



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 09:00 am BST

PDB ID : 6CJ6
Title : Structure of the poxvirus protein F9
Authors : Diesterbeck, U.S.; Gittis, A.G.; Garboczi, D.N.; Moss, B.
Deposited on : 2018-02-26
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

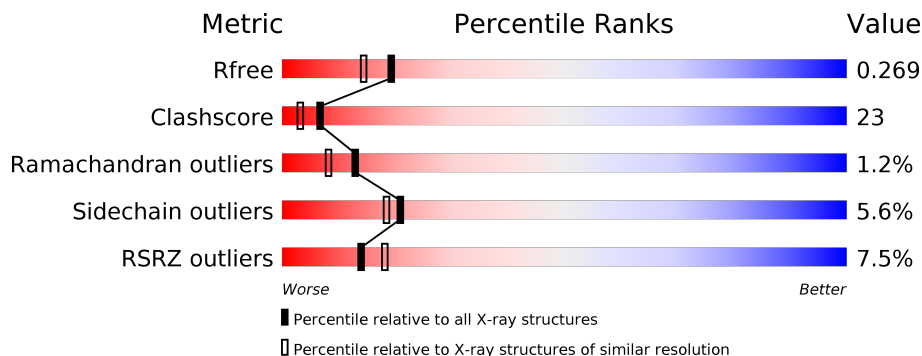
1 Overall quality at a glance

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 ≥ 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	176	 10% 64% 28% • 6%
1	B	176	 6% 65% 22% 5% 9%
1	C	176	 6% 68% 22% • 9%
1	D	176	 7% 66% 26% • 6%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	PGO	A	247	-	-	X	-
10	PGO	B	230	X	-	-	-
10	PGO	D	245	-	-	X	-
10	PGO	D	246	-	-	X	-
11	ETX	A	250	-	-	X	-
11	ETX	B	236	-	-	-	X
11	ETX	C	242	-	-	-	X
11	ETX	D	249	-	-	X	-
11	ETX	D	250	-	-	X	-
14	P33	C	207	-	-	X	-
15	P6G	D	209	-	-	X	-
2	PG4	D	202	-	-	X	-
3	PG0	A	204	-	-	X	-
4	PEG	A	207	-	-	X	-
4	PEG	C	203	-	-	X	-
4	PEG	C	205	-	X	X	-
4	PEG	D	205	-	-	X	-
4	PEG	D	206	-	-	X	X
5	EDO	A	213	-	-	-	X
5	EDO	B	209	-	-	-	X
5	EDO	D	216	-	-	-	X
5	EDO	D	220	-	-	-	X
6	GOL	A	218	-	X	-	-
6	GOL	C	216	-	-	-	X
6	GOL	C	217	-	X	-	-
6	GOL	C	218	-	X	-	-
6	GOL	C	219	-	X	-	-
7	PDO	A	221	-	-	X	-
7	PDO	D	224	-	-	X	-
8	EOH	A	226	-	-	X	-
8	EOH	A	236	-	-	X	-
8	EOH	B	217	-	-	X	-
8	EOH	B	220	-	-	X	-
8	EOH	B	223	-	-	X	-
8	EOH	C	225	-	-	X	-
8	EOH	C	226	-	-	X	-
8	EOH	C	230	-	-	-	X
8	EOH	D	230	-	-	X	-
9	MOH	A	243	-	-	-	X
9	MOH	B	229	-	-	X	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 6060 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 Protein F9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	165	1239	784	206	240	9	0	0	0
1	B	161	1210	764	202	235	9	0	0	0
1	C	161	1225	771	204	241	9	0	1	0
1	D	166	1271	801	214	246	10	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

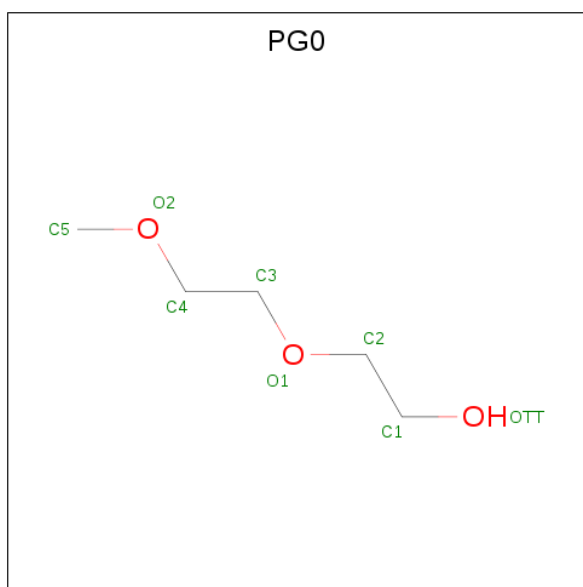
Chain	Residue	Modelled	Actual	Comment	Reference
A	84	ALA	ARG	conflict	UNP P24361
A	147	ALA	ARG	conflict	UNP P24361
B	84	ALA	ARG	conflict	UNP P24361
B	147	ALA	ARG	conflict	UNP P24361
C	84	ALA	ARG	conflict	UNP P24361
C	147	ALA	ARG	conflict	UNP P24361
D	84	ALA	ARG	conflict	UNP P24361
D	147	ALA	ARG	conflict	UNP P24361

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		
2	A	1	Total	C	O	0	0
			13	8	5		
2	B	1	Total	C	O	0	0
			13	8	5		
2	D	1	Total	C	O	0	0
			13	8	5		
2	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 3 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: C₅H₁₂O₃).



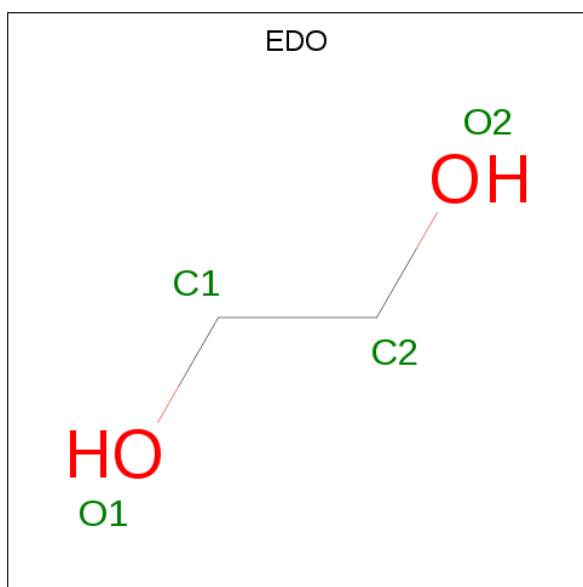
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	5	3		
3	A	1	Total	C	O	0	0
			8	5	3		
3	A	1	Total	C	O	0	0
			8	5	3		
3	A	1	Total	C	O	0	0
			8	5	3		
3	B	1	Total	C	O	0	0
			8	5	3		
3	C	1	Total	C	O	0	0
			8	5	3		
3	C	1	Total	C	O	0	0
			8	5	3		
3	D	1	Total	C	O	0	0
			8	5	3		
3	D	1	Total	C	O	0	0
			8	5	3		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



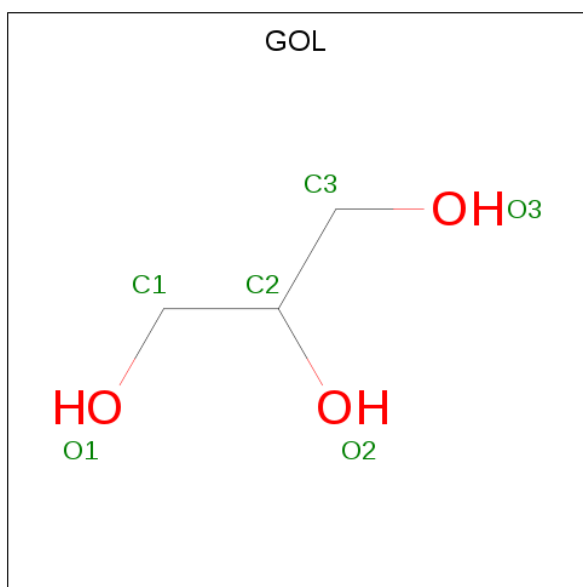
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

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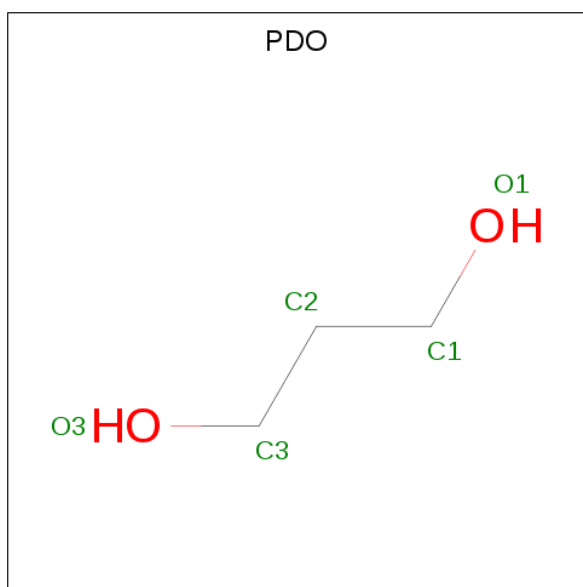
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



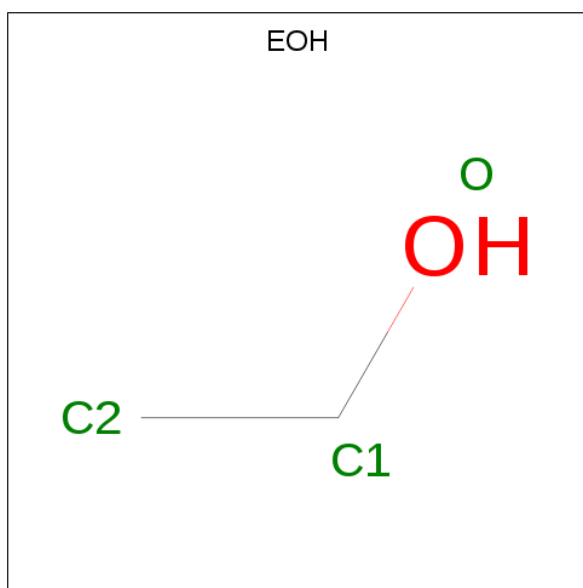
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is 1,3-PROPANDIOL (three-letter code: PDO) (formula: C₃H₈O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 5 3 2	0	0
7	A	1	Total C O 5 3 2	0	0
7	A	1	Total C O 5 3 2	0	0
7	A	1	Total C O 5 3 2	0	0
7	A	1	Total C O 5 3 2	0	0
7	A	1	Total C O 5 3 2	0	0
7	A	1	Total C O 5 3 2	0	0
7	B	1	Total C O 5 3 2	0	0
7	B	1	Total C O 5 3 2	0	0
7	B	1	Total C O 5 3 2	0	0
7	C	1	Total C O 5 3 2	0	0
7	C	1	Total C O 5 3 2	0	0
7	D	1	Total C O 5 3 2	0	0
7	D	1	Total C O 5 3 2	0	0

- Molecule 8 is ETHANOL (three-letter code: EOH) (formula: C₂H₆O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 3 2 1	0	0
8	A	1	Total C O 3 2 1	0	0
8	A	1	Total C O 3 2 1	0	0
8	A	1	Total C O 3 2 1	0	0
8	A	1	Total C O 3 2 1	0	0
8	A	1	Total C O 3 2 1	0	0
8	A	1	Total C O 3 2 1	0	0
8	A	1	Total C O 3 2 1	0	0
8	A	1	Total C O 3 2 1	0	0
8	A	1	Total C O 3 2 1	0	0
8	A	1	Total C O 3 2 1	0	0
8	A	1	Total C O 3 2 1	0	0
8	A	1	Total C O 3 2 1	0	0

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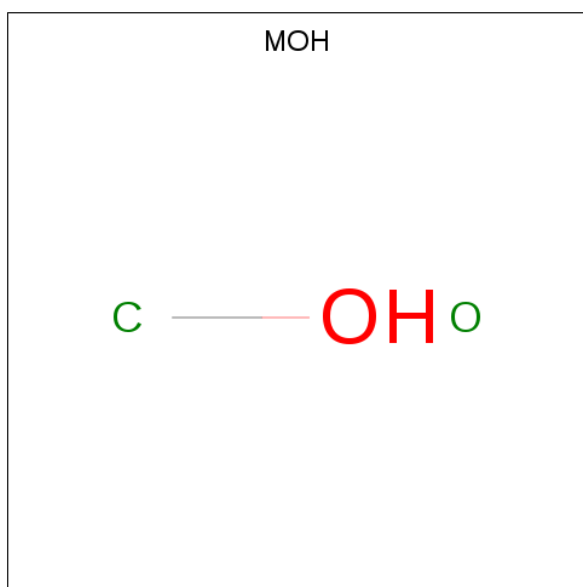
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total 3	C 2	O 1	0	0
8	B	1	Total 3	C 2	O 1	0	0
8	B	1	Total 3	C 2	O 1	0	0
8	B	1	Total 3	C 2	O 1	0	0
8	B	1	Total 3	C 2	O 1	0	0
8	B	1	Total 3	C 2	O 1	0	0
8	B	1	Total 3	C 2	O 1	0	0
8	B	1	Total 3	C 2	O 1	0	0
8	B	1	Total 3	C 2	O 1	0	0
8	B	1	Total 3	C 2	O 1	0	0
8	B	1	Total 3	C 2	O 1	0	0
8	B	1	Total 3	C 2	O 1	0	0
8	B	1	Total 3	C 2	O 1	0	0
8	C	1	Total 3	C 2	O 1	0	0
8	C	1	Total 3	C 2	O 1	0	0
8	C	1	Total 3	C 2	O 1	0	0
8	C	1	Total 3	C 2	O 1	0	0
8	C	1	Total 3	C 2	O 1	0	0
8	C	1	Total 3	C 2	O 1	0	0
8	C	1	Total 3	C 2	O 1	0	0
8	C	1	Total 3	C 2	O 1	0	0
8	C	1	Total 3	C 2	O 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			3	2	1		
8	D	1	Total	C	O	0	0
			3	2	1		
8	D	1	Total	C	O	0	0
			3	2	1		
8	D	1	Total	C	O	0	0
			3	2	1		
8	D	1	Total	C	O	0	0
			3	2	1		
8	D	1	Total	C	O	0	0
			3	2	1		
8	D	1	Total	C	O	0	0
			3	2	1		
8	D	1	Total	C	O	0	0
			3	2	1		
8	D	1	Total	C	O	0	0
			3	2	1		
8	D	1	Total	C	O	0	0
			3	2	1		

- Molecule 9 is METHANOL (three-letter code: MOH) (formula: CH₄O).



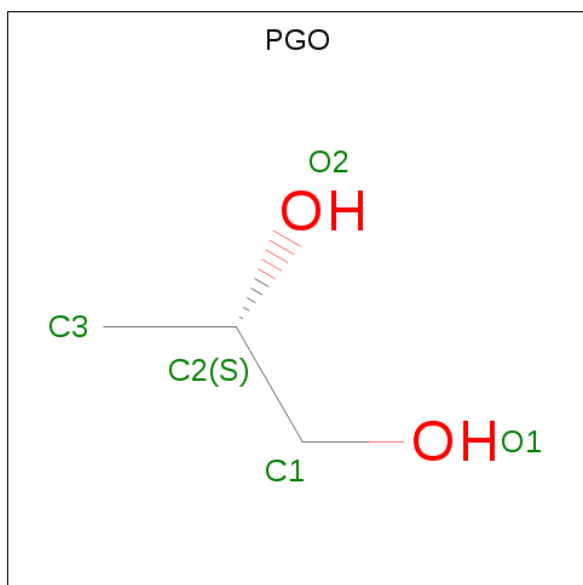
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			2	1	1		
9	A	1	Total	C	O	0	0
			2	1	1		
9	A	1	Total	C	O	0	0
			2	1	1		
9	A	1	Total	C	O	0	0
			2	1	1		
9	A	1	Total	C	O	0	0
			2	1	1		
9	A	1	Total	C	O	0	0
			2	1	1		
9	A	1	Total	C	O	0	0
			2	1	1		
9	B	1	Total	C	O	0	0
			2	1	1		
9	B	1	Total	C	O	0	0
			2	1	1		
9	B	1	Total	C	O	0	0
			2	1	1		
9	C	1	Total	C	O	0	0
			2	1	1		
9	C	1	Total	C	O	0	0
			2	1	1		
9	C	1	Total	C	O	0	0
			2	1	1		

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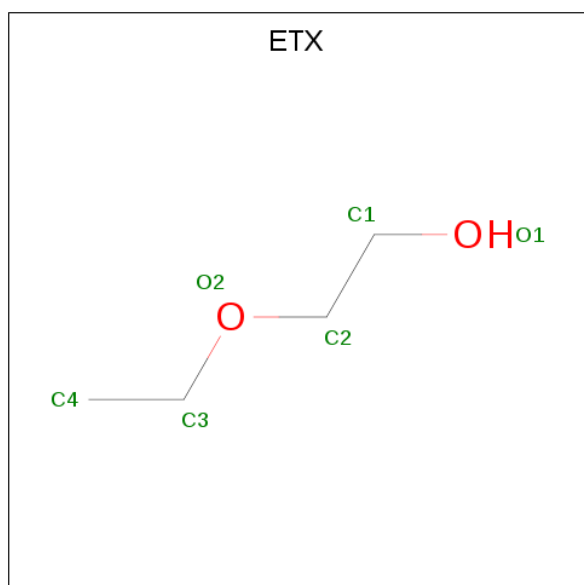
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C O 2 1 1	0	0
9	C	1	Total C O 2 1 1	0	0
9	C	1	Total C O 2 1 1	0	0
9	D	1	Total C O 2 1 1	0	0
9	D	1	Total C O 2 1 1	0	0
9	D	1	Total C O 2 1 1	0	0
9	D	1	Total C O 2 1 1	0	0
9	D	1	Total C O 2 1 1	0	0
9	D	1	Total C O 2 1 1	0	0
9	D	1	Total C O 2 1 1	0	0
9	D	1	Total C O 2 1 1	0	0

- Molecule 10 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: C₃H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			5	3	2		
10	A	1	Total	C	O	0	0
			5	3	2		
10	A	1	Total	C	O	0	0
			5	3	2		
10	B	1	Total	C	O	0	0
			5	3	2		
10	B	1	Total	C	O	0	0
			5	3	2		
10	B	1	Total	C	O	0	0
			5	3	2		
10	C	1	Total	C	O	0	0
			5	3	2		
10	D	1	Total	C	O	0	0
			5	3	2		
10	D	1	Total	C	O	0	0
			5	3	2		
10	D	1	Total	C	O	0	0
			5	3	2		

- Molecule 11 is 2-ETHOXYETHANOL (three-letter code: ETX) (formula: C₄H₁₀O₂).



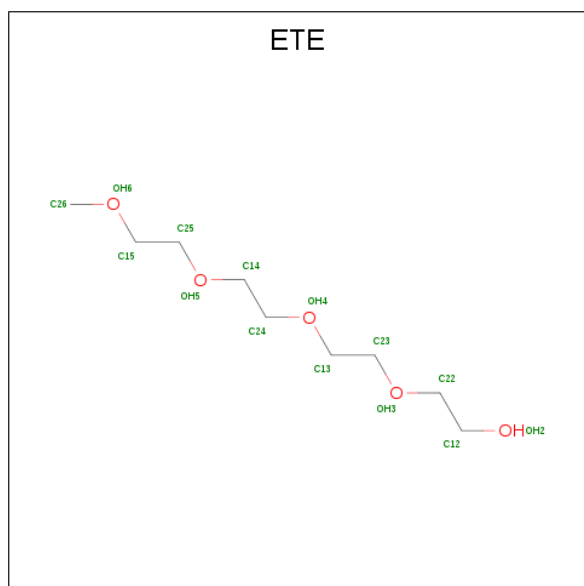
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			6	4	2		
11	A	1	Total	C	O	0	0
			6	4	2		

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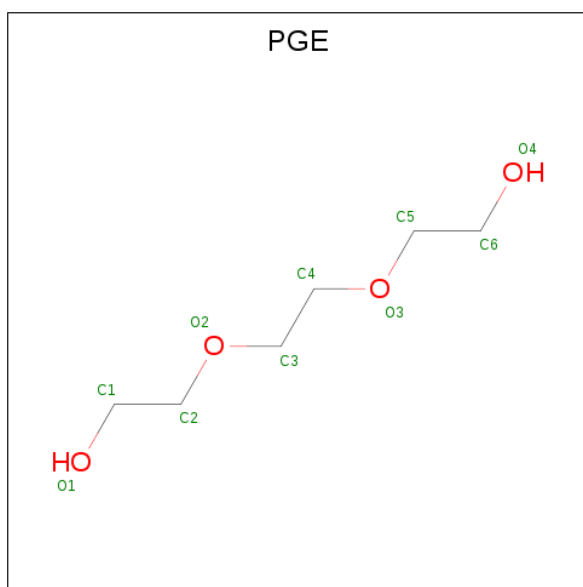
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			6	4	2		
11	B	1	Total	C	O	0	0
			6	4	2		
11	B	1	Total	C	O	0	0
			6	4	2		
11	C	1	Total	C	O	0	0
			6	4	2		
11	D	1	Total	C	O	0	0
			6	4	2		
11	D	1	Total	C	O	0	0
			6	4	2		

- Molecule 12 is 2-{2-[2-2-(METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: ETE) (formula: C₉H₂₀O₅).



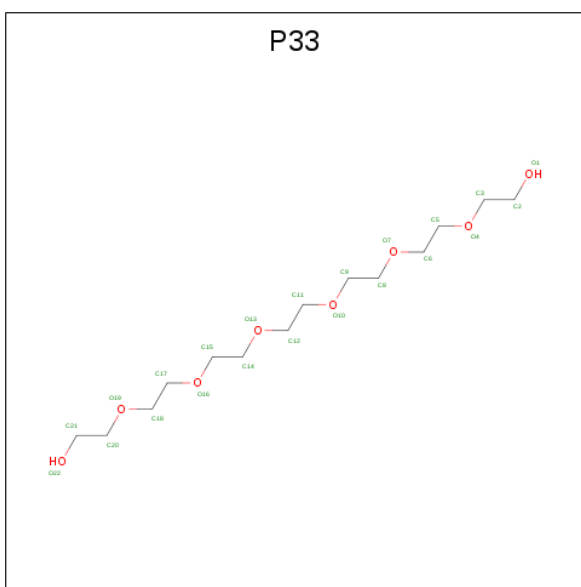
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	C	O	0	0
			14	9	5		
12	C	1	Total	C	O	0	0
			14	9	5		

- Molecule 13 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



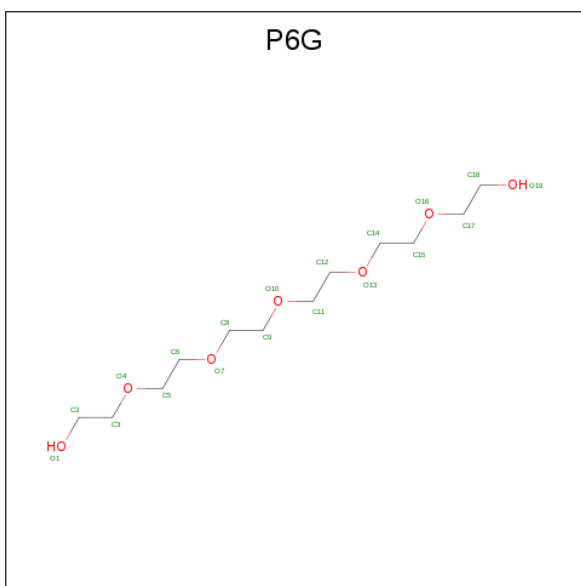
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	B	1	Total	C	O	0	0
			10	6	4		
13	C	1	Total	C	O	0	0
			10	6	4		
13	C	1	Total	C	O	0	0
			10	6	4		
13	C	1	Total	C	O	0	0
			10	6	4		
13	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 14 is 3,6,9,12,15,18-HEXA-OXAICOSANE-1,20-DIOL (three-letter code: P33) (formula: C₁₄H₃₀O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	C	O	0	0
			22	14	8		

- Molecule 15 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	D	1	Total	C	O	0	0
			19	12	7		
15	D	1	Total	C	O	0	0
			19	12	7		
15	D	1	Total	C	O	0	0
			19	12	7		

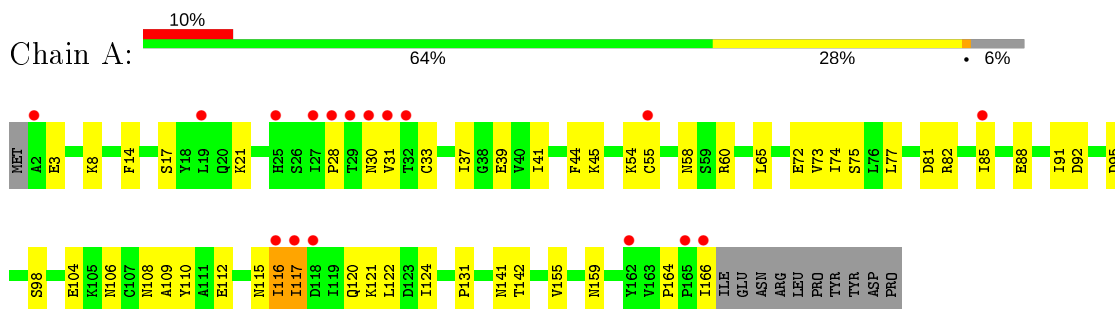
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	53	Total 53	O 53	0	0
16	B	60	Total 60	O 60	0	0
16	C	57	Total 58	O 58	0	1
16	D	46	Total 46	O 46	0	0

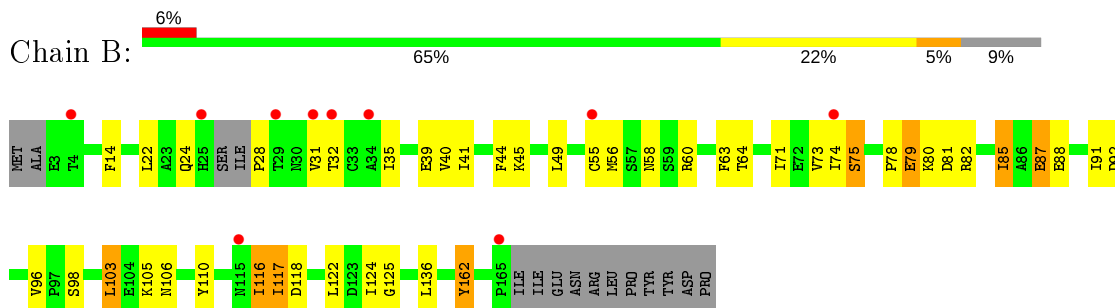
3 Residue-property plots [i](#)

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

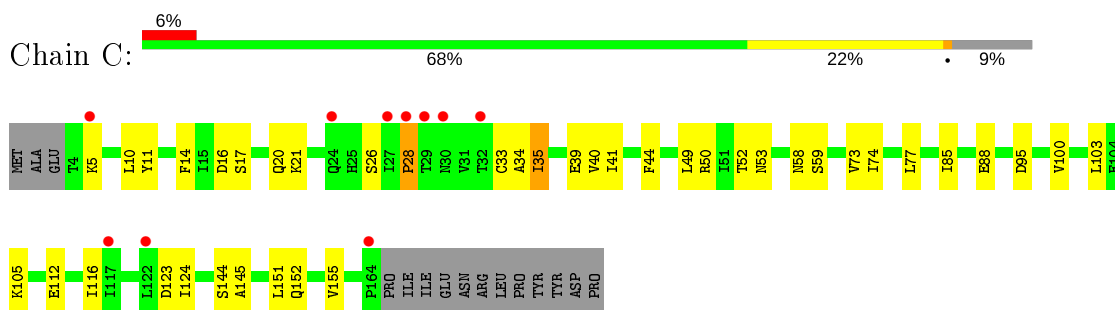
- Molecule 1: Protein F9



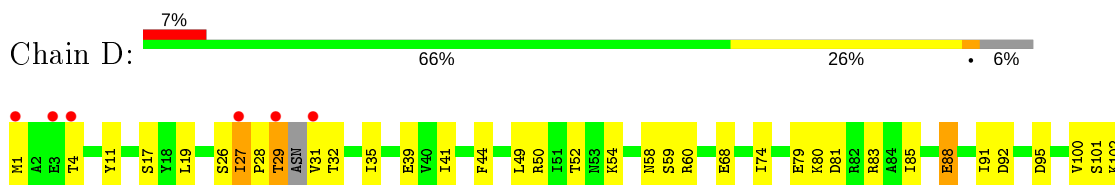
- Molecule 1: Protein F9

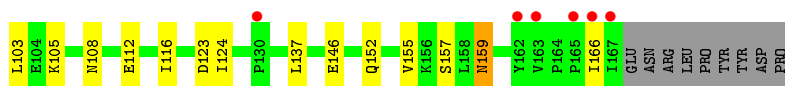


- Molecule 1: Protein F9



- Molecule 1: Protein F9





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.45Å 75.08Å 136.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.86 – 2.10 39.96 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.8 (38.86-2.10) 93.9 (39.96-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.10Å)	Xtrriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.226 , 0.269 0.226 , 0.269	Depositor DCC
R_{free} test set	2000 reflections (5.33%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtrriage
Anisotropy	0.854	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 68.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6060	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.08 % 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 1.1740e-03. 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: GOL, PGE, P6G, PGO, ETX, EOH, EDO, PDO, PG4, MOH, PG0, ETE, P33, PEG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.32	0/1257	0.44	0/1706
1	B	0.39	1/1225 (0.1%)	0.51	1/1659 (0.1%)
1	C	0.35	0/1240	0.49	1/1680 (0.1%)
1	D	0.28	0/1287	0.48	0/1742
All	All	0.34	1/5009 (0.0%)	0.48	2/6787 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	162	TYR	CB-CG	-6.29	1.42	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	28	PRO	N-CA-CB	6.10	110.62	103.30
1	B	28	PRO	N-CA-CB	5.91	110.39	103.30

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	1239	0	1217	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1210	0	1189	34	0
1	C	1225	0	1198	41	0
1	D	1271	0	1264	65	0
2	A	26	0	36	1	0
2	B	13	0	17	2	0
2	D	26	0	35	9	0
3	A	32	0	48	16	0
3	B	8	0	12	2	0
3	C	16	0	24	8	0
3	D	16	0	24	9	0
4	A	14	0	20	4	0
4	B	14	0	20	0	0
4	C	28	0	39	13	0
4	D	21	0	30	12	0
5	A	36	0	53	7	0
5	B	24	0	35	5	0
5	C	28	0	36	6	0
5	D	44	0	64	3	0
6	A	6	0	6	0	0
6	C	24	0	29	2	0
6	D	6	0	6	2	0
7	A	35	0	54	13	0
7	B	15	0	24	1	0
7	C	10	0	16	1	0
7	D	10	0	16	11	0
8	A	39	0	76	6	0
8	B	36	0	70	7	0
8	C	30	0	60	11	0
8	D	36	0	70	12	0
9	A	16	0	0	0	0
9	B	6	0	0	2	0
9	C	12	0	0	0	0
9	D	16	0	0	2	0
10	A	15	0	24	11	0
10	B	15	0	22	2	0
10	C	5	0	7	0	0
10	D	15	0	23	9	0
11	A	12	0	19	8	0
11	B	18	0	30	3	0
11	C	6	0	10	0	0
11	D	12	0	20	16	0
12	B	14	0	20	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	C	14	0	20	1	0
13	B	10	0	14	3	0
13	C	30	0	41	8	0
13	D	10	0	14	1	0
14	C	22	0	30	14	0
15	D	57	0	78	22	0
16	A	53	0	0	3	0
16	B	60	0	0	2	0
16	C	58	0	0	6	0
16	D	46	0	0	1	0
All	All	6060	0	6160	281	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 23.

All (281) 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:D:101:SER:HA	7:D:224:PDO:H32	1.21	1.16
4:A:207:PEG:H11	7:A:219:PDO:H31	1.22	1.15
10:A:247:PGO:C3	11:A:250:ETX:H12	1.78	1.12
12:B:205:ETE:H141	11:D:250:ETX:H41	1.20	1.11
10:A:247:PGO:H31	11:A:250:ETX:H12	1.17	1.09
3:C:201:PG0:H42	16:C:324:HOH:O	1.56	1.05
14:C:207:P33:H152	14:C:207:P33:H202	1.33	1.04
15:D:209:P6G:H142	15:D:209:P6G:H181	1.38	1.03
14:C:207:P33:H212	14:C:207:P33:H171	1.38	1.03
15:D:209:P6G:H112	15:D:209:P6G:H51	1.40	1.03
5:D:212:EDO:H21	6:D:222:GOL:H11	1.42	1.01
1:D:100:VAL:HG11	2:D:202:PG4:H32	1.41	1.00
10:A:247:PGO:H31	11:A:250:ETX:C1	1.93	0.99
4:A:207:PEG:C1	7:A:219:PDO:H31	1.93	0.98
2:B:201:PG4:H41	2:B:201:PG4:H12	1.45	0.98
4:A:207:PEG:H11	7:A:219:PDO:C3	1.93	0.97
1:A:108:ASN:HB3	7:A:221:PDO:H12	1.45	0.97
1:D:17:SER:HA	4:D:205:PEG:H21	1.46	0.96
4:C:203:PEG:H32	5:C:212:EDO:H12	1.47	0.94
1:D:101:SER:CA	7:D:224:PDO:H32	1.98	0.93
12:B:205:ETE:C14	11:D:250:ETX:H41	1.99	0.92
2:D:201:PG4:C3	2:D:202:PG4:H82	2.00	0.92
3:A:203:PG0:H51	3:D:204:PG0:C5	2.03	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:D:209:P6G:C5	15:D:209:P6G:H151	2.04	0.87
15:D:209:P6G:H151	15:D:209:P6G:H51	1.56	0.87
1:C:144:SER:HA	4:C:203:PEG:H42	1.55	0.86
12:B:205:ETE:H141	11:D:250:ETX:C4	2.02	0.86
3:D:203:PG0:H21	4:D:205:PEG:H12	1.57	0.85
1:D:101:SER:HA	7:D:224:PDO:C3	2.05	0.84
4:C:205:PEG:H41	8:C:226:EOH:H12	1.59	0.83
15:D:209:P6G:C14	15:D:209:P6G:H181	2.02	0.83
14:C:207:P33:C15	14:C:207:P33:H202	2.08	0.83
8:D:230:EOH:H11	11:D:249:ETX:O2	1.80	0.82
10:A:247:PGO:C3	11:A:250:ETX:C1	2.55	0.82
1:A:88:GLU:HA	3:A:206:PG0:H11	1.62	0.81
1:A:33:CYS:SG	5:A:212:EDO:H22	2.21	0.81
7:A:222:PDO:H31	8:A:226:EOH:H11	1.64	0.80
1:D:92:ASP:H	7:D:224:PDO:H22	1.48	0.79
1:D:92:ASP:H	7:D:224:PDO:C2	1.97	0.78
1:C:53:ASN:HB2	13:C:241:PGE:H2	1.63	0.78
1:C:5:LYS:HE3	8:C:227:EOH:H21	1.66	0.78
1:A:120:GLN:HA	3:A:204:PG0:H12	1.65	0.77
8:D:230:EOH:C1	11:D:249:ETX:H12	2.15	0.77
1:C:33:CYS:SG	13:C:241:PGE:H42	2.25	0.77
2:D:201:PG4:H31	2:D:202:PG4:H82	1.66	0.76
1:A:8:LYS:NZ	10:A:247:PGO:H2	2.00	0.76
1:A:3:GLU:HB3	4:A:207:PEG:H41	1.69	0.74
8:D:230:EOH:H21	11:D:249:ETX:C1	2.17	0.74
5:A:209:EDO:H11	1:C:52:THR:HG21	1.68	0.74
15:D:209:P6G:C11	15:D:209:P6G:H51	2.15	0.74
8:D:230:EOH:H21	11:D:249:ETX:H12	1.69	0.74
14:C:207:P33:C21	14:C:207:P33:H171	2.05	0.73
3:D:203:PG0:H21	4:D:205:PEG:C1	2.20	0.72
1:C:88:GLU:HG2	5:C:210:EDO:O2	1.90	0.72
5:D:212:EDO:H21	6:D:222:GOL:C1	2.18	0.72
1:D:27:ILE:HG23	10:D:246:PGO:H12	1.71	0.72
3:A:206:PG0:C5	3:A:206:PG0:H22	2.20	0.71
1:B:75:SER:HA	1:B:82:ARG:HE	1.54	0.70
1:D:88:GLU:HB2	15:D:210:P6G:H92	1.74	0.70
3:A:206:PG0:O2	3:A:206:PG0:H22	1.90	0.70
1:B:96:VAL:HG21	8:B:223:EOH:H21	1.74	0.70
3:D:203:PG0:H11	8:D:230:EOH:H12	1.73	0.69
15:D:209:P6G:H112	15:D:209:P6G:H151	1.73	0.69
1:C:95:ASP:OD2	7:C:221:PDO:H12	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASN:HB2	7:A:221:PDO:H32	1.74	0.68
1:B:125:GLY:HA2	3:B:202:PG0:H11	1.76	0.67
3:A:203:PG0:H51	3:D:204:PG0:H52	1.76	0.67
1:D:31:VAL:HG12	1:D:32:THR:HG23	1.77	0.67
1:A:109:ALA:N	7:A:221:PDO:H31	2.09	0.66
1:A:121:LYS:H	3:A:204:PG0:H22	1.60	0.66
1:D:54:LYS:HE3	10:D:245:PGO:H2	1.77	0.66
1:D:88:GLU:HB2	15:D:210:P6G:C9	2.26	0.65
1:D:44:PHE:HE1	1:D:124:ILE:HD11	1.61	0.65
1:D:54:LYS:NZ	4:D:206:PEG:O1	2.25	0.65
1:D:17:SER:CA	4:D:205:PEG:H21	2.24	0.65
15:D:209:P6G:H112	15:D:209:P6G:C5	2.23	0.65
15:D:209:P6G:H142	15:D:209:P6G:C18	2.21	0.65
8:D:230:EOH:C2	11:D:249:ETX:H12	2.26	0.65
3:B:202:PG0:C3	5:B:206:EDO:H12	2.27	0.65
1:D:35:ILE:HD11	1:D:116:ILE:HG22	1.78	0.65
1:B:39:GLU:HG3	1:D:41:ILE:HG22	1.77	0.65
1:A:75:SER:HA	1:A:82:ARG:HD3	1.79	0.64
3:A:203:PG0:H51	3:D:204:PG0:H53	1.78	0.64
8:C:225:EOH:H23	16:C:310:HOH:O	1.96	0.64
10:A:247:PGO:H32	11:A:250:ETX:H12	1.75	0.63
1:B:40:VAL:HG11	1:B:49:LEU:HD21	1.79	0.63
1:D:105:LYS:HE2	2:D:202:PG4:H22	1.80	0.63
1:B:60:ARG:HG3	11:B:236:ETX:H12	1.82	0.62
1:B:87:GLU:CG	5:B:207:EDO:H21	2.30	0.61
1:A:108:ASN:CB	7:A:221:PDO:H32	2.31	0.61
1:B:32:THR:CA	7:B:212:PDO:H21	2.31	0.60
2:D:201:PG4:O2	2:D:202:PG4:H82	2.01	0.60
1:C:10:LEU:HD21	1:C:77:LEU:HD11	1.82	0.60
1:C:145:ALA:H	4:C:203:PEG:H42	1.67	0.60
1:D:112:GLU:OE1	16:D:301:HOH:O	2.17	0.60
4:C:205:PEG:H32	6:C:219:GOL:H12	1.82	0.59
1:C:20:GLN:HB3	14:C:207:P33:H31	1.85	0.59
10:A:247:PGO:C3	11:A:250:ETX:C2	2.81	0.59
1:C:100:VAL:HB	4:C:204:PEG:H41	1.85	0.58
1:A:60:ARG:NH2	1:A:98:SER:O	2.36	0.58
1:D:19:LEU:HD22	1:D:54:LYS:HZ3	1.67	0.58
9:B:229:MOH:C	11:B:234:ETX:H42	2.34	0.58
1:D:19:LEU:HD13	4:D:206:PEG:H22	1.85	0.58
4:C:205:PEG:H41	8:C:226:EOH:C1	2.32	0.57
1:A:166:ILE:N	16:A:303:HOH:O	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:LYS:HD2	8:C:224:EOH:H11	1.87	0.57
1:D:52:THR:CG2	4:D:206:PEG:H41	2.35	0.57
1:C:144:SER:HB3	4:C:203:PEG:H21	1.87	0.57
3:A:205:PG0:H12	5:A:214:EDO:O1	2.06	0.56
1:A:115:ASN:O	1:A:117:ILE:N	2.38	0.56
1:A:17:SER:CB	7:A:220:PDO:H21	2.36	0.56
1:C:16:ASP:OD2	3:C:202:PG0:H31	2.06	0.56
1:D:95:ASP:CB	7:D:224:PDO:H11	2.36	0.56
1:C:112:GLU:OE2	5:C:215:EDO:H12	2.06	0.56
1:A:91:ILE:HG23	8:A:236:EOH:H11	1.86	0.55
1:B:24:GLN:CG	1:B:24:GLN:O	2.54	0.55
1:C:40:VAL:HG11	1:C:49:LEU:HD21	1.87	0.55
11:D:249:ETX:H43	11:D:250:ETX:H22	1.88	0.55
1:B:64:THR:HG21	13:B:233:PGE:H5	1.87	0.55
1:D:52:THR:HG23	4:D:206:PEG:H41	1.88	0.55
1:C:144:SER:CA	4:C:203:PEG:H42	2.35	0.55
3:A:206:PG0:H52	3:A:206:PG0:H22	1.89	0.55
1:A:41:ILE:HG22	1:C:39:GLU:HG3	1.89	0.55
1:B:162:TYR:HB2	5:B:209:EDO:H11	1.90	0.54
3:D:203:PG0:C2	4:D:205:PEG:C1	2.84	0.54
10:B:230:PGO:H12	1:C:105:LYS:HB3	1.89	0.54
1:C:144:SER:HA	4:C:203:PEG:C4	2.35	0.54
1:D:74:ILE:HD11	1:D:85:ILE:HG21	1.89	0.53
14:C:207:P33:H61	13:C:239:PGE:O2	2.08	0.53
15:D:209:P6G:H112	15:D:209:P6G:O7	2.02	0.53
1:B:22:LEU:HD22	1:B:56:MET:HE1	1.91	0.53
1:A:8:LYS:HZ3	10:A:247:PGO:H2	1.72	0.53
1:A:39:GLU:HG3	1:C:41:ILE:HG22	1.90	0.53
1:B:87:GLU:HG3	5:B:207:EDO:H21	1.90	0.53
3:C:202:PG0:H32	8:C:225:EOH:H11	1.91	0.53
2:D:202:PG4:O2	3:D:204:PG0:H31	2.08	0.53
3:C:202:PG0:H31	8:C:225:EOH:H21	1.91	0.52
1:B:92:ASP:HB3	8:B:217:EOH:H21	1.91	0.52
1:A:106:ASN:ND2	16:A:301:HOH:O	2.30	0.52
1:B:87:GLU:HG2	5:B:207:EDO:H21	1.90	0.52
1:C:11:TYR:CZ	1:C:155:VAL:HG22	2.46	0.51
8:C:225:EOH:C2	16:C:310:HOH:O	2.57	0.51
15:D:209:P6G:H122	15:D:209:P6G:H181	1.92	0.51
1:D:108:ASN:CG	15:D:208:P6G:H141	2.31	0.51
1:D:54:LYS:HE3	10:D:245:PGO:C2	2.41	0.51
1:D:54:LYS:HG2	10:D:245:PGO:C2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:230:EOH:C1	11:D:249:ETX:C1	2.85	0.51
1:A:120:GLN:HG3	3:A:204:PG0:C1	2.40	0.51
1:A:121:LYS:HE3	3:A:204:PG0:H32	1.93	0.51
11:D:249:ETX:C4	11:D:250:ETX:H22	2.41	0.51
8:D:230:EOH:C2	11:D:249:ETX:C1	2.85	0.50
5:A:210:EDO:O1	8:A:226:EOH:H23	2.12	0.50
15:D:209:P6G:C11	15:D:209:P6G:H151	2.40	0.50
4:C:205:PEG:C4	8:C:226:EOH:H12	2.37	0.50
1:D:100:VAL:HG11	2:D:202:PG4:C3	2.28	0.50
1:B:96:VAL:HG21	8:B:223:EOH:C2	2.40	0.50
1:B:136:LEU:HD21	1:D:1:MET:HE3	1.94	0.49
1:A:155:VAL:O	1:A:159:ASN:HB2	2.12	0.49
1:C:35:ILE:HD11	1:C:116:ILE:HG22	1.93	0.49
1:D:101:SER:CB	7:D:224:PDO:H32	2.41	0.49
1:A:17:SER:OG	7:A:220:PDO:H21	2.11	0.49
1:A:95:ASP:HB2	8:A:236:EOH:H23	1.93	0.49
12:C:208:ETE:H252	8:C:231:EOH:H23	1.93	0.49
1:B:81:ASP:O	1:B:85:ILE:HG22	2.13	0.49
1:D:29:THR:O	1:D:29:THR:OG1	2.20	0.49
15:D:209:P6G:C5	15:D:209:P6G:C15	2.85	0.49
14:C:207:P33:H61	13:C:239:PGE:C3	2.43	0.49
3:D:204:PG0:H42	5:D:220:EDO:C2	2.43	0.49
1:A:55:CYS:HA	1:A:142:THR:HA	1.95	0.49
1:C:17:SER:HB2	14:C:207:P33:H92	1.93	0.49
8:D:230:EOH:H21	11:D:249:ETX:H11	1.92	0.49
1:D:58:ASN:HD22	1:D:60:ARG:HB2	1.77	0.48
1:C:14:PHE:HA	1:C:73:VAL:HG21	1.95	0.48
4:C:203:PEG:H32	5:C:212:EDO:C1	2.30	0.48
1:C:74:ILE:HD11	1:C:85:ILE:HG21	1.95	0.48
8:D:230:EOH:H11	11:D:249:ETX:C1	2.43	0.48
1:B:41:ILE:HG12	1:D:39:GLU:HG3	1.96	0.48
1:C:16:ASP:OD2	3:C:202:PG0:H21	2.14	0.48
10:A:247:PGO:C3	11:A:250:ETX:H22	2.44	0.48
1:D:92:ASP:H	7:D:224:PDO:H21	1.74	0.48
12:B:205:ETE:H141	11:D:250:ETX:C3	2.42	0.47
1:C:44:PHE:HE1	1:C:124:ILE:HD11	1.79	0.47
1:C:77:LEU:O	5:C:214:EDO:O2	2.32	0.47
1:D:68:GLU:HA	9:D:237:MOH:C	2.44	0.47
1:B:79:GLU:CB	8:B:220:EOH:H12	2.44	0.47
1:C:34:ALA:HA	5:C:209:EDO:H22	1.95	0.47
1:D:100:VAL:CG1	2:D:202:PG4:H32	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:C:207:P33:H182	14:C:207:P33:H151	1.60	0.47
1:D:17:SER:OG	4:D:205:PEG:H41	2.14	0.47
1:A:121:LYS:N	3:A:204:PG0:H22	2.28	0.47
1:D:124:ILE:HD12	1:D:137:LEU:HD23	1.97	0.47
1:C:44:PHE:CE1	1:C:124:ILE:HD11	2.50	0.47
1:D:19:LEU:HD13	4:D:206:PEG:C2	2.45	0.46
1:D:80:LYS:HA	9:D:239:MOH:O	2.15	0.46
1:A:44:PHE:HE1	1:A:124:ILE:HD11	1.80	0.46
1:B:106:ASN:ND2	16:B:302:HOH:O	2.44	0.46
5:A:209:EDO:H11	1:C:52:THR:CG2	2.41	0.46
13:C:239:PGE:H1	13:C:239:PGE:H32	1.55	0.46
1:A:122:LEU:HD12	1:A:122:LEU:HA	1.83	0.46
8:A:230:EOH:H22	8:A:231:EOH:H21	1.95	0.46
15:D:209:P6G:C12	15:D:209:P6G:H181	2.46	0.46
1:A:121:LYS:H	3:A:204:PG0:C2	2.25	0.46
1:D:85:ILE:HD11	1:D:157:SER:HB3	1.96	0.46
1:A:60:ARG:HD2	1:A:104:GLU:OE2	2.15	0.46
1:B:117:ILE:HG21	8:B:226:EOH:H21	1.98	0.46
1:D:92:ASP:HB3	7:D:224:PDO:H22	1.98	0.46
1:C:11:TYR:CE1	1:C:155:VAL:HG22	2.51	0.46
1:A:81:ASP:O	1:A:85:ILE:HG22	2.16	0.45
1:B:91:ILE:HG23	8:B:217:EOH:H12	1.98	0.45
3:A:206:PG0:H52	3:A:206:PG0:C2	2.46	0.45
3:C:202:PG0:H12	16:C:309:HOH:O	2.17	0.45
1:D:54:LYS:HG2	10:D:245:PGO:O2	2.17	0.45
1:A:58:ASN:CB	5:A:216:EDO:H21	2.47	0.45
1:B:64:THR:CG2	13:B:233:PGE:H5	2.47	0.45
1:D:26:SER:O	1:D:28:PRO:HD3	2.16	0.45
1:B:79:GLU:H	8:B:220:EOH:H12	1.81	0.45
1:A:112:GLU:HG3	7:A:221:PDO:H11	1.99	0.45
1:B:105:LYS:HB3	10:B:230:PGO:H31	1.98	0.45
15:D:210:P6G:H182	13:D:248:PGE:H6	1.98	0.44
2:B:201:PG4:C4	2:B:201:PG4:H12	2.18	0.44
14:C:207:P33:H81	13:C:239:PGE:H2	2.00	0.44
1:D:11:TYR:CZ	1:D:155:VAL:HG22	2.51	0.44
1:A:44:PHE:CE1	1:A:124:ILE:HD11	2.53	0.44
10:A:247:PGO:H33	11:A:250:ETX:H22	1.99	0.44
1:D:91:ILE:HA	7:D:224:PDO:H21	2.00	0.44
1:C:17:SER:N	14:C:207:P33:H91	2.33	0.44
1:D:26:SER:O	10:D:246:PGO:H11	2.18	0.44
1:B:98:SER:HB3	13:B:233:PGE:H6	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:ARG:CB	4:D:206:PEG:H42	2.48	0.44
1:A:164:PRO:HB2	8:A:232:EOH:H12	1.99	0.43
1:C:123:ASP:O	1:C:152:GLN:HG3	2.18	0.43
1:D:155:VAL:O	1:D:159:ASN:HB2	2.18	0.43
1:B:14:PHE:HA	1:B:73:VAL:HG21	2.00	0.43
15:D:209:P6G:H151	15:D:209:P6G:H52	1.97	0.43
1:B:63:PHE:HE1	1:B:103:LEU:HD13	1.83	0.43
1:C:112:GLU:HA	3:C:201:PG0:H21	2.01	0.43
1:D:95:ASP:HB2	7:D:224:PDO:H11	2.00	0.43
1:A:109:ALA:CA	7:A:221:PDO:H31	2.48	0.43
1:B:58:ASN:HB2	16:B:334:HOH:O	2.17	0.43
1:A:131:PRO:HB2	2:A:202:PG4:H52	2.01	0.43
13:C:240:PGE:H4	13:C:240:PGE:H22	1.47	0.43
1:C:21:LYS:HG3	14:C:207:P33:H32	2.00	0.43
14:C:207:P33:C6	13:C:239:PGE:O2	2.67	0.43
1:A:77:LEU:O	1:A:82:ARG:NE	2.51	0.42
3:C:201:PG0:H52	16:C:324:HOH:O	2.18	0.42
1:D:146:GLU:H	1:D:146:GLU:CD	2.23	0.42
1:D:27:ILE:CG2	10:D:246:PGO:H12	2.45	0.42
1:A:120:GLN:CA	3:A:204:PG0:H12	2.43	0.42
7:A:221:PDO:H22	1:D:102:LYS:NZ	2.34	0.42
1:D:123:ASP:O	1:D:152:GLN:HG3	2.20	0.42
1:D:81:ASP:O	1:D:85:ILE:HG22	2.20	0.42
2:D:201:PG4:C4	2:D:202:PG4:H82	2.47	0.42
1:A:92:ASP:HB2	10:A:249:PGO:C1	2.50	0.42
1:B:78:PRO:O	1:B:82:ARG:HG3	2.20	0.42
8:D:230:EOH:H11	11:D:249:ETX:H12	2.00	0.42
1:D:74:ILE:HA	1:D:74:ILE:HD12	1.89	0.42
8:C:222:EOH:H23	16:C:341:HOH:O	2.20	0.41
1:A:21:LYS:HB3	1:A:65:LEU:HD13	2.02	0.41
1:A:45:LYS:O	1:C:52:THR:HA	2.20	0.41
1:D:27:ILE:HG23	10:D:246:PGO:C1	2.45	0.41
1:B:45:LYS:O	1:D:52:THR:HA	2.21	0.41
1:A:37:ILE:HG12	1:A:141:ASN:HB2	2.02	0.41
1:D:88:GLU:HB2	15:D:210:P6G:H91	2.01	0.41
1:A:41:ILE:HD13	1:A:121:LYS:HD3	2.03	0.41
1:A:58:ASN:HB2	5:A:216:EDO:H21	2.01	0.41
1:C:59:SER:OG	6:C:217:GOL:H32	2.21	0.41
1:D:59:SER:OG	15:D:208:P6G:H171	2.21	0.41
1:C:151:LEU:O	1:C:155:VAL:HG23	2.20	0.41
1:A:72:GLU:HG2	16:A:323:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ILE:HD11	1:A:85:ILE:HG21	2.02	0.41
1:D:79:GLU:HG2	1:D:83[B]:ARG:NH1	2.36	0.41
1:D:137:LEU:HD11	1:D:159:ASN:OD1	2.21	0.41
1:D:26:SER:N	10:D:246:PGO:H2	2.36	0.41
1:A:14:PHE:HA	1:A:73:VAL:HG21	2.03	0.40
1:D:102:LYS:HZ2	8:D:225:EOH:H21	1.86	0.40
1:B:71:ILE:HA	1:B:74:ILE:HG22	2.03	0.40
1:C:145:ALA:N	4:C:203:PEG:H42	2.34	0.40
14:C:207:P33:H52	14:C:207:P33:H21	1.57	0.40
1:B:44:PHE:CE1	1:B:124:ILE:HD11	2.57	0.40
9:B:229:MOH:C	11:B:234:ETX:C4	3.00	0.40
15:D:210:P6G:H112	15:D:210:P6G:H142	1.33	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	163/176 (93%)	151 (93%)	10 (6%)	2 (1%)	13 8
1	B	157/176 (89%)	144 (92%)	9 (6%)	4 (2%)	5 2
1	C	160/176 (91%)	149 (93%)	10 (6%)	1 (1%)	25 21
1	D	163/176 (93%)	153 (94%)	9 (6%)	1 (1%)	25 21
All	All	643/704 (91%)	597 (93%)	38 (6%)	8 (1%)	13 8

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	ILE
1	B	117	ILE
1	A	28	PRO

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Mol	Chain	Res	Type
1	B	116	ILE
1	C	28	PRO
1	B	31	VAL
1	B	79	GLU
1	D	166	ILE

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	135/157 (86%)	129 (96%)	6 (4%)	28	28
1	B	132/157 (84%)	120 (91%)	12 (9%)	9	6
1	C	134/157 (85%)	129 (96%)	5 (4%)	34	35
1	D	141/157 (90%)	134 (95%)	7 (5%)	24	23
All	All	542/628 (86%)	512 (94%)	30 (6%)	21	19

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	31	VAL
1	A	54	LYS
1	A	110	TYR
1	A	116	ILE
1	A	117	ILE
1	B	35	ILE
1	B	55	CYS
1	B	75	SER
1	B	80	LYS
1	B	85	ILE
1	B	87	GLU
1	B	88	GLU
1	B	103	LEU
1	B	110	TYR
1	B	116	ILE

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Mol	Chain	Res	Type
1	B	118	ASP
1	B	122	LEU
1	C	26	SER
1	C	35	ILE
1	C	50	ARG
1	C	58	ASN
1	C	103	LEU
1	D	4	THR
1	D	27	ILE
1	D	29	THR
1	D	49	LEU
1	D	88	GLU
1	D	103	LEU
1	D	159	ASN

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](#)

179 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
5	EDO	D	220	-	3,3,3	0.30	0	2,2,2	0.67	0
9	MOH	B	228	-	1,1,1	0.08	0	-		
8	EOH	C	224	-	2,2,2	0.39	0	1,1,1	0.38	0
5	EDO	B	207	-	3,3,3	0.53	0	2,2,2	1.23	0
15	P6G	D	209	-	18,18,18	0.55	0	17,17,17	0.80	1 (5%)
6	GOL	C	216	-	5,5,5	0.96	0	5,5,5	0.97	0
7	PDO	A	220	-	4,4,4	0.33	0	3,3,3	0.37	0
14	P33	C	207	-	21,21,21	0.48	0	20,20,20	0.31	0
7	PDO	B	214	-	4,4,4	0.41	0	3,3,3	0.95	0
5	EDO	A	209	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	A	217	-	3,3,3	0.46	0	2,2,2	0.34	0
8	EOH	A	227	-	2,2,2	0.39	0	1,1,1	0.38	0
4	PEG	A	207	-	6,6,6	0.53	0	5,5,5	2.06	2 (40%)
9	MOH	D	239	-	1,1,1	0.11	0	-		
9	MOH	A	242	-	1,1,1	0.06	0	-		
8	EOH	B	225	-	2,2,2	0.61	0	1,1,1	0.43	0
5	EDO	A	210	-	3,3,3	0.46	0	2,2,2	0.34	0
8	EOH	A	233	-	2,2,2	0.23	0	1,1,1	0.40	0
5	EDO	C	213	-	3,3,3	0.46	0	2,2,2	0.34	0
3	PG0	D	204	-	7,7,7	0.44	0	6,6,6	0.26	0
8	EOH	D	230	-	2,2,2	0.40	0	1,1,1	0.39	0
9	MOH	C	234	-	1,1,1	0.07	0	-		
5	EDO	D	218	-	3,3,3	1.21	1 (33%)	2,2,2	0.53	0
3	PG0	A	205	-	7,7,7	0.32	0	6,6,6	1.44	2 (33%)
7	PDO	B	213	-	4,4,4	0.33	0	3,3,3	0.37	0
13	PGE	B	233	-	9,9,9	0.44	0	8,8,8	0.29	0
8	EOH	A	237	-	2,2,2	0.70	0	1,1,1	0.73	0
5	EDO	C	211	-	3,3,3	0.46	0	2,2,2	0.34	0
8	EOH	D	226	-	2,2,2	0.40	0	1,1,1	0.38	0
9	MOH	C	233	-	1,1,1	0.08	0	-		
5	EDO	A	213	-	3,3,3	0.59	0	2,2,2	0.14	0
9	MOH	D	244	-	1,1,1	0.31	0	-		
12	ETE	C	208	-	13,13,13	0.66	0	12,12,12	1.37	3 (25%)
9	MOH	D	241	-	1,1,1	0.05	0	-		
5	EDO	C	209	-	3,3,3	1.16	0	2,2,2	1.39	0
8	EOH	D	228	-	2,2,2	0.40	0	1,1,1	0.39	0
7	PDO	A	222	-	4,4,4	0.32	0	3,3,3	0.37	0
7	PDO	D	224	-	4,4,4	0.32	0	3,3,3	0.37	0
9	MOH	C	232	-	1,1,1	0.20	0	-		
5	EDO	D	213	-	3,3,3	0.45	0	2,2,2	0.46	0
9	MOH	B	227	-	1,1,1	0.07	0	-		
9	MOH	C	237	-	1,1,1	0.12	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	C	218	-	5,5,5	1.63	1 (20%)	5,5,5	2.37	2 (40%)
8	EOH	B	223	-	2,2,2	0.39	0	1,1,1	0.39	0
8	EOH	C	229	-	2,2,2	0.40	0	1,1,1	0.39	0
5	EDO	C	210	-	3,3,3	0.46	0	2,2,2	0.34	0
4	PEG	C	203	-	6,6,6	0.43	0	5,5,5	0.31	0
5	EDO	A	211	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	B	206	-	3,3,3	0.45	0	2,2,2	0.33	0
8	EOH	A	228	-	2,2,2	0.40	0	1,1,1	0.39	0
9	MOH	A	240	-	1,1,1	0.07	0	-		
3	PG0	D	203	-	7,7,7	0.44	0	6,6,6	0.27	0
8	EOH	B	226	-	2,2,2	0.37	0	1,1,1	0.17	0
9	MOH	A	244	-	1,1,1	0.08	0	-		
8	EOH	D	231	-	2,2,2	0.40	0	1,1,1	0.39	0
10	PGO	D	246	-	3,4,4	0.25	0	1,4,4	0.03	0
6	GOL	A	218	-	5,5,5	1.41	1 (20%)	5,5,5	2.62	3 (60%)
10	PGO	D	247	-	3,4,4	1.57	1 (33%)	1,4,4	0.95	0
13	PGE	C	240	-	9,9,9	0.45	0	8,8,8	0.29	0
3	PG0	C	202	-	7,7,7	0.74	0	6,6,6	0.84	0
7	PDO	C	221	-	4,4,4	0.32	0	3,3,3	0.37	0
9	MOH	A	245	-	1,1,1	0.07	0	-		
3	PG0	A	203	-	7,7,7	0.77	0	6,6,6	0.69	0
9	MOH	C	235	-	1,1,1	0.08	0	-		
9	MOH	D	237	-	1,1,1	0.07	0	-		
5	EDO	D	217	-	3,3,3	0.91	0	2,2,2	0.73	0
7	PDO	D	223	-	4,4,4	0.32	0	3,3,3	0.37	0
4	PEG	C	204	-	6,6,6	0.42	0	5,5,5	0.31	0
3	PG0	C	201	-	7,7,7	0.55	0	6,6,6	1.60	1 (16%)
5	EDO	A	214	-	3,3,3	0.39	0	2,2,2	0.84	0
11	ETX	D	250	-	5,5,5	0.64	0	4,4,4	0.82	0
6	GOL	C	217	-	5,5,5	1.29	1 (20%)	5,5,5	1.31	1 (20%)
9	MOH	A	246	-	1,1,1	0.07	0	-		
5	EDO	B	211	-	3,3,3	0.84	0	2,2,2	0.40	0
5	EDO	D	215	-	3,3,3	0.46	0	2,2,2	0.34	0
7	PDO	A	225	-	4,4,4	0.94	0	3,3,3	0.81	0
9	MOH	A	239	-	1,1,1	0.07	0	-		
2	PG4	A	202	-	12,12,12	0.58	0	11,11,11	1.25	3 (27%)
11	ETX	B	236	-	5,5,5	0.53	0	4,4,4	1.21	1 (25%)
5	EDO	D	221	-	3,3,3	0.46	0	2,2,2	0.34	0
15	P6G	D	210	-	18,18,18	0.82	0	17,17,17	1.65	4 (23%)
8	EOH	C	223	-	2,2,2	0.39	0	1,1,1	0.38	0
8	EOH	C	230	-	2,2,2	0.39	0	1,1,1	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PG0	A	204	-	7,7,7	0.45	0	6,6,6	0.27	0
10	PGO	B	231	-	3,4,4	0.25	0	1,4,4	0.02	0
8	EOH	A	226	-	2,2,2	0.05	0	1,1,1	0.13	0
9	MOH	D	240	-	1,1,1	0.07	0	-		
8	EOH	B	222	-	2,2,2	0.39	0	1,1,1	0.38	0
10	PGO	A	249	-	3,4,4	0.54	0	1,4,4	0.19	0
8	EOH	C	227	-	2,2,2	0.39	0	1,1,1	0.38	0
9	MOH	A	241	-	1,1,1	0.07	0	-		
8	EOH	D	229	-	2,2,2	0.39	0	1,1,1	0.38	0
6	GOL	D	222	-	5,5,5	1.52	1 (20%)	5,5,5	0.78	0
8	EOH	A	238	-	2,2,2	0.17	0	1,1,1	0.28	0
9	MOH	D	242	-	1,1,1	0.07	0	-		
9	MOH	C	236	-	1,1,1	0.01	0	-		
13	PGE	C	241	-	9,9,9	1.26	2 (22%)	8,8,8	2.12	2 (25%)
8	EOH	B	215	-	2,2,2	0.39	0	1,1,1	0.38	0
8	EOH	B	220	-	2,2,2	0.39	0	1,1,1	0.38	0
5	EDO	D	212	-	3,3,3	0.43	0	2,2,2	0.48	0
8	EOH	B	221	-	2,2,2	0.40	0	1,1,1	0.65	0
5	EDO	D	211	-	3,3,3	0.49	0	2,2,2	0.34	0
4	PEG	D	207	-	6,6,6	0.47	0	5,5,5	0.92	0
8	EOH	A	236	-	2,2,2	0.55	0	1,1,1	0.13	0
5	EDO	D	214	-	3,3,3	0.58	0	2,2,2	0.46	0
8	EOH	B	219	-	2,2,2	0.39	0	1,1,1	0.38	0
7	PDO	A	219	-	4,4,4	0.58	0	3,3,3	2.03	1 (33%)
8	EOH	D	234	-	2,2,2	0.54	0	1,1,1	0.27	0
8	EOH	C	226	-	2,2,2	0.49	0	1,1,1	0.38	0
11	ETX	C	242	-	5,5,5	0.44	0	4,4,4	0.29	0
9	MOH	D	243	-	1,1,1	0.07	0	-		
8	EOH	A	235	-	2,2,2	0.39	0	1,1,1	0.39	0
5	EDO	D	216	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	A	216	-	3,3,3	0.80	0	2,2,2	0.80	0
5	EDO	C	212	-	3,3,3	0.45	0	2,2,2	0.34	0
5	EDO	B	210	-	3,3,3	0.71	0	2,2,2	1.02	0
2	PG4	B	201	-	12,12,12	0.95	0	11,11,11	1.42	1 (9%)
11	ETX	B	235	-	5,5,5	0.44	0	4,4,4	0.29	0
2	PG4	A	201	-	12,12,12	0.54	0	11,11,11	0.46	0
8	EOH	A	232	-	2,2,2	0.63	0	1,1,1	0.85	0
11	ETX	B	234	-	5,5,5	0.33	0	4,4,4	0.79	0
7	PDO	A	221	-	4,4,4	0.33	0	3,3,3	0.37	0
8	EOH	D	235	-	2,2,2	0.57	0	1,1,1	0.84	0
10	PGO	D	245	-	3,4,4	1.12	0	1,4,4	2.44	1 (100%)
7	PDO	A	224	-	4,4,4	0.33	0	3,3,3	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	MOH	A	243	-	1,1,1	0.12	0	-		
8	EOH	D	227	-	2,2,2	0.40	0	1,1,1	0.39	0
8	EOH	A	234	-	2,2,2	0.40	0	1,1,1	0.39	0
5	EDO	D	219	-	3,3,3	0.46	0	2,2,2	0.34	0
8	EOH	D	233	-	2,2,2	0.39	0	1,1,1	0.38	0
4	PEG	D	205	-	6,6,6	0.43	0	5,5,5	0.31	0
4	PEG	C	206	-	6,6,6	0.60	0	5,5,5	1.25	0
8	EOH	B	224	-	2,2,2	0.48	0	1,1,1	0.42	0
8	EOH	B	217	-	2,2,2	0.39	0	1,1,1	0.38	0
8	EOH	C	225	-	2,2,2	0.40	0	1,1,1	0.39	0
8	EOH	D	225	-	2,2,2	0.44	0	1,1,1	0.28	0
4	PEG	C	205	-	6,6,6	0.66	0	5,5,5	2.42	3 (60%)
12	ETE	B	205	-	13,13,13	0.70	0	12,12,12	1.48	2 (16%)
8	EOH	C	228	-	2,2,2	0.39	0	1,1,1	0.38	0
4	PEG	A	208	-	6,6,6	0.60	0	5,5,5	1.13	1 (20%)
8	EOH	C	222	-	2,2,2	0.39	0	1,1,1	0.38	0
11	ETX	A	251	-	5,5,5	0.81	0	4,4,4	1.62	1 (25%)
5	EDO	B	209	-	3,3,3	0.48	0	2,2,2	0.22	0
4	PEG	B	204	-	6,6,6	0.30	0	5,5,5	1.34	1 (20%)
9	MOH	B	229	-	1,1,1	0.06	0	-		
10	PGO	C	238	-	3,4,4	1.32	0	1,4,4	0.72	0
8	EOH	A	229	-	2,2,2	0.20	0	1,1,1	0.56	0
13	PGE	D	248	-	9,9,9	0.44	0	8,8,8	0.29	0
5	EDO	A	215	-	3,3,3	0.45	0	2,2,2	0.34	0
2	PG4	D	202	-	12,12,12	0.45	0	11,11,11	0.28	0
3	PG0	A	206	-	7,7,7	1.07	1 (14%)	6,6,6	1.92	3 (50%)
3	PG0	B	202	-	7,7,7	0.44	0	6,6,6	0.27	0
9	MOH	D	238	-	1,1,1	0.08	0	-		
8	EOH	D	236	-	2,2,2	0.39	0	1,1,1	0.38	0
13	PGE	C	239	-	9,9,9	0.44	0	8,8,8	0.29	0
5	EDO	B	208	-	3,3,3	0.36	0	2,2,2	0.25	0
10	PGO	A	248	-	3,4,4	0.45	0	1,4,4	0.48	0
11	ETX	A	250	-	5,5,5	0.44	0	4,4,4	0.29	0
7	PDO	A	223	-	4,4,4	0.32	0	3,3,3	0.37	0
10	PGO	B	232	-	3,4,4	0.31	0	1,4,4	1.18	0
11	ETX	D	249	-	5,5,5	0.41	0	4,4,4	0.56	0
8	EOH	B	216	-	2,2,2	0.40	0	1,1,1	0.38	0
5	EDO	C	215	-	3,3,3	1.44	1 (33%)	2,2,2	0.40	0
10	PGO	B	230	-	3,4,4	3.20	1 (33%)	1,4,4	2.01	1 (100%)
4	PEG	D	206	-	6,6,6	0.43	0	5,5,5	0.31	0
2	PG4	D	201	-	12,12,12	1.33	2 (16%)	11,11,11	1.64	2 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	212	-	3,3,3	0.46	0	2,2,2	0.34	0
4	PEG	B	203	-	6,6,6	0.43	0	5,5,5	0.31	0
10	PGO	A	247	-	3,4,4	0.65	0	1,4,4	1.44	0
8	EOH	B	218	-	2,2,2	0.40	0	1,1,1	0.38	0
8	EOH	A	230	-	2,2,2	0.40	0	1,1,1	0.39	0
5	EDO	C	214	-	3,3,3	1.00	0	2,2,2	1.16	0
8	EOH	A	231	-	2,2,2	0.40	0	1,1,1	0.38	0
7	PDO	C	220	-	4,4,4	0.32	0	3,3,3	0.37	0
8	EOH	D	232	-	2,2,2	0.39	0	1,1,1	0.38	0
7	PDO	B	212	-	4,4,4	0.32	0	3,3,3	0.37	0
15	P6G	D	208	-	18,18,18	0.46	0	17,17,17	0.27	0
6	GOL	C	219	-	5,5,5	1.15	0	5,5,5	2.21	3 (60%)
8	EOH	C	231	-	2,2,2	0.39	0	1,1,1	0.38	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	EDO	D	220	-	-	1/1/1/1	-
5	EDO	B	207	-	-	1/1/1/1	-
15	P6G	D	209	-	-	7/16/16/16	-
6	GOL	C	216	-	-	2/4/4/4	-
11	ETX	B	236	-	-	2/3/3/3	-
14	P33	C	207	-	-	11/19/19/19	-
7	PDO	B	214	-	-	1/2/2/2	-
5	EDO	A	209	-	-	0/1/1/1	-
5	EDO	A	217	-	-	1/1/1/1	-
4	PEG	A	207	-	-	3/4/4/4	-
5	EDO	C	213	-	-	1/1/1/1	-
3	PG0	D	204	-	-	3/5/5/5	-
5	EDO	D	218	-	-	1/1/1/1	-
3	PG0	A	205	-	-	3/5/5/5	-
7	PDO	B	213	-	-	1/2/2/2	-
13	PGE	B	233	-	-	3/7/7/7	-
5	EDO	C	211	-	-	1/1/1/1	-
5	EDO	A	213	-	-	1/1/1/1	-
10	PGO	C	238	-	-	0/2/2/2	-
12	ETE	C	208	-	-	6/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PDO	A	222	-	-	2/2/2/2	-
7	PDO	D	224	-	-	1/2/2/2	-
5	EDO	D	213	-	-	0/1/1/1	-
6	GOL	C	218	-	-	4/4/4/4	-
5	EDO	C	210	-	-	1/1/1/1	-
4	PEG	C	203	-	-	1/4/4/4	-
5	EDO	A	211	-	-	1/1/1/1	-
5	EDO	B	206	-	-	1/1/1/1	-
5	EDO	D	219	-	-	1/1/1/1	-
11	ETX	D	249	-	-	2/3/3/3	-
10	PGO	D	246	-	-	0/2/2/2	-
6	GOL	A	218	-	-	4/4/4/4	-
10	PGO	D	247	-	-	2/2/2/2	-
13	PGE	C	240	-	-	3/7/7/7	-
3	PG0	C	202	-	-	4/5/5/5	-
7	PDO	C	221	-	-	1/2/2/2	-
3	PG0	A	203	-	-	3/5/5/5	-
5	EDO	D	217	-	-	0/1/1/1	-
7	PDO	D	223	-	-	1/2/2/2	-
4	PEG	C	204	-	-	3/4/4/4	-
3	PG0	C	201	-	-	1/5/5/5	-
5	EDO	A	214	-	-	1/1/1/1	-
11	ETX	D	250	-	-	2/3/3/3	-
6	GOL	C	217	-	-	4/4/4/4	-
5	EDO	B	211	-	-	0/1/1/1	-
5	EDO	D	215	-	-	1/1/1/1	-
7	PDO	A	225	-	-	1/2/2/2	-
2	PG4	A	202	-	-	6/10/10/10	-
5	EDO	D	221	-	-	1/1/1/1	-
3	PG0	A	204	-	-	4/5/5/5	-
10	PGO	B	231	-	-	2/2/2/2	-
13	PGE	C	239	-	-	4/7/7/7	-
10	PGO	A	249	-	-	2/2/2/2	-
5	EDO	A	210	-	-	1/1/1/1	-
6	GOL	D	222	-	-	4/4/4/4	-
13	PGE	C	241	-	-	4/7/7/7	-
5	EDO	D	212	-	-	1/1/1/1	-
5	EDO	D	211	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	D	207	-	-	3/4/4/4	-
5	EDO	D	214	-	-	0/1/1/1	-
7	PDO	A	219	-	-	1/2/2/2	-
15	P6G	D	210	-	-	9/16/16/16	-
11	ETX	C	242	-	-	3/3/3/3	-
5	EDO	D	216	-	-	1/1/1/1	-
5	EDO	A	216	-	-	1/1/1/1	-
5	EDO	C	212	-	-	1/1/1/1	-
5	EDO	B	210	-	-	0/1/1/1	-
2	PG4	B	201	-	-	6/10/10/10	-
11	ETX	B	235	-	-	1/3/3/3	-
2	PG4	A	201	-	-	4/10/10/10	-
7	PDO	A	224	-	-	2/2/2/2	-
11	ETX	B	234	-	-	2/3/3/3	-
7	PDO	A	221	-	-	1/2/2/2	-
10	PGO	D	245	-	-	2/2/2/2	-
13	PGE	D	248	-	-	6/7/7/7	-
3	PG0	D	203	-	-	1/5/5/5	-
4	PEG	D	205	-	-	2/4/4/4	-
4	PEG	C	206	-	-	2/4/4/4	-
4	PEG	C	205	-	-	3/4/4/4	-
12	ETE	B	205	-	-	6/11/11/11	-
4	PEG	A	208	-	-	3/4/4/4	-
11	ETX	A	251	-	-	2/3/3/3	-
5	EDO	B	209	-	-	1/1/1/1	-
4	PEG	B	204	-	-	2/4/4/4	-
5	EDO	A	215	-	-	0/1/1/1	-
2	PG4	D	202	-	-	2/10/10/10	-
3	PG0	A	206	-	-	2/5/5/5	-
3	PG0	B	202	-	-	1/5/5/5	-
5	EDO	B	208	-	-	1/1/1/1	-
10	PGO	A	248	-	-	2/2/2/2	-
7	PDO	A	220	-	-	1/2/2/2	-
11	ETX	A	250	-	-	2/3/3/3	-
7	PDO	A	223	-	-	1/2/2/2	-
10	PGO	B	232	-	-	2/2/2/2	-
5	EDO	C	215	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PGO	B	230	-	1/1/1/1	1/2/2/2	-
4	PEG	D	206	-	-	4/4/4/4	-
2	PG4	D	201	-	-	6/10/10/10	-
5	EDO	A	212	-	-	0/1/1/1	-
4	PEG	B	203	-	-	3/4/4/4	-
10	PGO	A	247	-	-	2/2/2/2	-
5	EDO	C	214	-	-	0/1/1/1	-
7	PDO	C	220	-	-	2/2/2/2	-
5	EDO	C	209	-	-	1/1/1/1	-
7	PDO	B	212	-	-	1/2/2/2	-
15	P6G	D	208	-	-	9/16/16/16	-
6	GOL	C	219	-	-	4/4/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	230	PGO	O2-C2	-5.54	1.19	1.43
6	C	218	GOL	O2-C2	-3.07	1.34	1.43
6	D	222	GOL	O2-C2	-2.84	1.34	1.43
6	A	218	GOL	O2-C2	-2.82	1.35	1.43
2	D	201	PG4	O4-C6	-2.34	1.31	1.42
10	D	247	PGO	O1-C1	-2.33	1.32	1.42
3	A	206	PG0	O1-C3	-2.33	1.31	1.42
6	C	217	GOL	O2-C2	-2.31	1.36	1.43
13	C	241	PGE	O1-C1	-2.31	1.30	1.42
2	D	201	PG4	O3-C5	-2.29	1.32	1.42
13	C	241	PGE	O2-C2	-2.17	1.32	1.42
5	C	215	EDO	O1-C1	-2.02	1.31	1.42
5	D	218	EDO	O1-C1	-2.01	1.31	1.42

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	241	PGE	C3-O2-C2	-4.33	94.52	113.29
6	C	218	GOL	O2-C2-C3	-4.04	91.34	109.12
15	D	210	P6G	O7-C6-C5	3.94	128.18	110.39
4	A	207	PEG	O2-C2-C1	3.78	126.65	110.07
6	A	218	GOL	O1-C1-C2	3.53	127.11	110.20
3	C	201	PG0	O1-C2-C1	3.41	125.04	110.07
2	D	201	PG4	C5-O3-C4	-3.35	98.79	113.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	219	PDO	O3-C3-C2	-3.25	90.31	111.66
2	B	201	PG4	O4-C7-C8	3.23	124.27	110.07
4	C	205	PEG	C3-O2-C2	3.09	126.66	113.29
13	C	241	PGE	O2-C2-C1	3.02	123.33	110.07
4	C	205	PEG	O2-C3-C4	-2.98	96.98	110.07
6	A	218	GOL	O2-C2-C3	-2.98	96.01	109.12
6	C	219	GOL	O2-C2-C3	2.97	122.20	109.12
12	B	205	ETE	C23-OH3-C22	2.92	125.94	113.29
6	C	218	GOL	O3-C3-C2	-2.91	96.26	110.20
3	A	206	PG0	O1-C2-C1	2.88	122.71	110.07
6	C	219	GOL	O3-C3-C2	2.87	123.95	110.20
12	B	205	ETE	OH5-C14-C24	2.77	122.89	110.39
3	A	206	PG0	C2-O1-C3	2.75	125.19	113.29
15	D	210	P6G	O7-C8-C9	2.70	122.59	110.39
11	A	251	ETX	O1-C1-C2	-2.64	96.48	111.81
4	C	205	PEG	O1-C1-C2	-2.60	96.71	111.81
4	A	207	PEG	O2-C3-C4	2.60	121.48	110.07
3	A	205	PG0	OTT-C1-C2	2.59	126.84	111.81
6	A	218	GOL	O2-C2-C1	2.57	120.46	109.12
12	C	208	ETE	OH5-C14-C24	2.49	121.62	110.39
10	D	245	PGO	O2-C2-C3	-2.44	98.81	109.38
3	A	206	PG0	O1-C3-C4	-2.37	99.70	110.39
11	B	236	ETX	C3-O2-C2	2.35	121.31	112.90
15	D	210	P6G	C14-O13-C12	-2.34	103.14	113.29
6	C	219	GOL	C3-C2-C1	-2.28	102.83	111.70
2	A	202	PG4	O4-C6-C5	2.26	120.61	110.39
4	A	208	PEG	C3-O2-C2	2.26	123.07	113.29
4	B	204	PEG	O2-C3-C4	-2.25	100.16	110.07
15	D	210	P6G	O13-C14-C15	2.24	120.49	110.39
2	A	202	PG4	C7-O4-C6	2.20	122.83	113.29
6	C	217	GOL	O3-C3-C2	2.18	120.64	110.20
12	C	208	ETE	OH3-C22-C12	2.18	119.63	110.07
15	D	209	P6G	O16-C17-C18	-2.15	100.64	110.07
12	C	208	ETE	OH4-C13-C23	-2.08	101.03	110.39
3	A	205	PG0	O1-C3-C4	2.07	119.73	110.39
2	D	201	PG4	O2-C2-C1	2.06	119.10	110.07
2	A	202	PG4	C3-O2-C2	-2.03	104.49	113.29
10	B	230	PGO	O2-C2-C3	2.01	118.09	109.38

All (1) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
10	B	230	PGO	C2

All (237) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	216	GOL	C1-C2-C3-O3
6	C	216	GOL	O2-C2-C3-O3
7	B	214	PDO	O1-C1-C2-C3
7	A	222	PDO	O1-C1-C2-C3
7	D	224	PDO	O1-C1-C2-C3
6	C	218	GOL	C1-C2-C3-O3
6	C	218	GOL	O2-C2-C3-O3
10	D	247	PGO	O1-C1-C2-C3
10	D	247	PGO	O1-C1-C2-O2
7	A	225	PDO	O1-C1-C2-C3
10	B	231	PGO	O1-C1-C2-C3
10	B	231	PGO	O1-C1-C2-O2
6	D	222	GOL	C1-C2-C3-O3
7	A	219	PDO	O1-C1-C2-C3
7	A	221	PDO	O1-C1-C2-C3
7	A	224	PDO	O1-C1-C2-C3
7	A	224	PDO	C1-C2-C3-O3
10	A	248	PGO	O1-C1-C2-C3
10	A	248	PGO	O1-C1-C2-O2
7	A	223	PDO	O1-C1-C2-C3
10	B	232	PGO	O1-C1-C2-C3
10	B	232	PGO	O1-C1-C2-O2
10	B	230	PGO	O1-C1-C2-O2
10	A	247	PGO	O1-C1-C2-C3
10	A	247	PGO	O1-C1-C2-O2
7	C	220	PDO	O1-C1-C2-C3
7	B	212	PDO	O1-C1-C2-C3
6	C	219	GOL	O1-C1-C2-C3
2	A	202	PG4	C5-C6-O4-C7
2	B	201	PG4	C1-C2-O2-C3
14	C	207	P33	C17-C18-O19-C20
13	C	239	PGE	C1-C2-O2-C3
14	C	207	P33	C8-C9-O10-C11
13	C	240	PGE	C4-C3-O2-C2
14	C	207	P33	C18-C17-O16-C15
14	C	207	P33	C2-C3-O4-C5

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Mol	Chain	Res	Type	Atoms
3	A	203	PG0	O1-C3-C4-O2
15	D	210	P6G	O7-C8-C9-O10
14	C	207	P33	O7-C8-C9-O10
2	A	202	PG4	O2-C3-C4-O3
13	C	240	PGE	O2-C3-C4-O3
15	D	208	P6G	O10-C11-C12-O13
15	D	209	P6G	O10-C11-C12-O13
13	B	233	PGE	O2-C3-C4-O3
12	B	205	ETE	OH6-C15-C25-OH5
15	D	208	P6G	O4-C5-C6-O7
13	C	241	PGE	O2-C3-C4-O3
14	C	207	P33	O16-C17-C18-O19
12	B	205	ETE	OH4-C13-C23-OH3
15	D	209	P6G	O13-C14-C15-O16
2	D	201	PG4	O3-C5-C6-O4
6	C	219	GOL	O1-C1-C2-O2
11	D	250	ETX	O1-C1-C2-O2
2	A	202	PG4	O1-C1-C2-O2
15	D	210	P6G	O1-C2-C3-O4
4	C	205	PEG	O2-C3-C4-O4
4	A	208	PEG	O2-C3-C4-O4
14	C	207	P33	O1-C2-C3-O4
4	B	204	PEG	O1-C1-C2-O2
13	D	248	PGE	O3-C5-C6-O4
3	B	202	PG0	OTT-C1-C2-O1
4	D	206	PEG	O2-C3-C4-O4
4	C	204	PEG	C4-C3-O2-C2
2	D	201	PG4	C4-C3-O2-C2
12	C	208	ETE	OH6-C15-C25-OH5
15	D	208	P6G	O13-C14-C15-O16
13	B	233	PGE	O1-C1-C2-O2
4	C	204	PEG	O1-C1-C2-O2
4	D	207	PEG	O1-C1-C2-O2
2	B	201	PG4	O4-C7-C8-O5
4	C	205	PEG	O1-C1-C2-O2
12	B	205	ETE	OH2-C12-C22-OH3
4	B	204	PEG	O2-C3-C4-O4
3	A	206	PG0	OTT-C1-C2-O1
4	D	206	PEG	O1-C1-C2-O2
4	D	207	PEG	C4-C3-O2-C2
14	C	207	P33	O10-C11-C12-O13
3	C	202	PG0	O1-C3-C4-O2

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Mol	Chain	Res	Type	Atoms
13	C	239	PGE	O2-C3-C4-O3
6	C	218	GOL	O1-C1-C2-C3
6	A	218	GOL	O1-C1-C2-C3
6	A	218	GOL	C1-C2-C3-O3
6	C	217	GOL	C1-C2-C3-O3
6	C	219	GOL	C1-C2-C3-O3
15	D	209	P6G	O4-C5-C6-O7
15	D	209	P6G	O7-C8-C9-O10
6	C	218	GOL	O1-C1-C2-O2
6	A	218	GOL	O1-C1-C2-O2
6	A	218	GOL	O2-C2-C3-O3
6	C	217	GOL	O2-C2-C3-O3
6	D	222	GOL	O2-C2-C3-O3
15	D	210	P6G	C11-C12-O13-C14
11	B	236	ETX	O1-C1-C2-O2
5	A	217	EDO	O1-C1-C2-O2
5	C	211	EDO	O1-C1-C2-O2
5	C	210	EDO	O1-C1-C2-O2
5	A	211	EDO	O1-C1-C2-O2
5	B	206	EDO	O1-C1-C2-O2
5	A	210	EDO	O1-C1-C2-O2
5	D	221	EDO	O1-C1-C2-O2
5	A	216	EDO	O1-C1-C2-O2
5	C	212	EDO	O1-C1-C2-O2
5	B	208	EDO	O1-C1-C2-O2
12	C	208	ETE	OH5-C14-C24-OH4
4	A	207	PEG	O1-C1-C2-O2
3	A	205	PG0	O1-C3-C4-O2
4	B	203	PEG	O2-C3-C4-O4
2	A	201	PG4	O3-C5-C6-O4
15	D	209	P6G	O1-C2-C3-O4
11	D	249	ETX	O1-C1-C2-O2
5	C	209	EDO	O1-C1-C2-O2
5	A	214	EDO	O1-C1-C2-O2
5	D	219	EDO	O1-C1-C2-O2
5	B	209	EDO	O1-C1-C2-O2
5	C	215	EDO	O1-C1-C2-O2
4	C	205	PEG	C1-C2-O2-C3
11	D	249	ETX	C4-C3-O2-C2
7	A	220	PDO	O1-C1-C2-C3
7	A	222	PDO	C1-C2-C3-O3
7	C	220	PDO	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
10	A	249	PGO	O1-C1-C2-O2
10	D	245	PGO	O1-C1-C2-O2
3	A	206	PG0	C3-C4-O2-C5
3	C	202	PG0	OTT-C1-C2-O1
15	D	208	P6G	O16-C17-C18-O19
15	D	209	P6G	C5-C6-O7-C8
6	C	219	GOL	O2-C2-C3-O3
15	D	210	P6G	C9-C8-O7-C6
3	A	204	PG0	C3-C4-O2-C5
5	D	220	EDO	O1-C1-C2-O2
5	D	211	EDO	O1-C1-C2-O2
5	D	216	EDO	O1-C1-C2-O2
4	A	207	PEG	O2-C3-C4-O4
13	C	241	PGE	O1-C1-C2-O2
13	C	241	PGE	O3-C5-C6-O4
4	C	206	PEG	O2-C3-C4-O4
2	D	201	PG4	O4-C7-C8-O5
2	D	201	PG4	C5-C6-O4-C7
14	C	207	P33	C15-C14-O13-C12
11	B	236	ETX	C4-C3-O2-C2
15	D	210	P6G	C8-C9-O10-C11
15	D	208	P6G	C18-C17-O16-C15
3	A	203	PG0	C1-C2-O1-C3
12	B	205	ETE	C24-C14-OH5-C25
11	B	234	ETX	C4-C3-O2-C2
10	A	249	PGO	O1-C1-C2-C3
15	D	210	P6G	C14-C15-O16-C17
13	C	239	PGE	C4-C3-O2-C2
15	D	210	P6G	C12-C11-O10-C9
15	D	208	P6G	C12-C11-O10-C9
3	D	204	PG0	C4-C3-O1-C2
12	C	208	ETE	C13-C23-OH3-C22
2	A	201	PG4	C3-C4-O3-C5
11	B	234	ETX	C1-C2-O2-C3
4	A	208	PEG	C4-C3-O2-C2
3	C	202	PG0	C1-C2-O1-C3
2	A	202	PG4	C1-C2-O2-C3
13	D	248	PGE	C1-C2-O2-C3
2	D	201	PG4	C8-C7-O4-C6
14	C	207	P33	C6-C5-O4-C3
11	C	242	ETX	C4-C3-O2-C2
2	D	201	PG4	C6-C5-O3-C4

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Mol	Chain	Res	Type	Atoms
4	D	206	PEG	C1-C2-O2-C3
13	D	248	PGE	C3-C4-O3-C5
15	D	208	P6G	C15-C14-O13-C12
4	D	205	PEG	O1-C1-C2-O2
4	B	203	PEG	O1-C1-C2-O2
4	C	206	PEG	C4-C3-O2-C2
13	B	233	PGE	C3-C4-O3-C5
13	D	248	PGE	C4-C3-O2-C2
15	D	209	P6G	C8-C9-O10-C11
4	C	203	PEG	C4-C3-O2-C2
3	D	204	PG0	C1-C2-O1-C3
12	C	208	ETE	C15-C25-OH5-C14
13	C	240	PGE	C6-C5-O3-C4
15	D	208	P6G	C11-C12-O13-C14
2	B	201	PG4	C4-C3-O2-C2
13	C	239	PGE	O1-C1-C2-O2
2	A	201	PG4	C1-C2-O2-C3
11	C	242	ETX	O1-C1-C2-O2
3	D	204	PG0	C3-C4-O2-C5
2	A	202	PG4	C4-C3-O2-C2
15	D	210	P6G	O4-C5-C6-O7
3	D	203	PG0	C4-C3-O1-C2
15	D	208	P6G	C2-C3-O4-C5
12	C	208	ETE	C14-C24-OH4-C13
5	B	207	EDO	O1-C1-C2-O2
4	A	208	PEG	C1-C2-O2-C3
12	B	205	ETE	C25-C15-OH6-C26
3	A	204	PG0	OTT-C1-C2-O1
11	A	251	ETX	O1-C1-C2-O2
11	C	242	ETX	C1-C2-O2-C3
11	A	251	ETX	C1-C2-O2-C3
6	C	217	GOL	O1-C1-C2-C3
4	A	207	PEG	C4-C3-O2-C2
3	C	202	PG0	C4-C3-O1-C2
3	A	205	PG0	C3-C4-O2-C5
2	B	201	PG4	C5-C6-O4-C7
4	B	203	PEG	C4-C3-O2-C2
13	D	248	PGE	C6-C5-O3-C4
3	A	205	PG0	OTT-C1-C2-O1
14	C	207	P33	C12-C11-O10-C9
13	C	241	PGE	C6-C5-O3-C4
11	A	250	ETX	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
6	D	222	GOL	O1-C1-C2-O2
11	A	250	ETX	C4-C3-O2-C2
3	A	203	PG0	C3-C4-O2-C5
12	B	205	ETE	C15-C25-OH5-C14
4	D	205	PEG	C4-C3-O2-C2
4	D	207	PEG	C1-C2-O2-C3
4	D	206	PEG	C4-C3-O2-C2
5	A	213	EDO	O1-C1-C2-O2
5	D	212	EDO	O1-C1-C2-O2
10	D	245	PGO	O1-C1-C2-C3
2	A	202	PG4	C3-C4-O3-C5
13	D	248	PGE	O2-C3-C4-O3
6	C	217	GOL	O1-C1-C2-O2
2	D	202	PG4	O4-C7-C8-O5
12	C	208	ETE	C25-C15-OH6-C26
4	C	204	PEG	C1-C2-O2-C3
11	D	250	ETX	C4-C3-O2-C2
6	D	222	GOL	O1-C1-C2-C3
2	B	201	PG4	O2-C3-C4-O3
3	A	204	PG0	C1-C2-O1-C3
7	B	213	PDO	C1-C2-C3-O3
7	C	221	PDO	C1-C2-C3-O3
7	D	223	PDO	O1-C1-C2-C3
5	C	213	EDO	O1-C1-C2-O2
5	D	218	EDO	O1-C1-C2-O2
5	D	215	EDO	O1-C1-C2-O2
11	B	235	ETX	C4-C3-O2-C2
15	D	210	P6G	O10-C11-C12-O13
2	A	201	PG4	O2-C3-C4-O3
3	C	201	PG0	O1-C3-C4-O2
3	A	204	PG0	O1-C3-C4-O2
2	D	202	PG4	O2-C3-C4-O3
2	B	201	PG4	O3-C5-C6-O4

There are no ring outliers.

85 monomers are involved in 213 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	220	EDO	1	0
8	C	224	EOH	1	0
5	B	207	EDO	3	0
15	D	209	P6G	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	220	PDO	2	0
14	C	207	P33	14	0
5	A	209	EDO	2	0
4	A	207	PEG	4	0
9	D	239	MOH	1	0
5	A	210	EDO	1	0
3	D	204	PG0	5	0
8	D	230	EOH	11	0
3	A	205	PG0	1	0
13	B	233	PGE	3	0
12	C	208	ETE	1	0
5	C	209	EDO	1	0
7	A	222	PDO	1	0
7	D	224	PDO	11	0
8	B	223	EOH	2	0
5	C	210	EDO	1	0
4	C	203	PEG	8	0
5	B	206	EDO	1	0
3	D	203	PG0	4	0
8	B	226	EOH	1	0
10	D	246	PGO	5	0
13	C	240	PGE	1	0
3	C	202	PG0	5	0
7	C	221	PDO	1	0
3	A	203	PG0	3	0
9	D	237	MOH	1	0
4	C	204	PEG	1	0
3	C	201	PG0	3	0
5	A	214	EDO	1	0
11	D	250	ETX	6	0
6	C	217	GOL	1	0
2	A	202	PG4	1	0
11	B	236	ETX	1	0
15	D	210	P6G	5	0
3	A	204	PG0	7	0
8	A	226	EOH	2	0
10	A	249	PGO	1	0
8	C	227	EOH	1	0
6	D	222	GOL	2	0
13	C	241	PGE	2	0
8	B	220	EOH	2	0
5	D	212	EDO	2	0

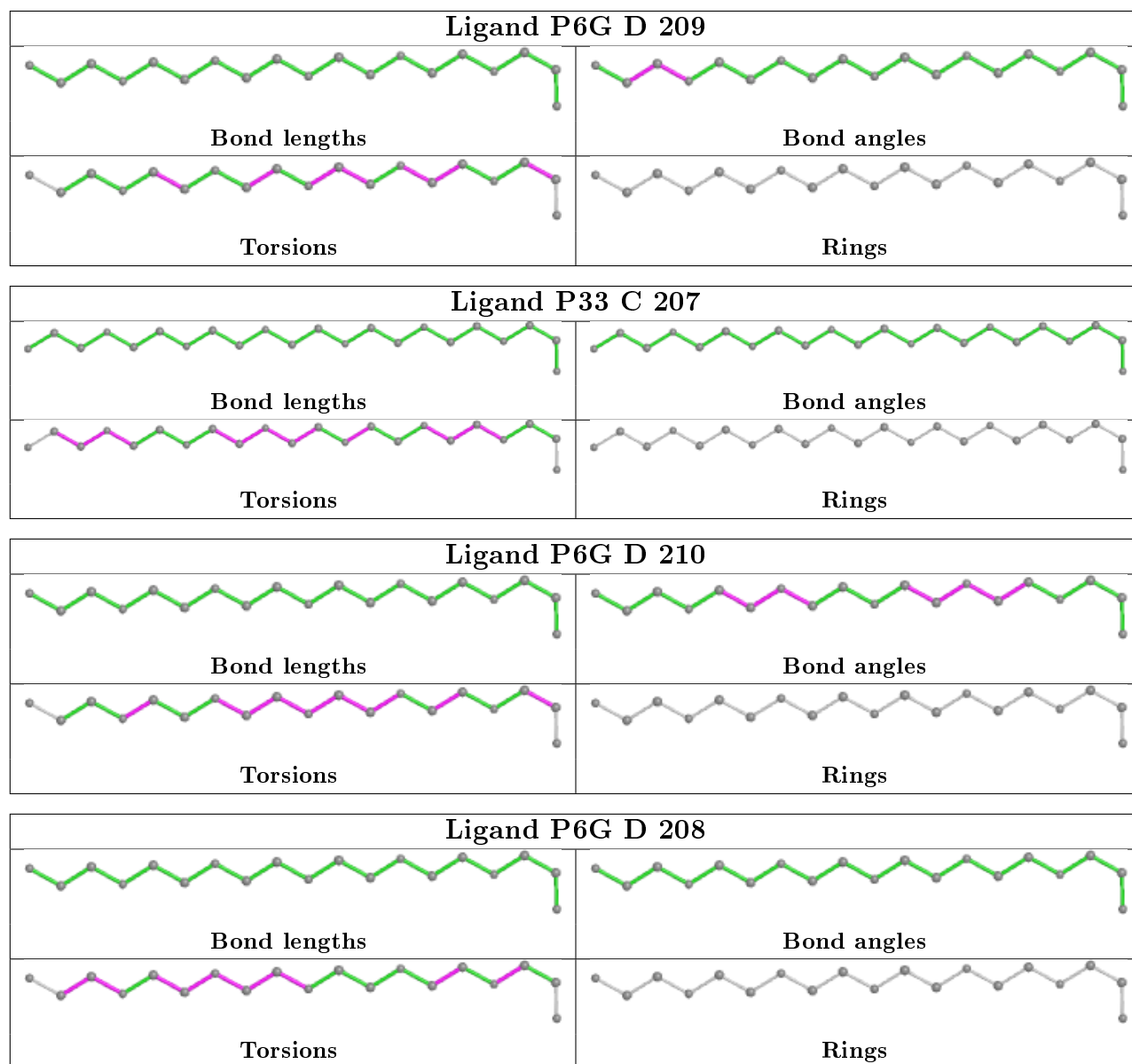
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	236	EOH	2	0
7	A	219	PDO	3	0
8	C	226	EOH	3	0
5	A	216	EDO	2	0
5	C	212	EDO	2	0
2	B	201	PG4	2	0
8	A	232	EOH	1	0
11	B	234	ETX	2	0
7	A	221	PDO	7	0
10	D	245	PGO	4	0
4	D	205	PEG	6	0
8	B	217	EOH	2	0
8	C	225	EOH	4	0
8	D	225	EOH	1	0
4	C	205	PEG	4	0
12	B	205	ETE	4	0
8	C	222	EOH	1	0
5	B	209	EDO	1	0
9	B	229	MOH	2	0
13	D	248	PGE	1	0
2	D	202	PG4	9	0
3	A	206	PG0	5	0
3	B	202	PG0	2	0
13	C	239	PGE	5	0
11	A	250	ETX	8	0
11	D	249	ETX	12	0
5	C	215	EDO	1	0
10	B	230	PGO	2	0
4	D	206	PEG	6	0
2	D	201	PG4	4	0
5	A	212	EDO	1	0
10	A	247	PGO	10	0
8	A	230	EOH	1	0
5	C	214	EDO	1	0
8	A	231	EOH	1	0
7	B	212	PDO	1	0
15	D	208	P6G	2	0
6	C	219	GOL	1	0
8	C	231	EOH	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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	165/176 (93%)	0.58	17 (10%) 6 8	23, 38, 71, 84	0
1	B	161/176 (91%)	0.40	10 (6%) 20 25	22, 38, 62, 76	0
1	C	161/176 (91%)	0.38	10 (6%) 20 25	21, 33, 56, 83	0
1	D	166/176 (94%)	0.48	12 (7%) 15 19	21, 36, 63, 91	0
All	All	653/704 (92%)	0.46	49 (7%) 14 18	21, 37, 64, 91	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	29	THR	8.8
1	A	2	ALA	6.8
1	A	32	THR	6.4
1	A	29	THR	5.3
1	A	28	PRO	5.2
1	A	166	ILE	4.3
1	D	165	PRO	4.3
1	B	74	ILE	4.1
1	D	166	ILE	4.0
1	A	116	ILE	3.8
1	D	31	VAL	3.8
1	C	32	THR	3.7
1	D	4	THR	3.5
1	D	167	ILE	3.5
1	C	164	PRO	3.4
1	B	32	THR	3.3
1	D	162	TYR	3.1
1	A	31	VAL	3.1
1	A	27	ILE	3.0
1	C	27	ILE	3.0
1	A	165	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	165	PRO	2.9
1	C	117	ILE	2.8
1	A	30	ASN	2.8
1	A	117	ILE	2.8
1	B	4	THR	2.7
1	D	1	MET	2.7
1	C	28	PRO	2.7
1	D	27	ILE	2.6
1	B	29	THR	2.6
1	B	31	VAL	2.6
1	C	5	LYS	2.5
1	D	130	PRO	2.4
1	D	3	GLU	2.3
1	A	19	LEU	2.3
1	D	29	THR	2.3
1	B	25	HIS	2.2
1	C	24	GLN	2.2
1	A	85	ILE	2.2
1	B	55	CYS	2.2
1	D	163	VAL	2.2
1	A	25	HIS	2.2
1	B	115	ASN	2.2
1	B	34	ALA	2.2
1	A	55	CYS	2.1
1	C	30	ASN	2.0
1	A	118	ASP	2.0
1	A	162	TYR	2.0
1	C	122	LEU	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 [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
8	EOH	D	230	3/3	0.26	0.24	57,57,60,62	0
6	GOL	C	216	6/6	0.41	0.55	59,64,71,72	0
8	EOH	A	227	3/3	0.44	0.29	48,48,62,67	0
11	ETX	C	242	6/6	0.45	0.59	52,63,63,70	0
9	MOH	D	239	2/2	0.47	0.29	62,62,62,62	0
15	P6G	D	210	19/19	0.49	0.38	56,71,87,88	0
4	PEG	C	206	7/7	0.50	0.26	50,55,61,66	0
10	PGO	D	246	5/5	0.53	0.26	54,55,59,60	0
13	PGE	C	239	10/10	0.55	0.24	68,71,76,76	0
5	EDO	B	209	4/4	0.56	0.51	63,64,64,65	0
11	ETX	B	236	6/6	0.57	0.44	61,64,70,73	0
3	PG0	A	205	8/8	0.57	0.32	55,61,65,70	0
5	EDO	D	220	4/4	0.58	0.80	68,68,72,73	0
9	MOH	A	243	2/2	0.59	0.44	65,65,65,67	0
5	EDO	B	210	4/4	0.59	0.24	75,76,77,80	0
3	PG0	A	206	8/8	0.60	0.32	64,68,72,73	0
9	MOH	A	244	2/2	0.60	0.29	62,62,62,70	0
11	ETX	D	250	6/6	0.61	0.26	58,62,65,66	0
12	ETE	C	208	14/14	0.61	0.25	56,69,75,80	0
8	EOH	A	233	3/3	0.61	0.28	50,50,54,57	0
5	EDO	B	207	4/4	0.61	0.27	56,61,61,67	0
6	GOL	C	219	6/6	0.61	0.32	66,71,74,78	0
4	PEG	B	204	7/7	0.62	0.38	61,67,74,76	0
2	PG4	A	202	13/13	0.62	0.34	52,61,76,77	0
4	PEG	A	207	7/7	0.63	0.22	63,70,73,74	0
9	MOH	D	243	2/2	0.64	0.23	56,56,56,58	0
10	PGO	A	249	5/5	0.64	0.29	42,44,48,48	0
8	EOH	C	224	3/3	0.64	0.20	57,57,59,63	0
9	MOH	C	234	2/2	0.65	0.20	46,46,46,49	0
8	EOH	B	221	3/3	0.65	0.18	67,67,71,73	0
12	ETE	B	205	14/14	0.66	0.22	61,69,76,77	0
11	ETX	A	250	6/6	0.66	0.34	63,74,75,78	0
5	EDO	D	221	4/4	0.66	0.27	70,70,75,77	0
9	MOH	A	241	2/2	0.67	0.33	34,34,34,41	0
13	PGE	C	240	10/10	0.67	0.39	56,71,77,83	0
3	PG0	A	204	8/8	0.68	0.27	36,49,55,58	0
9	MOH	C	232	2/2	0.68	0.24	45,45,45,48	0
7	PDO	A	225	5/5	0.68	0.27	48,54,56,61	0
8	EOH	C	230	3/3	0.68	0.43	68,68,70,74	0
15	P6G	D	209	19/19	0.69	0.40	79,90,96,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PG0	C	202	8/8	0.69	0.27	49,59,62,68	0
6	GOL	D	222	6/6	0.69	0.35	56,58,65,65	0
9	MOH	C	236	2/2	0.69	0.29	50,50,50,64	0
3	PG0	D	204	8/8	0.69	0.32	42,49,57,66	0
7	PDO	A	223	5/5	0.69	0.18	44,45,50,57	0
4	PEG	D	207	7/7	0.69	0.32	62,75,81,84	0
8	EOH	B	226	3/3	0.70	0.29	64,64,70,71	0
7	PDO	A	224	5/5	0.70	0.34	70,71,72,72	0
3	PG0	D	203	8/8	0.71	0.34	57,62,63,64	0
7	PDO	A	219	5/5	0.71	0.34	68,70,76,77	0
2	PG4	A	201	13/13	0.71	0.31	55,63,68,69	0
10	PGO	D	245	5/5	0.71	0.39	49,51,54,66	0
8	EOH	A	238	3/3	0.71	0.30	60,60,62,65	0
8	EOH	A	229	3/3	0.72	0.23	59,59,68,71	0
4	PEG	C	205	7/7	0.72	0.18	55,59,62,67	0
9	MOH	B	227	2/2	0.73	0.23	45,45,45,45	0
3	PG0	B	202	8/8	0.73	0.25	43,57,59,64	0
5	EDO	D	214	4/4	0.73	0.26	50,51,54,54	0
14	P33	C	207	22/22	0.74	0.37	44,59,74,77	0
8	EOH	A	228	3/3	0.74	0.26	58,58,61,64	0
10	PGO	A	248	5/5	0.74	0.23	49,50,57,58	0
8	EOH	D	235	3/3	0.74	0.25	46,46,46,51	0
9	MOH	D	244	2/2	0.74	0.25	44,44,44,47	0
4	PEG	D	206	7/7	0.74	0.48	30,39,50,51	0
4	PEG	B	203	7/7	0.74	0.20	56,60,63,64	0
8	EOH	C	226	3/3	0.74	0.37	55,55,56,58	0
5	EDO	D	219	4/4	0.75	0.28	73,75,77,88	0
9	MOH	D	241	2/2	0.75	0.23	60,60,60,63	0
5	EDO	A	212	4/4	0.75	0.25	55,58,60,62	0
13	PGE	D	248	10/10	0.75	0.29	54,65,76,79	0
7	PDO	B	214	5/5	0.75	0.22	50,54,65,75	0
7	PDO	B	213	5/5	0.76	0.24	60,64,70,71	0
8	EOH	A	237	3/3	0.76	0.23	64,64,66,70	0
4	PEG	A	208	7/7	0.76	0.19	68,73,78,81	0
5	EDO	D	218	4/4	0.76	0.32	50,56,60,67	0
4	PEG	D	205	7/7	0.76	0.24	38,45,52,52	0
10	PGO	A	247	5/5	0.76	0.18	62,65,69,77	0
5	EDO	A	217	4/4	0.76	0.20	70,74,74,79	0
5	EDO	B	211	4/4	0.77	0.24	47,52,52,52	0
9	MOH	B	229	2/2	0.77	0.20	65,65,65,65	0
8	EOH	D	232	3/3	0.77	0.28	49,49,53,53	0
5	EDO	A	211	4/4	0.77	0.21	67,70,71,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	ETX	B	234	6/6	0.78	0.30	55,62,69,73	0
8	EOH	A	226	3/3	0.78	0.20	49,49,52,55	0
8	EOH	C	225	3/3	0.78	0.17	50,50,54,60	0
11	ETX	D	249	6/6	0.78	0.17	60,64,67,70	0
5	EDO	C	213	4/4	0.78	0.20	58,58,59,60	0
3	PG0	A	203	8/8	0.78	0.26	45,50,60,63	0
5	EDO	D	217	4/4	0.78	0.40	41,42,43,43	0
11	ETX	A	251	6/6	0.78	0.17	59,71,74,78	0
3	PG0	C	201	8/8	0.78	0.20	47,51,58,59	0
5	EDO	B	208	4/4	0.78	0.24	56,58,62,62	0
5	EDO	A	213	4/4	0.79	0.51	54,55,57,61	0
7	PDO	D	223	5/5	0.79	0.22	40,41,45,48	0
4	PEG	C	204	7/7	0.79	0.19	30,32,36,37	0
5	EDO	D	216	4/4	0.79	0.41	44,47,51,54	0
13	PGE	B	233	10/10	0.79	0.34	56,63,69,84	0
8	EOH	C	228	3/3	0.79	0.29	49,49,52,55	0
10	PGO	B	231	5/5	0.79	0.17	51,60,64,65	0
9	MOH	C	237	2/2	0.80	0.22	51,51,51,55	0
7	PDO	C	221	5/5	0.80	0.20	29,34,40,40	0
6	GOL	C	218	6/6	0.80	0.29	53,57,63,66	0
5	EDO	D	213	4/4	0.80	0.18	47,51,51,58	0
10	PGO	D	247	5/5	0.80	0.19	40,44,49,52	0
7	PDO	B	212	5/5	0.80	0.18	40,46,49,51	0
8	EOH	B	225	3/3	0.80	0.22	48,48,49,57	0
8	EOH	D	233	3/3	0.81	0.23	48,48,51,51	0
8	EOH	B	220	3/3	0.81	0.39	54,54,58,59	0
5	EDO	B	206	4/4	0.81	0.28	36,40,42,42	0
7	PDO	C	220	5/5	0.81	0.19	53,55,59,60	0
7	PDO	A	220	5/5	0.81	0.22	46,51,54,55	0
8	EOH	A	232	3/3	0.81	0.19	55,55,67,69	0
5	EDO	A	214	4/4	0.81	0.19	63,69,72,73	0
8	EOH	A	236	3/3	0.82	0.50	41,41,45,47	0
7	PDO	A	222	5/5	0.82	0.19	55,56,60,66	0
5	EDO	A	216	4/4	0.82	0.14	47,51,52,56	0
9	MOH	B	228	2/2	0.82	0.19	47,47,47,54	0
5	EDO	C	214	4/4	0.82	0.24	52,56,56,56	0
2	PG4	B	201	13/13	0.82	0.15	54,58,63,66	0
5	EDO	D	215	4/4	0.82	0.19	44,46,50,51	0
8	EOH	B	223	3/3	0.82	0.27	46,46,49,57	0
5	EDO	A	215	4/4	0.82	0.26	54,55,56,65	0
8	EOH	A	230	3/3	0.83	0.19	65,65,72,80	0
11	ETX	B	235	6/6	0.83	0.16	45,55,56,61	0

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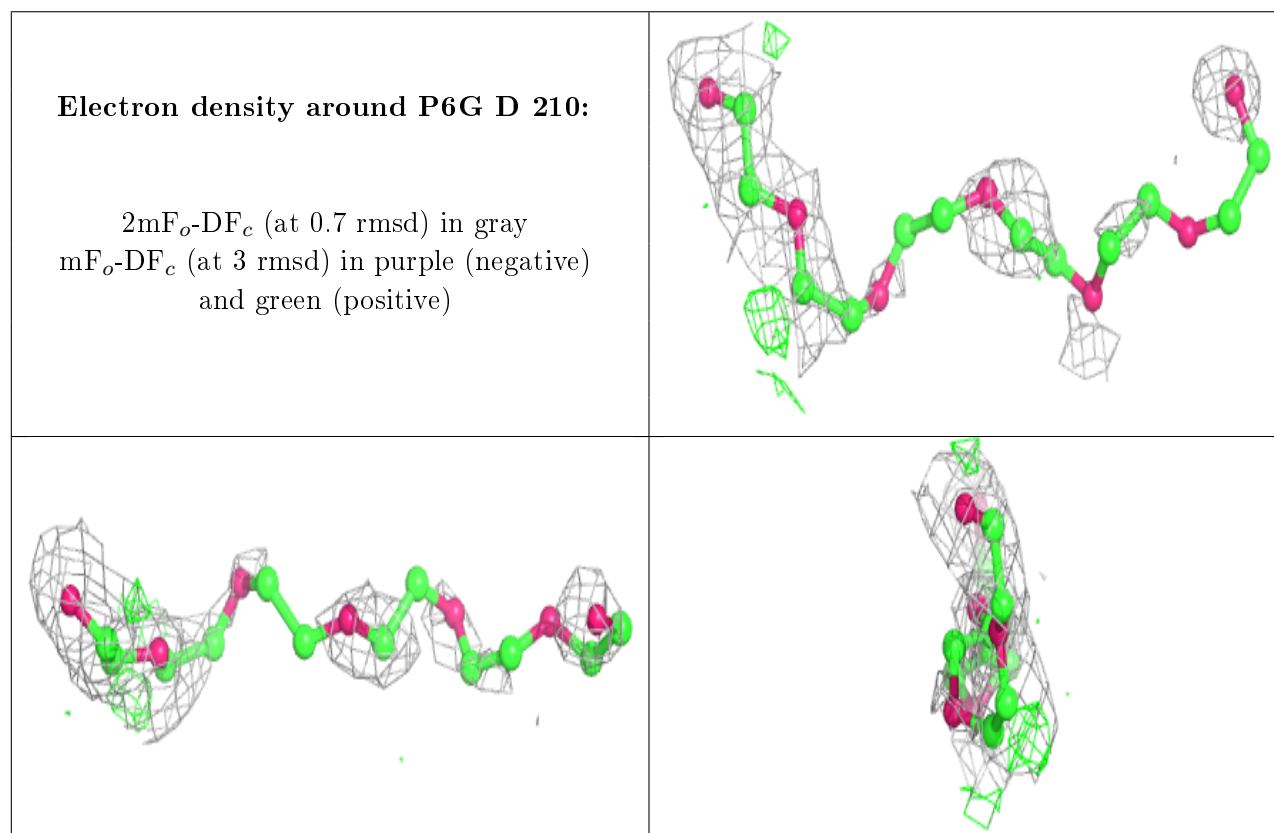
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	A	210	4/4	0.83	0.17	43,46,46,52	0
6	GOL	A	218	6/6	0.83	0.18	48,50,53,66	0
10	PGO	B	230	5/5	0.83	0.16	30,35,41,45	0
8	EOH	B	218	3/3	0.83	0.18	52,52,55,56	0
9	MOH	C	233	2/2	0.84	0.24	39,39,39,44	0
9	MOH	A	245	2/2	0.84	0.20	55,55,55,60	0
8	EOH	B	222	3/3	0.84	0.31	55,55,59,68	0
5	EDO	C	209	4/4	0.84	0.29	52,57,57,61	0
9	MOH	A	239	2/2	0.84	0.23	40,40,40,42	0
2	PG4	D	202	13/13	0.84	0.34	30,42,48,53	0
8	EOH	D	229	3/3	0.84	0.19	32,32,32,44	0
8	EOH	B	216	3/3	0.84	0.31	53,53,56,58	0
9	MOH	A	246	2/2	0.84	0.25	55,55,55,68	0
15	P6G	D	208	19/19	0.84	0.16	27,47,51,61	0
2	PG4	D	201	13/13	0.84	0.28	41,47,52,56	0
9	MOH	C	235	2/2	0.85	0.24	63,63,63,65	0
8	EOH	C	229	3/3	0.85	0.24	49,49,58,59	0
6	GOL	C	217	6/6	0.85	0.22	42,47,51,59	0
5	EDO	C	211	4/4	0.85	0.15	62,70,70,74	0
5	EDO	A	209	4/4	0.85	0.20	51,55,55,60	0
9	MOH	D	238	2/2	0.85	0.13	51,51,51,56	0
8	EOH	B	215	3/3	0.85	0.15	59,59,59,69	0
10	PGO	C	238	5/5	0.85	0.16	40,44,52,53	0
8	EOH	D	228	3/3	0.85	0.28	41,41,48,51	0
5	EDO	C	210	4/4	0.86	0.20	37,45,45,46	0
13	PGE	C	241	10/10	0.86	0.24	38,51,59,63	0
8	EOH	C	222	3/3	0.86	0.20	55,55,55,59	0
4	PEG	C	203	7/7	0.86	0.49	35,39,44,50	0
8	EOH	C	227	3/3	0.86	0.15	53,53,54,61	0
7	PDO	A	221	5/5	0.86	0.25	35,35,38,50	0
8	EOH	D	234	3/3	0.86	0.25	45,45,48,56	0
10	PGO	B	232	5/5	0.86	0.13	44,50,60,61	0
8	EOH	A	231	3/3	0.87	0.12	59,59,63,63	0
8	EOH	A	234	3/3	0.87	0.29	50,50,51,61	0
7	PDO	D	224	5/5	0.87	0.25	21,26,32,35	0
8	EOH	B	224	3/3	0.88	0.25	54,54,58,61	0
9	MOH	A	242	2/2	0.88	0.22	29,29,29,34	0
5	EDO	C	212	4/4	0.89	0.26	48,51,57,58	0
8	EOH	D	227	3/3	0.89	0.17	46,46,51,63	0
5	EDO	C	215	4/4	0.89	0.19	38,48,51,54	0
8	EOH	B	217	3/3	0.90	0.24	30,30,36,42	0
9	MOH	D	242	2/2	0.90	0.26	45,45,45,48	0

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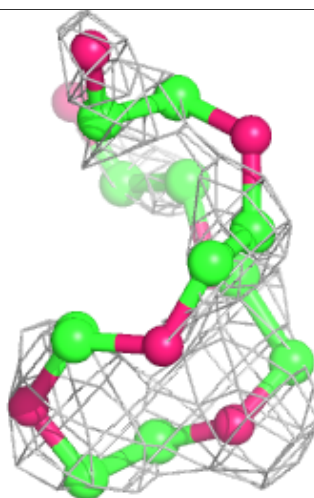
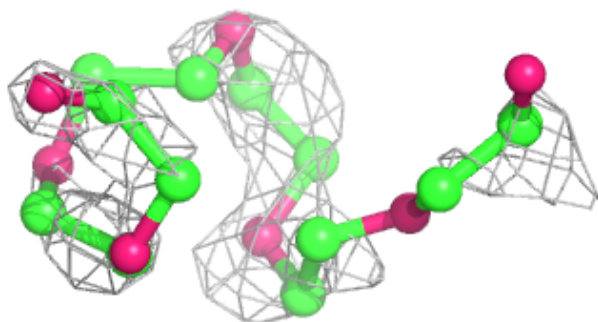
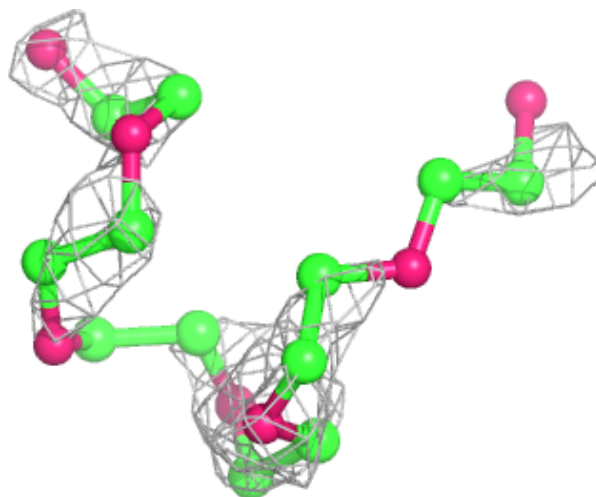
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	EOH	B	219	3/3	0.90	0.11	39,39,46,56	0
5	EDO	D	211	4/4	0.91	0.20	40,42,47,59	0
9	MOH	D	237	2/2	0.91	0.47	35,35,35,41	0
8	EOH	C	223	3/3	0.91	0.19	42,42,44,50	0
5	EDO	D	212	4/4	0.91	0.15	41,43,43,44	0
9	MOH	A	240	2/2	0.91	0.17	39,39,39,39	0
8	EOH	A	235	3/3	0.91	0.20	31,31,38,42	0
8	EOH	D	231	3/3	0.92	0.16	44,44,51,64	0
8	EOH	C	231	3/3	0.92	0.21	61,61,63,63	0
9	MOH	D	240	2/2	0.93	0.13	54,54,54,57	0
8	EOH	D	236	3/3	0.93	0.58	50,50,55,61	0
8	EOH	D	226	3/3	0.93	0.22	46,46,50,50	0
8	EOH	D	225	3/3	0.94	0.12	33,33,35,42	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.



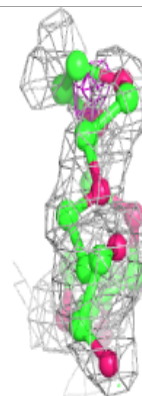
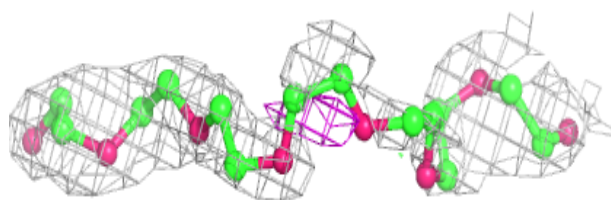
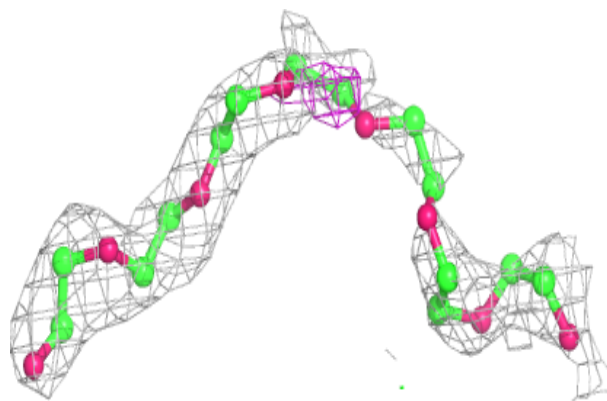
Electron density around P6G D 209:

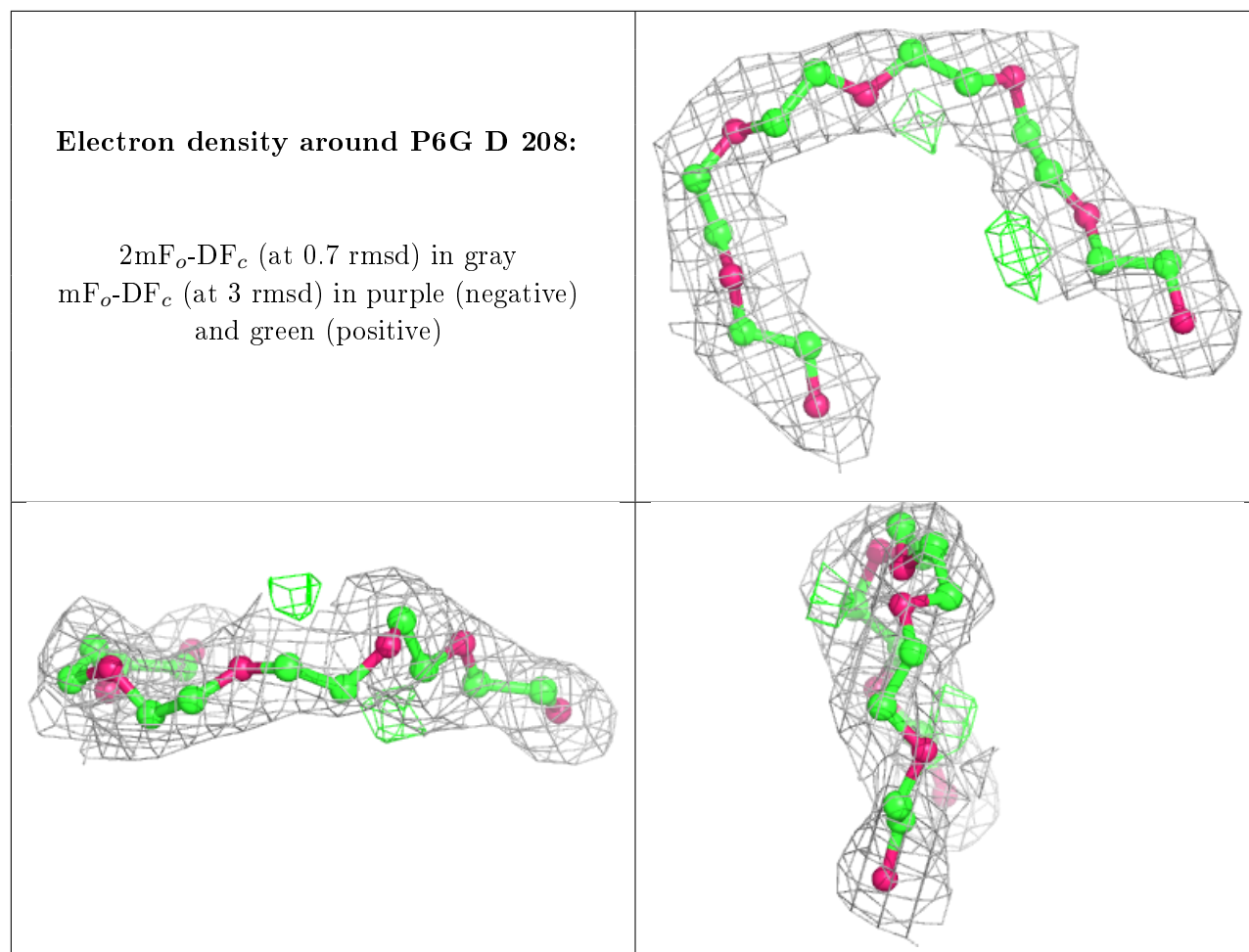
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around P33 C 207:

$2mF_o-DF_c$ (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.