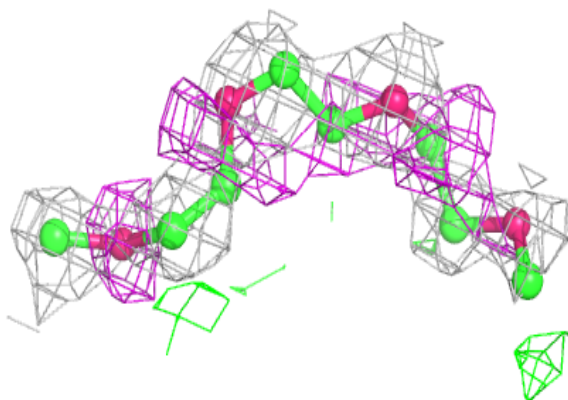


**Electron density around PG6 E 210:**

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

**Electron density around PG6 E 209:**

$2mF_o-DF_c$  (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.