



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 05:18 AM UTC

PDB ID : 6CJ6 / pdb_00006cj6
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

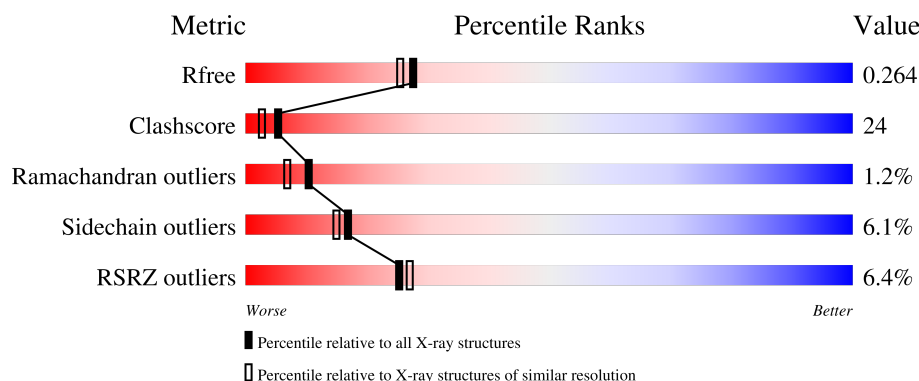
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	176	7% 63% 29% • 6%
1	B	176	5% 63% 24% 5% 9%
1	C	176	5% 67% 22% • 9%
1	D	176	7% 66% 25% • 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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	PGO	A	247	-	-	X	-
10	PGO	A	249	-	X	-	-
10	PGO	B	230	X	X	-	-
10	PGO	D	245	-	-	X	-
10	PGO	D	246	-	-	X	-
10	PGO	D	247	-	X	-	-
11	ETX	A	250	-	-	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	X	-
4	PEG	C	203	-	-	X	-
4	PEG	C	205	-	X	X	-
4	PEG	D	205	-	-	X	-
4	PEG	D	206	-	-	X	-
6	GOL	A	218	-	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	D	230	-	-	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.

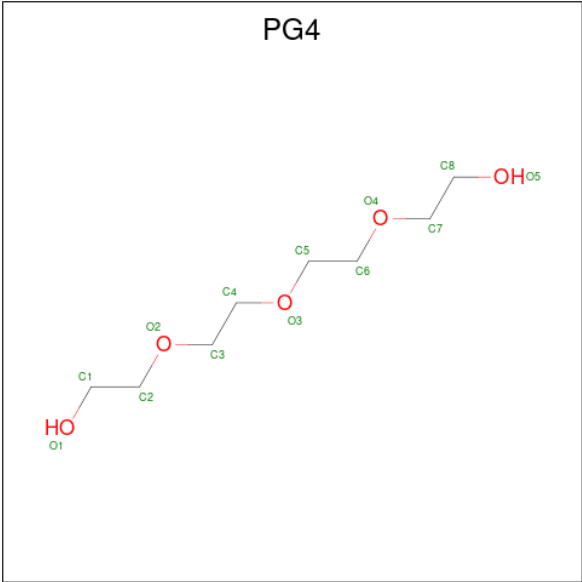
- Molecule 1 is a protein called Protein F9.

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

There are 8 discrepancies between the modelled and reference sequences:

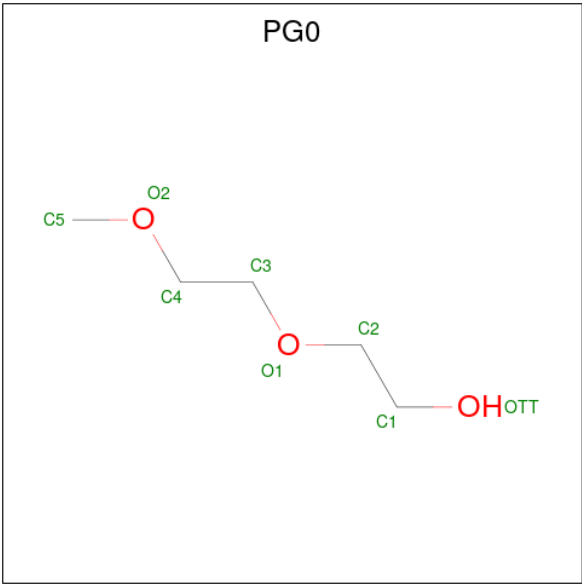
Chain	Residue	Modelled	Actual	Comment	Reference
A	84	ALA	ARG	conflict	UNP P24361
A	147	ALA	ARG	conflict	UNP P24361
B	84	ALA	ARG	conflict	UNP P24361
B	147	ALA	ARG	conflict	UNP P24361
C	84	ALA	ARG	conflict	UNP P24361
C	147	ALA	ARG	conflict	UNP P24361
D	84	ALA	ARG	conflict	UNP P24361
D	147	ALA	ARG	conflict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

- Molecule 2 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



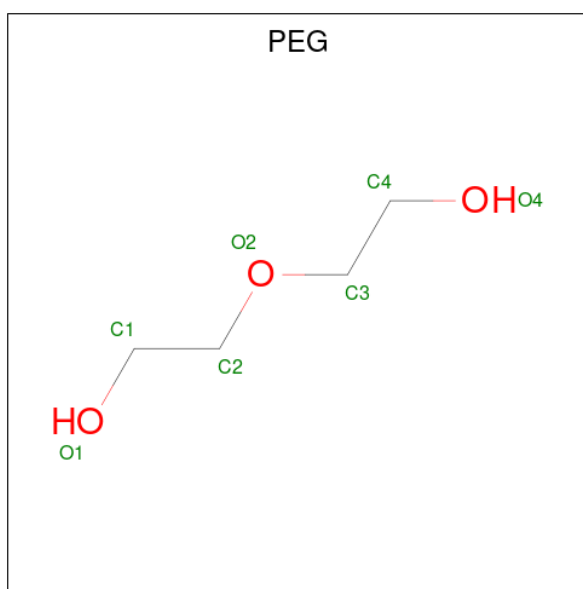
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		
2	A	1	Total	C	O	0	0
			13	8	5		
2	B	1	Total	C	O	0	0
			13	8	5		
2	D	1	Total	C	O	0	0
			13	8	5		
2	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 3 is 2-(2-METHOXYETHOXY)ETHANOL (CCD ID: 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 (CCD ID: PEG) (formula: C₄H₁₀O₃).



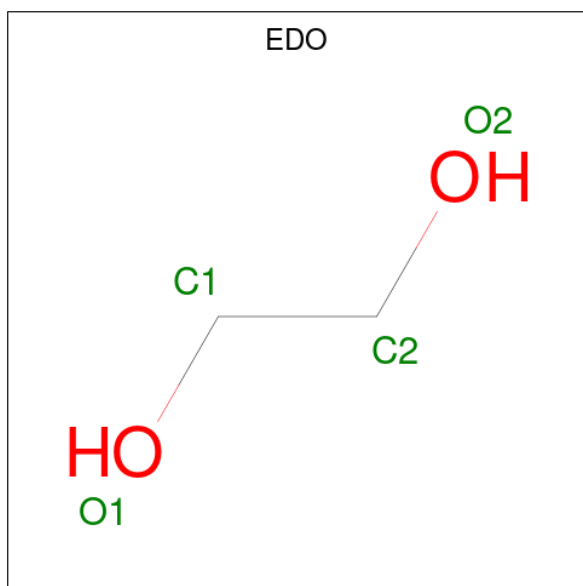
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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 (CCD ID: EDO) (formula: C₂H₆O₂).



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

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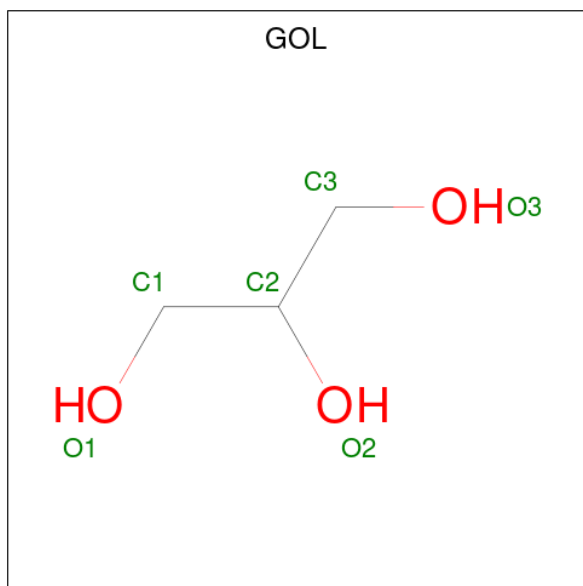
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total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

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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



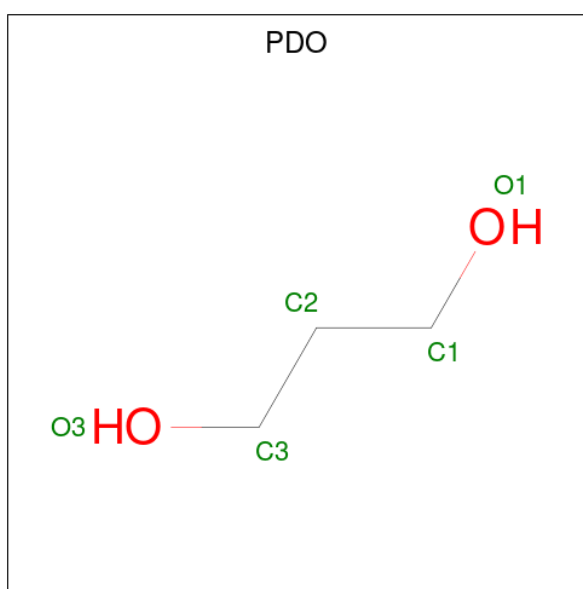
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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 (CCD ID: PDO) (formula: $C_3H_8O_2$).



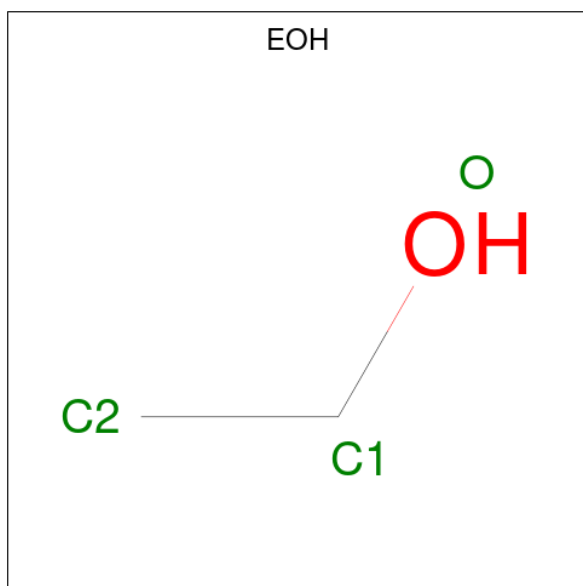
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			5	3	2		
7	A	1	Total	C	O	0	0
			5	3	2		
7	A	1	Total	C	O	0	0
			5	3	2		
7	A	1	Total	C	O	0	0
			5	3	2		
7	A	1	Total	C	O	0	0
			5	3	2		
7	A	1	Total	C	O	0	0
			5	3	2		

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

- Molecule 8 is ETHANOL (CCD ID: EOH) (formula: C₂H₆O).



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

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

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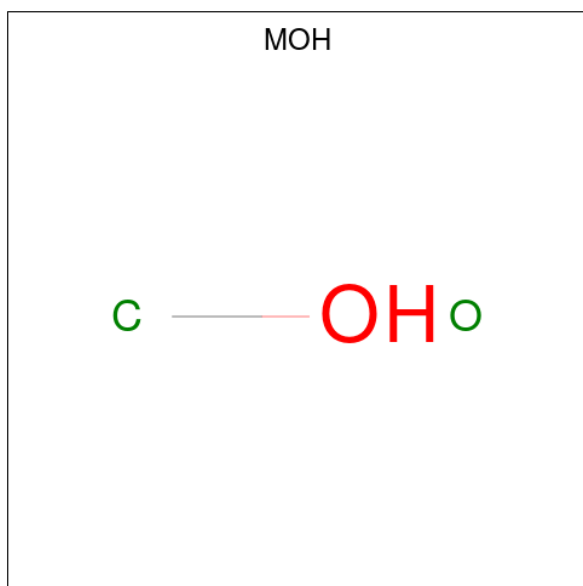
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			3	2	1		
8	C	1	Total	C	O	0	0
			3	2	1		
8	C	1	Total	C	O	0	0
			3	2	1		
8	C	1	Total	C	O	0	0
			3	2	1		
8	C	1	Total	C	O	0	0
			3	2	1		
8	C	1	Total	C	O	0	0
			3	2	1		
8	C	1	Total	C	O	0	0
			3	2	1		
8	C	1	Total	C	O	0	0
			3	2	1		
8	D	1	Total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

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

- Molecule 9 is METHANOL (CCD ID: MOH) (formula: CH₄O).



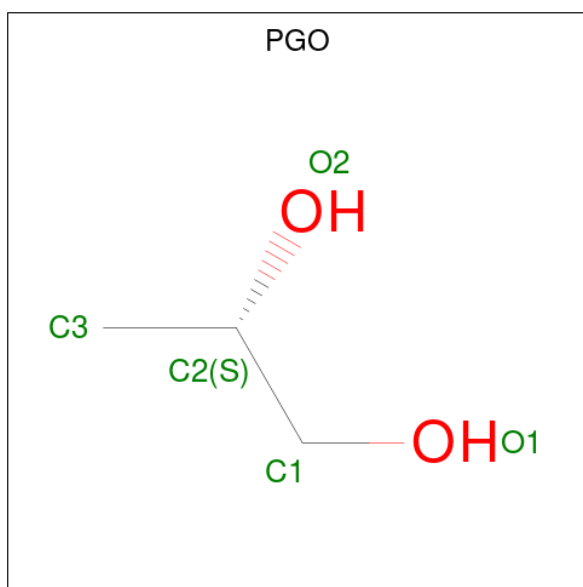
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			2	1	1		
9	A	1	Total	C	O	0	0
			2	1	1		
9	A	1	Total	C	O	0	0
			2	1	1		
9	A	1	Total	C	O	0	0
			2	1	1		
9	A	1	Total	C	O	0	0
			2	1	1		
9	A	1	Total	C	O	0	0
			2	1	1		
9	A	1	Total	C	O	0	0
			2	1	1		
9	B	1	Total	C	O	0	0
			2	1	1		
9	B	1	Total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

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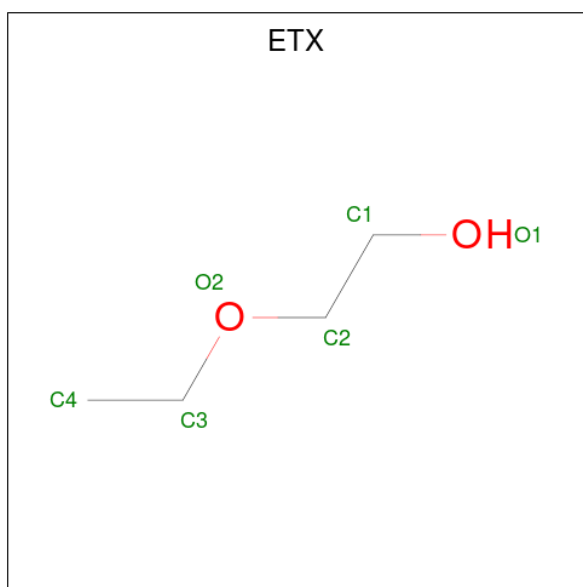
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			2	1	1		
9	C	1	Total	C	O	0	0
			2	1	1		
9	C	1	Total	C	O	0	0
			2	1	1		
9	C	1	Total	C	O	0	0
			2	1	1		
9	C	1	Total	C	O	0	0
			2	1	1		
9	C	1	Total	C	O	0	0
			2	1	1		
9	D	1	Total	C	O	0	0
			2	1	1		
9	D	1	Total	C	O	0	0
			2	1	1		
9	D	1	Total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

- Molecule 10 is S-1,2-PROPANEDIOL (CCD ID: PGO) (formula: C₃H₈O₂).



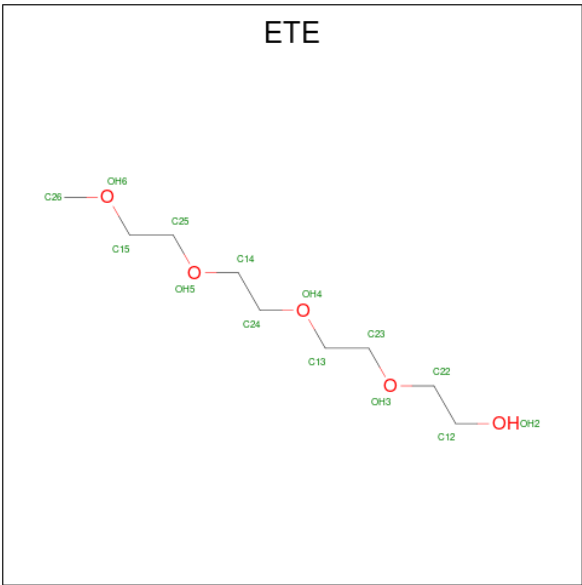
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			5	3	2		
10	A	1	Total	C	O	0	0
			5	3	2		
10	A	1	Total	C	O	0	0
			5	3	2		
10	B	1	Total	C	O	0	0
			5	3	2		
10	B	1	Total	C	O	0	0
			5	3	2		
10	B	1	Total	C	O	0	0
			5	3	2		
10	C	1	Total	C	O	0	0
			5	3	2		
10	D	1	Total	C	O	0	0
			5	3	2		
10	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 (CCD ID: ETX) (formula: C₄H₁₀O₂).



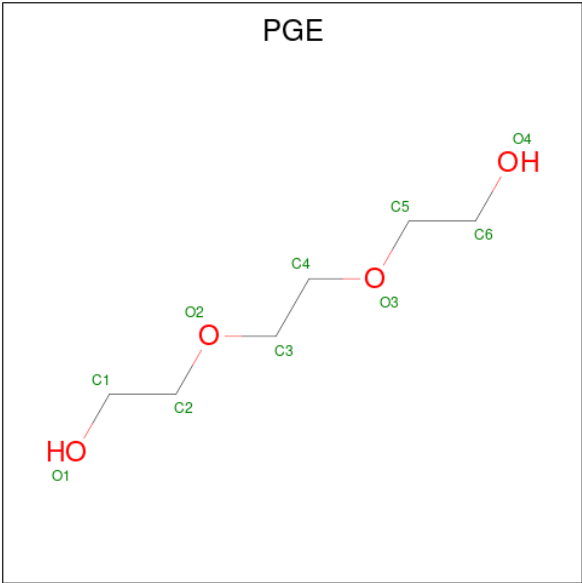
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			6	4	2		
11	A	1	Total	C	O	0	0
			6	4	2		
11	B	1	Total	C	O	0	0
			6	4	2		
11	B	1	Total	C	O	0	0
			6	4	2		
11	B	1	Total	C	O	0	0
			6	4	2		
11	C	1	Total	C	O	0	0
			6	4	2		
11	D	1	Total	C	O	0	0
			6	4	2		
11	D	1	Total	C	O	0	0
			6	4	2		

- Molecule 12 is 2-{2-[2-(Methoxyethoxy)-ethoxy]-ethoxy}-ethanol (CCD ID: 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 (CCD ID: PGE) (formula: C₆H₁₄O₄).



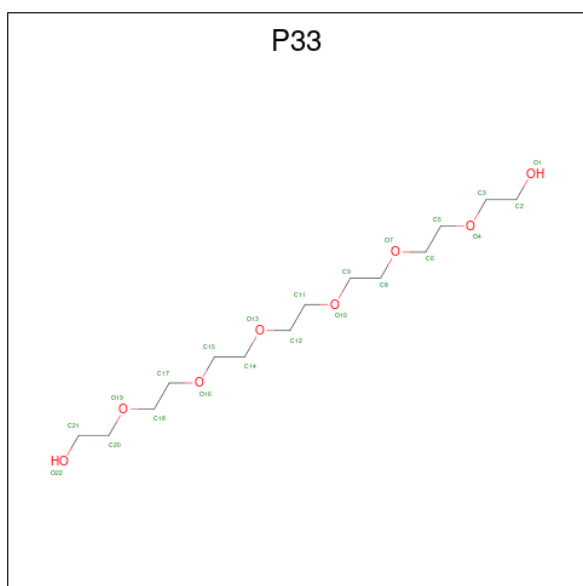
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	B	1	Total	C	O	0	0
			10	6	4		
13	C	1	Total	C	O	0	0
			10	6	4		

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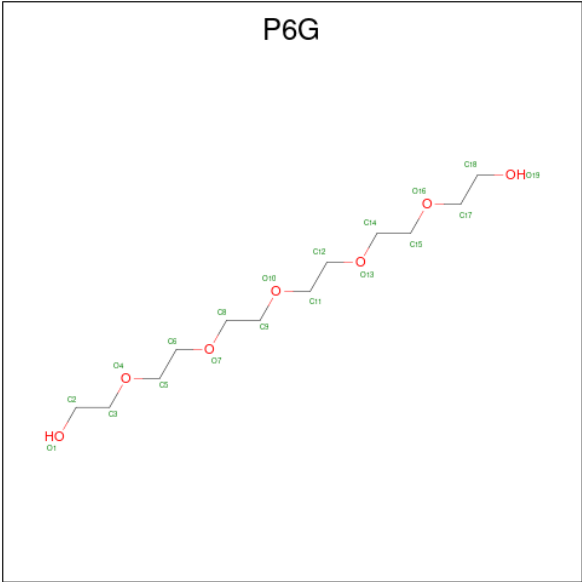
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	O	0	0
			10	6	4		
13	C	1	Total	C	O	0	0
			10	6	4		
13	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 14 is 3,6,9,12,15,18-HEXA OXAICOSANE-1,20-DIOL (CCD ID: P33) (formula: $C_{14}H_{30}O_8$).



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

- Molecule 15 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



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		

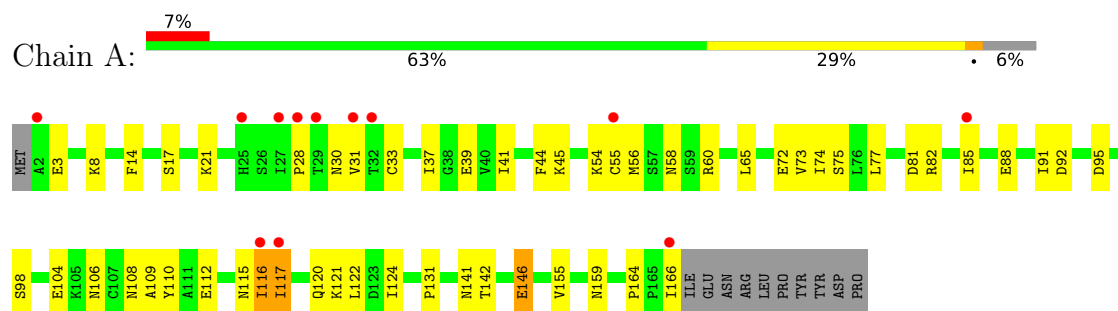
- Molecule 16 is water.

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

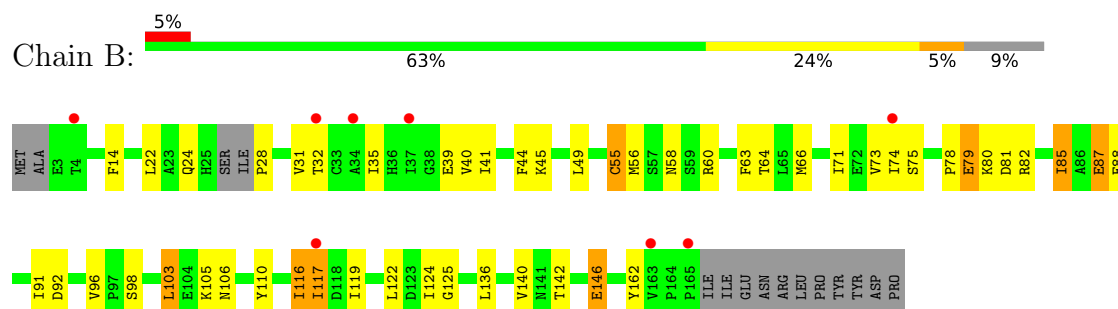
3 Residue-property plots [i](#)

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

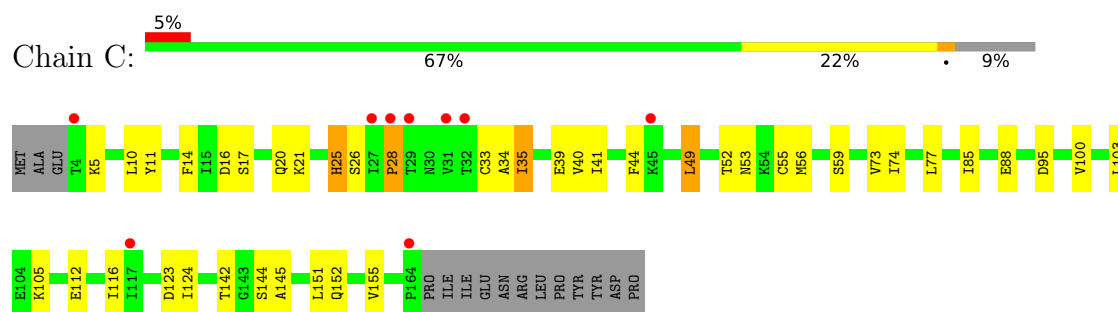
• Molecule 1: Protein F9



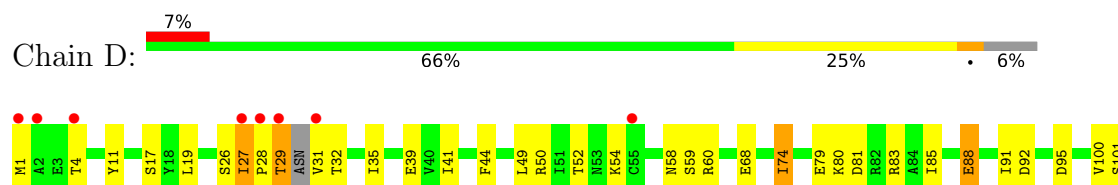
• Molecule 1: Protein F9

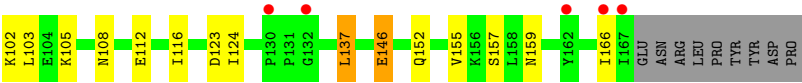


• Molecule 1: Protein F9



• 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 38.86 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.8 (38.86-2.10) 93.8 (38.86-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.226 , 0.269 (Not available) , 0.264	Depositor DCC
R_{free} test set	2000 reflections (5.33%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.854	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PGO, P33, MOH, PG0, GOL, PG4, ETE, P6G, ETX, PGE, PEG, EOH, PDO, EDO

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	0.22	0/1257	0.38	0/1706
1	B	0.28	0/1225	0.42	1/1659 (0.1%)
1	C	0.28	1/1240 (0.1%)	0.41	1/1680 (0.1%)
1	D	0.16	0/1287	0.35	0/1742
All	All	0.24	1/5009 (0.0%)	0.39	2/6787 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	25	HIS	CB-CG	-5.63	1.42	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	28	PRO	N-CA-CB	7.02	110.62	103.25
1	B	28	PRO	N-CA-CB	6.72	110.39	103.00

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	1239	0	1217	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1210	0	1189	37	0
1	C	1225	0	1198	43	0
1	D	1271	0	1264	66	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	3	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	289	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 24.

The worst 5 of 289 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

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%)	10 7
1	B	157/176 (89%)	144 (92%)	9 (6%)	4 (2%)	4 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	160/176 (91%)	149 (93%)	10 (6%)	1 (1%)	21	18
1	D	163/176 (93%)	153 (94%)	9 (6%)	1 (1%)	21	18
All	All	643/704 (91%)	597 (93%)	38 (6%)	8 (1%)	10	7

5 of 8 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	135/157 (86%)	128 (95%)	7 (5%)	21	20
1	B	132/157 (84%)	119 (90%)	13 (10%)	7	5
1	C	134/157 (85%)	130 (97%)	4 (3%)	36	41
1	D	141/157 (90%)	132 (94%)	9 (6%)	16	14
All	All	542/628 (86%)	509 (94%)	33 (6%)	17	15

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	74	ILE
1	D	88	GLU
1	D	146	GLU
1	B	88	GLU
1	B	87	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	133	GLN
1	D	46	ASN
1	D	134	HIS
1	A	148	ASN
1	A	138	GLN

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 oligosaccharides 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	$\# Z > 2$
7	PDO	C	221	-	4,4,4	0.32	0	3,3,3	0.35	0
13	PGE	C	240	-	9,9,9	0.45	0	8,8,8	0.29	0
8	EOH	B	224	-	2,2,2	0.50	0	1,1,1	0.43	0
13	PGE	C	241	-	9,9,9	1.28	2 (22%)	8,8,8	2.10	2 (25%)
4	PEG	B	203	-	6,6,6	0.44	0	5,5,5	0.31	0
10	PGO	B	232	-	4,4,4	0.60	0	4,4,4	0.79	0
8	EOH	C	230	-	2,2,2	0.39	0	1,1,1	0.39	0
5	EDO	A	217	-	3,3,3	0.43	0	2,2,2	0.38	0
10	PGO	B	231	-	4,4,4	0.65	0	4,4,4	0.74	0
3	PG0	A	204	-	7,7,7	0.45	0	6,6,6	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PG4	A	202	-	12,12,12	0.59	0	11,11,11	1.24	3 (27%)
13	PGE	D	248	-	9,9,9	0.45	0	8,8,8	0.28	0
15	P6G	D	208	-	18,18,18	0.46	0	17,17,17	0.26	0
3	PG0	D	204	-	7,7,7	0.44	0	6,6,6	0.26	0
8	EOH	A	237	-	2,2,2	0.72	0	1,1,1	0.74	0
8	EOH	B	216	-	2,2,2	0.40	0	1,1,1	0.39	0
9	MOH	A	242	-	1,1,1	0.07	0	-		
5	EDO	A	212	-	3,3,3	0.42	0	2,2,2	0.38	0
8	EOH	A	228	-	2,2,2	0.40	0	1,1,1	0.39	0
8	EOH	D	228	-	2,2,2	0.40	0	1,1,1	0.39	0
8	EOH	C	224	-	2,2,2	0.39	0	1,1,1	0.39	0
9	MOH	C	233	-	1,1,1	0.08	0	-		
4	PEG	D	207	-	6,6,6	0.48	0	5,5,5	0.91	0
6	GOL	C	217	-	5,5,5	1.33	1 (20%)	5,5,5	1.38	1 (20%)
8	EOH	D	236	-	2,2,2	0.39	0	1,1,1	0.39	0
9	MOH	D	238	-	1,1,1	0.09	0	-		
5	EDO	B	208	-	3,3,3	0.32	0	2,2,2	0.19	0
5	EDO	D	212	-	3,3,3	0.39	0	2,2,2	0.52	0
4	PEG	B	204	-	6,6,6	0.31	0	5,5,5	1.34	1 (20%)
11	ETX	A	250	-	5,5,5	0.43	0	4,4,4	0.30	0
8	EOH	A	230	-	2,2,2	0.40	0	1,1,1	0.39	0
4	PEG	C	205	-	6,6,6	0.65	0	5,5,5	2.40	3 (60%)
12	ETE	C	208	-	13,13,13	0.68	0	12,12,12	1.36	3 (25%)
8	EOH	D	232	-	2,2,2	0.39	0	1,1,1	0.38	0
8	EOH	B	222	-	2,2,2	0.40	0	1,1,1	0.39	0
8	EOH	D	227	-	2,2,2	0.40	0	1,1,1	0.39	0
9	MOH	D	241	-	1,1,1	0.06	0	-		
4	PEG	C	206	-	6,6,6	0.61	0	5,5,5	1.23	0
8	EOH	A	231	-	2,2,2	0.40	0	1,1,1	0.39	0
8	EOH	C	223	-	2,2,2	0.39	0	1,1,1	0.39	0
3	PG0	A	205	-	7,7,7	0.34	0	6,6,6	1.42	2 (33%)
9	MOH	D	243	-	1,1,1	0.08	0	-		
6	GOL	C	216	-	5,5,5	1.02	0	5,5,5	1.04	0
11	ETX	B	236	-	5,5,5	0.53	0	4,4,4	1.21	1 (25%)
11	ETX	D	249	-	5,5,5	0.41	0	4,4,4	0.58	0
5	EDO	A	213	-	3,3,3	0.57	0	2,2,2	0.14	0
8	EOH	A	229	-	2,2,2	0.20	0	1,1,1	0.57	0
11	ETX	B	235	-	5,5,5	0.44	0	4,4,4	0.30	0
6	GOL	C	219	-	5,5,5	1.17	0	5,5,5	2.33	3 (60%)
6	GOL	A	218	-	5,5,5	1.45	1 (20%)	5,5,5	2.77	4 (80%)
9	MOH	C	232	-	1,1,1	0.21	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PEG	C	204	-	6,6,6	0.43	0	5,5,5	0.30	0
5	EDO	D	215	-	3,3,3	0.43	0	2,2,2	0.38	0
5	EDO	D	219	-	3,3,3	0.43	0	2,2,2	0.38	0
2	PG4	D	201	-	12,12,12	1.34	2 (16%)	11,11,11	1.62	2 (18%)
8	EOH	B	218	-	2,2,2	0.40	0	1,1,1	0.39	0
10	PGO	B	230	-	4,4,4	3.00	1 (25%)	4,4,4	1.73	2 (50%)
4	PEG	A	207	-	6,6,6	0.54	0	5,5,5	2.05	2 (40%)
9	MOH	C	235	-	1,1,1	0.09	0	-		
5	EDO	D	220	-	3,3,3	0.30	0	2,2,2	0.61	0
8	EOH	D	230	-	2,2,2	0.40	0	1,1,1	0.39	0
8	EOH	B	221	-	2,2,2	0.40	0	1,1,1	0.66	0
9	MOH	C	234	-	1,1,1	0.07	0	-		
9	MOH	D	244	-	1,1,1	0.33	0	-		
2	PG4	B	201	-	12,12,12	0.96	0	11,11,11	1.41	1 (9%)
15	P6G	D	210	-	18,18,18	0.83	0	17,17,17	1.63	4 (23%)
7	PDO	B	214	-	4,4,4	0.42	0	3,3,3	1.00	0
5	EDO	B	206	-	3,3,3	0.42	0	2,2,2	0.38	0
8	EOH	C	225	-	2,2,2	0.40	0	1,1,1	0.39	0
8	EOH	A	233	-	2,2,2	0.22	0	1,1,1	0.40	0
9	MOH	A	239	-	1,1,1	0.08	0	-		
9	MOH	D	240	-	1,1,1	0.08	0	-		
5	EDO	C	209	-	3,3,3	1.18	0	2,2,2	1.34	0
7	PDO	A	223	-	4,4,4	0.32	0	3,3,3	0.35	0
8	EOH	D	226	-	2,2,2	0.40	0	1,1,1	0.39	0
8	EOH	D	235	-	2,2,2	0.59	0	1,1,1	0.86	0
8	EOH	C	228	-	2,2,2	0.39	0	1,1,1	0.39	0
5	EDO	A	214	-	3,3,3	0.37	0	2,2,2	0.81	0
8	EOH	A	227	-	2,2,2	0.39	0	1,1,1	0.39	0
12	ETE	B	205	-	13,13,13	0.71	0	12,12,12	1.47	2 (16%)
5	EDO	D	221	-	3,3,3	0.43	0	2,2,2	0.39	0
9	MOH	A	241	-	1,1,1	0.08	0	-		
5	EDO	B	210	-	3,3,3	0.70	0	2,2,2	1.03	0
7	PDO	B	213	-	4,4,4	0.32	0	3,3,3	0.35	0
5	EDO	C	210	-	3,3,3	0.43	0	2,2,2	0.39	0
8	EOH	B	226	-	2,2,2	0.37	0	1,1,1	0.17	0
3	PG0	B	202	-	7,7,7	0.45	0	6,6,6	0.26	0
8	EOH	C	227	-	2,2,2	0.39	0	1,1,1	0.39	0
3	PG0	D	203	-	7,7,7	0.44	0	6,6,6	0.26	0
8	EOH	C	229	-	2,2,2	0.40	0	1,1,1	0.39	0
2	PG4	A	201	-	12,12,12	0.56	0	11,11,11	0.45	0
10	PGO	A	248	-	4,4,4	0.79	0	4,4,4	0.87	0
5	EDO	B	207	-	3,3,3	0.52	0	2,2,2	1.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PEG	D	206	-	6,6,6	0.43	0	5,5,5	0.31	0
10	PGO	C	238	-	4,4,4	1.17	0	4,4,4	1.10	0
8	EOH	B	215	-	2,2,2	0.39	0	1,1,1	0.39	0
9	MOH	C	237	-	1,1,1	0.12	0	-		
5	EDO	D	218	-	3,3,3	1.22	1 (33%)	2,2,2	0.56	0
8	EOH	B	223	-	2,2,2	0.39	0	1,1,1	0.39	0
5	EDO	C	213	-	3,3,3	0.42	0	2,2,2	0.38	0
5	EDO	D	217	-	3,3,3	0.90	0	2,2,2	0.71	0
9	MOH	D	237	-	1,1,1	0.08	0	-		
9	MOH	B	228	-	1,1,1	0.09	0	-		
6	GOL	C	218	-	5,5,5	1.70	1 (20%)	5,5,5	2.53	2 (40%)
9	MOH	A	244	-	1,1,1	0.09	0	-		
9	MOH	B	229	-	1,1,1	0.07	0	-		
7	PDO	C	220	-	4,4,4	0.32	0	3,3,3	0.35	0
8	EOH	D	231	-	2,2,2	0.40	0	1,1,1	0.39	0
8	EOH	C	222	-	2,2,2	0.39	0	1,1,1	0.39	0
9	MOH	A	246	-	1,1,1	0.08	0	-		
3	PG0	C	201	-	7,7,7	0.57	0	6,6,6	1.59	1 (16%)
4	PEG	A	208	-	6,6,6	0.61	0	5,5,5	1.12	1 (20%)
10	PGO	D	245	-	4,4,4	1.23	0	4,4,4	1.54	1 (25%)
9	MOH	A	240	-	1,1,1	0.08	0	-		
8	EOH	D	234	-	2,2,2	0.57	0	1,1,1	0.27	0
9	MOH	B	227	-	1,1,1	0.08	0	-		
8	EOH	A	235	-	2,2,2	0.40	0	1,1,1	0.39	0
7	PDO	D	223	-	4,4,4	0.32	0	3,3,3	0.35	0
5	EDO	C	214	-	3,3,3	1.02	0	2,2,2	1.15	0
5	EDO	D	213	-	3,3,3	0.41	0	2,2,2	0.50	0
8	EOH	D	229	-	2,2,2	0.39	0	1,1,1	0.39	0
9	MOH	A	243	-	1,1,1	0.12	0	-		
7	PDO	A	219	-	4,4,4	0.61	0	3,3,3	2.10	1 (33%)
8	EOH	C	226	-	2,2,2	0.50	0	1,1,1	0.39	0
8	EOH	D	225	-	2,2,2	0.44	0	1,1,1	0.28	0
5	EDO	A	216	-	3,3,3	0.82	0	2,2,2	0.74	0
10	PGO	D	247	-	4,4,4	1.42	1 (25%)	4,4,4	1.57	2 (50%)
8	EOH	A	236	-	2,2,2	0.56	0	1,1,1	0.14	0
10	PGO	D	246	-	4,4,4	0.65	0	4,4,4	0.74	0
5	EDO	A	210	-	3,3,3	0.42	0	2,2,2	0.38	0
11	ETX	D	250	-	5,5,5	0.65	0	4,4,4	0.83	0
8	EOH	C	231	-	2,2,2	0.39	0	1,1,1	0.39	0
5	EDO	D	216	-	3,3,3	0.43	0	2,2,2	0.38	0
3	PG0	A	206	-	7,7,7	1.08	1 (14%)	6,6,6	1.90	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PDO	A	222	-	4,4,4	0.32	0	3,3,3	0.35	0
8	EOH	A	238	-	2,2,2	0.16	0	1,1,1	0.28	0
8	EOH	B	217	-	2,2,2	0.39	0	1,1,1	0.39	0
5	EDO	A	215	-	3,3,3	0.42	0	2,2,2	0.38	0
9	MOH	A	245	-	1,1,1	0.08	0	-		
7	PDO	B	212	-	4,4,4	0.32	0	3,3,3	0.35	0
5	EDO	B	211	-	3,3,3	0.84	0	2,2,2	0.42	0
10	PGO	A	247	-	4,4,4	0.60	0	4,4,4	1.21	0
8	EOH	B	220	-	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
7	PDO	A	225	-	4,4,4	0.97	0	3,3,3	0.84	0
5	EDO	C	212	-	3,3,3	0.42	0	2,2,2	0.39	0
9	MOH	C	236	-	1,1,1	0.01	0	-		
9	MOH	D	242	-	1,1,1	0.08	0	-		
14	P33	C	207	-	21,21,21	0.48	0	20,20,20	0.31	0
4	PEG	D	205	-	6,6,6	0.44	0	5,5,5	0.31	0
5	EDO	C	215	-	3,3,3	1.46	1 (33%)	2,2,2	0.41	0
8	EOH	A	226	-	2,2,2	0.07	0	1,1,1	0.12	0
8	EOH	B	219	-	2,2,2	0.39	0	1,1,1	0.39	0
15	P6G	D	209	-	18,18,18	0.56	0	17,17,17	0.79	1 (5%)
7	PDO	A	220	-	4,4,4	0.32	0	3,3,3	0.35	0
13	PGE	C	239	-	9,9,9	0.45	0	8,8,8	0.29	0
3	PG0	C	202	-	7,7,7	0.76	0	6,6,6	0.83	0
5	EDO	A	211	-	3,3,3	0.43	0	2,2,2	0.39	0
5	EDO	C	211	-	3,3,3	0.43	0	2,2,2	0.38	0
11	ETX	C	242	-	5,5,5	0.43	0	4,4,4	0.31	0
2	PG4	D	202	-	12,12,12	0.45	0	11,11,11	0.28	0
10	PGO	A	249	-	4,4,4	0.70	0	4,4,4	1.90	2 (50%)
8	EOH	A	232	-	2,2,2	0.65	0	1,1,1	0.87	0
13	PGE	B	233	-	9,9,9	0.44	0	8,8,8	0.29	0
8	EOH	D	233	-	2,2,2	0.39	0	1,1,1	0.39	0
9	MOH	D	239	-	1,1,1	0.11	0	-		
5	EDO	D	211	-	3,3,3	0.46	0	2,2,2	0.39	0
7	PDO	A	221	-	4,4,4	0.32	0	3,3,3	0.35	0
6	GOL	D	222	-	5,5,5	1.55	1 (20%)	5,5,5	0.82	0
7	PDO	A	224	-	4,4,4	0.32	0	3,3,3	0.35	0
4	PEG	C	203	-	6,6,6	0.43	0	5,5,5	0.31	0
5	EDO	B	209	-	3,3,3	0.47	0	2,2,2	0.16	0
5	EDO	A	209	-	3,3,3	0.43	0	2,2,2	0.38	0
8	EOH	B	225	-	2,2,2	0.63	0	1,1,1	0.44	0
11	ETX	A	251	-	5,5,5	0.82	0	4,4,4	1.60	1 (25%)
11	ETX	B	234	-	5,5,5	0.32	0	4,4,4	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	D	214	-	3,3,3	0.57	0	2,2,2	0.44	0
3	PG0	A	203	-	7,7,7	0.79	0	6,6,6	0.71	0
7	PDO	D	224	-	4,4,4	0.31	0	3,3,3	0.35	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
7	PDO	C	221	-	-	1/2/2/2	-
13	PGE	C	240	-	-	3/7/7/7	-
13	PGE	C	241	-	-	4/7/7/7	-
4	PEG	B	203	-	-	3/4/4/4	-
10	PGO	B	232	-	-	2/2/2/2	-
5	EDO	A	217	-	-	1/1/1/1	-
10	PGO	B	231	-	-	2/2/2/2	-
3	PG0	A	204	-	-	4/5/5/5	-
2	PG4	A	202	-	-	7/10/10/10	-
13	PGE	D	248	-	-	6/7/7/7	-
15	P6G	D	208	-	-	10/16/16/16	-
3	PG0	D	204	-	-	3/5/5/5	-
5	EDO	A	212	-	-	0/1/1/1	-
4	PEG	D	207	-	-	3/4/4/4	-
6	GOL	C	217	-	-	4/4/4/4	-
5	EDO	B	208	-	-	1/1/1/1	-
5	EDO	D	212	-	-	1/1/1/1	-
4	PEG	B	204	-	-	2/4/4/4	-
11	ETX	A	250	-	-	2/3/3/3	-
4	PEG	C	205	-	-	3/4/4/4	-
12	ETE	C	208	-	-	6/11/11/11	-
4	PEG	C	206	-	-	2/4/4/4	-
3	PG0	A	205	-	-	3/5/5/5	-
6	GOL	C	216	-	-	2/4/4/4	-
11	ETX	B	236	-	-	2/3/3/3	-
11	ETX	D	249	-	-	2/3/3/3	-
5	EDO	A	213	-	-	1/1/1/1	-
11	ETX	B	235	-	-	1/3/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	C	219	-	-	4/4/4/4	-
6	GOL	A	218	-	-	4/4/4/4	-
4	PEG	C	204	-	-	3/4/4/4	-
5	EDO	D	215	-	-	1/1/1/1	-
5	EDO	D	219	-	-	1/1/1/1	-
2	PG4	D	201	-	-	6/10/10/10	-
10	PGO	B	230	-	1/1/1/1	1/2/2/2	-
4	PEG	A	207	-	-	4/4/4/4	-
5	EDO	D	220	-	-	1/1/1/1	-
2	PG4	B	201	-	-	5/10/10/10	-
15	P6G	D	210	-	-	10/16/16/16	-
7	PDO	B	214	-	-	1/2/2/2	-
5	EDO	B	206	-	-	1/1/1/1	-
5	EDO	C	209	-	-	1/1/1/1	-
7	PDO	A	223	-	-	1/2/2/2	-
5	EDO	A	214	-	-	1/1/1/1	-
12	ETE	B	205	-	-	7/11/11/11	-
5	EDO	D	221	-	-	1/1/1/1	-
5	EDO	B	210	-	-	1/1/1/1	-
7	PDO	B	213	-	-	1/2/2/2	-
5	EDO	C	210	-	-	1/1/1/1	-
3	PG0	B	202	-	-	1/5/5/5	-
3	PG0	D	203	-	-	1/5/5/5	-
2	PG4	A	201	-	-	3/10/10/10	-
10	PGO	A	248	-	-	2/2/2/2	-
5	EDO	B	207	-	-	1/1/1/1	-
4	PEG	D	206	-	-	4/4/4/4	-
10	PGO	C	238	-	-	0/2/2/2	-
5	EDO	D	218	-	-	1/1/1/1	-
5	EDO	C	213	-	-	1/1/1/1	-
5	EDO	D	217	-	-	0/1/1/1	-
6	GOL	C	218	-	-	4/4/4/4	-
7	PDO	C	220	-	-	2/2/2/2	-
3	PG0	C	201	-	-	0/5/5/5	-
4	PEG	A	208	-	-	3/4/4/4	-
10	PGO	D	245	-	-	1/2/2/2	-
7	PDO	D	223	-	-	1/2/2/2	-
5	EDO	C	214	-	-	0/1/1/1	-
5	EDO	D	213	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PDO	A	219	-	-	1/2/2/2	-
5	EDO	A	216	-	-	1/1/1/1	-
10	PGO	D	247	-	-	2/2/2/2	-
11	ETX	D	250	-	-	2/3/3/3	-
10	PGO	D	246	-	-	0/2/2/2	-
5	EDO	A	210	-	-	1/1/1/1	-
5	EDO	D	216	-	-	1/1/1/1	-
3	PG0	A	206	-	-	2/5/5/5	-
7	PDO	A	222	-	-	2/2/2/2	-
5	EDO	A	215	-	-	0/1/1/1	-
7	PDO	B	212	-	-	1/2/2/2	-
5	EDO	B	211	-	-	0/1/1/1	-
10	PGO	A	247	-	-	2/2/2/2	-
7	PDO	A	225	-	-	1/2/2/2	-
5	EDO	C	212	-	-	1/1/1/1	-
14	P33	C	207	-	-	11/19/19/19	-
4	PEG	D	205	-	-	2/4/4/4	-
5	EDO	C	215	-	-	1/1/1/1	-
15	P6G	D	209	-	-	7/16/16/16	-
7	PDO	A	220	-	-	1/2/2/2	-
13	PGE	C	239	-	-	4/7/7/7	-
3	PG0	C	202	-	-	4/5/5/5	-
5	EDO	A	211	-	-	1/1/1/1	-
5	EDO	C	211	-	-	1/1/1/1	-
11	ETX	C	242	-	-	3/3/3/3	-
2	PG4	D	202	-	-	1/10/10/10	-
10	PGO	A	249	-	-	2/2/2/2	-
13	PGE	B	233	-	-	3/7/7/7	-
5	EDO	D	211	-	-	1/1/1/1	-
7	PDO	A	221	-	-	1/2/2/2	-
6	GOL	D	222	-	-	3/4/4/4	-
7	PDO	A	224	-	-	2/2/2/2	-
4	PEG	C	203	-	-	1/4/4/4	-
5	EDO	B	209	-	-	1/1/1/1	-
5	EDO	A	209	-	-	0/1/1/1	-
11	ETX	A	251	-	-	2/3/3/3	-
11	ETX	B	234	-	-	2/3/3/3	-
5	EDO	D	214	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PG0	A	203	-	-	3/5/5/5	-
7	PDO	D	224	-	-	1/2/2/2	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	230	PGO	O2-C2	-5.84	1.19	1.43
6	C	218	GOL	O2-C2	-3.15	1.34	1.43
6	D	222	GOL	O2-C2	-2.91	1.34	1.43
6	A	218	GOL	O2-C2	-2.89	1.35	1.43
6	C	217	GOL	O2-C2	-2.37	1.36	1.43

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	218	GOL	O2-C2-C3	-4.31	91.34	109.18
13	C	241	PGE	C3-O2-C2	-4.28	94.52	113.26
15	D	210	P6G	O7-C6-C5	3.91	128.18	110.35
4	A	207	PEG	O2-C2-C1	3.75	126.65	110.11
6	A	218	GOL	O1-C1-C2	3.72	127.11	110.38

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	B	230	PGO	C2

5 of 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
6	C	218	GOL	C1-C2-C3-O3
6	C	218	GOL	O2-C2-C3-O3
6	C	219	GOL	O1-C1-C2-C3

There are no ring outliers.

86 monomers are involved in 214 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	221	PDO	1	0
13	C	240	PGE	1	0

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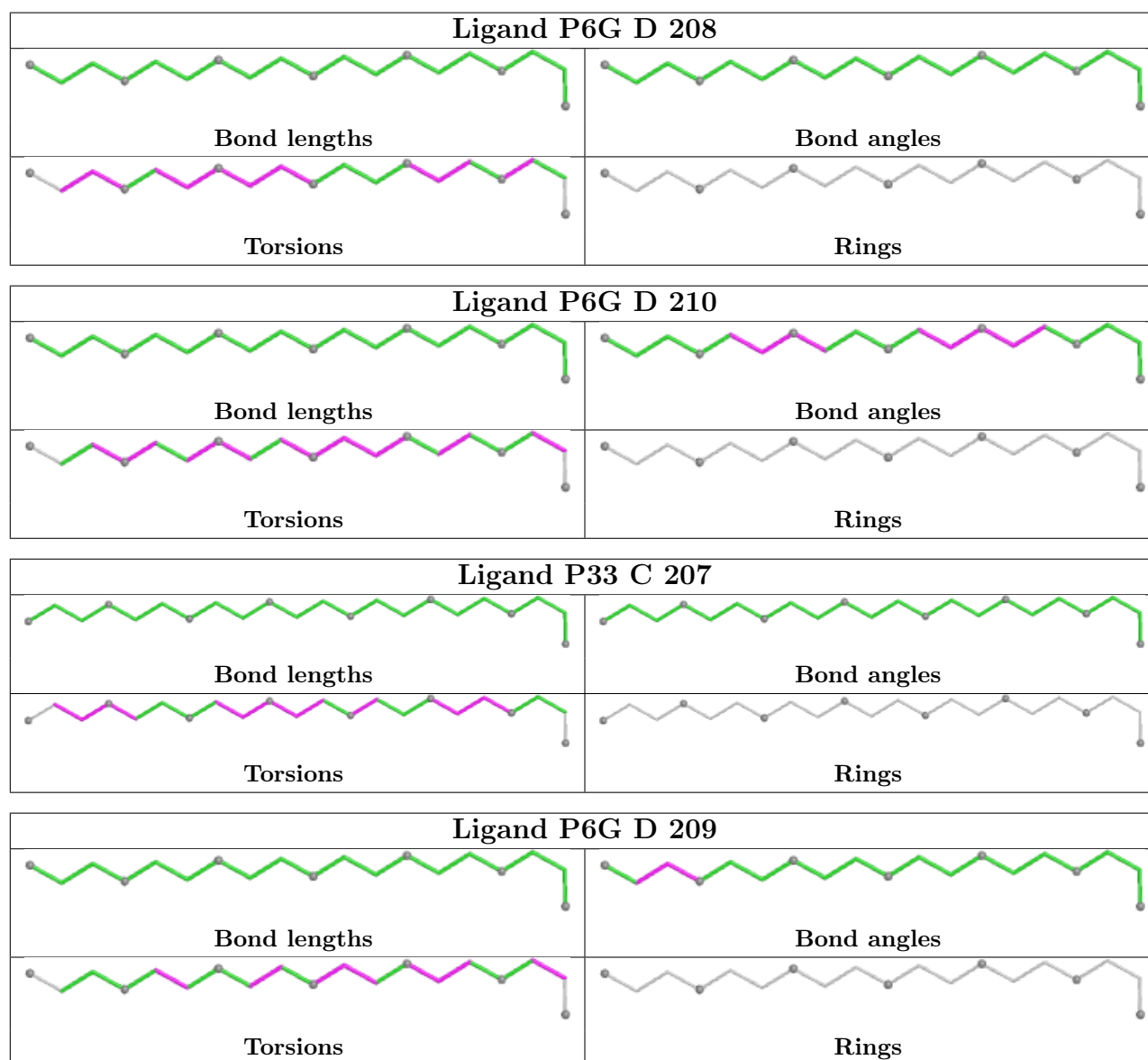
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	241	PGE	2	0
10	B	232	PGO	1	0
3	A	204	PG0	7	0
2	A	202	PG4	1	0
13	D	248	PGE	1	0
15	D	208	P6G	2	0
3	D	204	PG0	5	0
5	A	212	EDO	1	0
8	C	224	EOH	1	0
6	C	217	GOL	1	0
5	D	212	EDO	2	0
11	A	250	ETX	8	0
8	A	230	EOH	1	0
4	C	205	PEG	4	0
12	C	208	ETE	1	0
8	A	231	EOH	1	0
3	A	205	PG0	1	0
11	B	236	ETX	1	0
11	D	249	ETX	12	0
6	C	219	GOL	1	0
4	C	204	PEG	1	0
2	D	201	PG4	4	0
10	B	230	PGO	2	0
4	A	207	PEG	4	0
5	D	220	EDO	1	0
8	D	230	EOH	11	0
2	B	201	PG4	2	0
15	D	210	P6G	5	0
5	B	206	EDO	1	0
8	C	225	EOH	4	0
5	C	209	EDO	1	0
5	A	214	EDO	1	0
12	B	205	ETE	4	0
5	C	210	EDO	1	0
8	B	226	EOH	1	0
3	B	202	PG0	2	0
8	C	227	EOH	1	0
3	D	203	PG0	4	0
5	B	207	EDO	3	0
4	D	206	PEG	6	0
8	B	223	EOH	2	0
9	D	237	MOH	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	229	MOH	2	0
8	C	222	EOH	1	0
3	C	201	PG0	3	0
10	D	245	PGO	4	0
5	C	214	EDO	1	0
7	A	219	PDO	3	0
8	C	226	EOH	3	0
8	D	225	EOH	1	0
5	A	216	EDO	2	0
8	A	236	EOH	2	0
10	D	246	PGO	5	0
5	A	210	EDO	1	0
11	D	250	ETX	6	0
8	C	231	EOH	1	0
3	A	206	PG0	5	0
7	A	222	PDO	1	0
8	B	217	EOH	2	0
7	B	212	PDO	1	0
10	A	247	PGO	10	0
8	B	220	EOH	2	0
5	C	212	EDO	2	0
14	C	207	P33	14	0
4	D	205	PEG	6	0
5	C	215	EDO	1	0
8	A	226	EOH	2	0
15	D	209	P6G	15	0
7	A	220	PDO	2	0
13	C	239	PGE	5	0
3	C	202	PG0	5	0
2	D	202	PG4	9	0
10	A	249	PGO	1	0
8	A	232	EOH	1	0
13	B	233	PGE	3	0
9	D	239	MOH	1	0
7	A	221	PDO	7	0
6	D	222	GOL	2	0
4	C	203	PEG	8	0
5	B	209	EDO	1	0
5	A	209	EDO	2	0
11	B	234	ETX	2	0
3	A	203	PG0	3	0
7	D	224	PDO	11	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	165/176 (93%)	0.60	12 (7%) 21 22	23, 38, 71, 84	0
1	B	161/176 (91%)	0.49	8 (4%) 34 36	22, 38, 62, 76	0
1	C	161/176 (91%)	0.40	9 (5%) 30 32	21, 33, 56, 83	1 (0%)
1	D	166/176 (94%)	0.50	13 (7%) 19 20	21, 36, 63, 91	1 (0%)
All	All	653/704 (92%)	0.50	42 (6%) 25 27	21, 36, 64, 91	2 (0%)

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	29	THR	5.4
1	A	2	ALA	4.3
1	D	166	ILE	3.4
1	D	4	THR	3.3
1	A	116	ILE	3.3

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	ETX	B	236	6/6	0.41	0.18	61,64,70,73	0
8	EOH	D	230	3/3	0.45	0.20	57,57,60,62	0
15	P6G	D	210	19/19	0.51	0.16	56,71,87,88	0
9	MOH	C	235	2/2	0.54	0.21	63,63,63,65	0
11	ETX	A	250	6/6	0.54	0.16	63,74,75,78	0
10	PGO	D	246	5/5	0.55	0.15	54,55,59,60	0
8	EOH	B	221	3/3	0.56	0.14	67,67,71,73	0
9	MOH	D	239	2/2	0.56	0.13	62,62,62,62	0
5	EDO	A	217	4/4	0.56	0.15	70,74,74,79	0
8	EOH	A	232	3/3	0.57	0.16	55,55,67,69	0
4	PEG	C	206	7/7	0.57	0.17	50,55,61,66	0
5	EDO	B	210	4/4	0.57	0.14	75,76,77,80	0
8	EOH	A	238	3/3	0.58	0.18	60,60,62,65	0
9	MOH	D	243	2/2	0.58	0.17	56,56,56,58	0
11	ETX	C	242	6/6	0.60	0.16	52,63,63,70	0
6	GOL	C	219	6/6	0.60	0.13	66,71,74,78	0
15	P6G	D	209	19/19	0.61	0.12	79,90,96,97	0
5	EDO	D	220	4/4	0.62	0.24	68,68,72,73	0
5	EDO	D	221	4/4	0.62	0.15	70,70,75,77	0
13	PGE	C	239	10/10	0.62	0.13	68,71,76,76	0
3	PG0	A	206	8/8	0.62	0.14	64,68,72,73	0
5	EDO	D	219	4/4	0.62	0.12	73,75,77,88	0
11	ETX	D	250	6/6	0.63	0.17	58,62,65,66	0
9	MOH	C	236	2/2	0.63	0.14	50,50,50,64	0
6	GOL	C	216	6/6	0.64	0.13	59,64,71,72	0
12	ETE	C	208	14/14	0.64	0.13	56,69,75,80	0
8	EOH	B	226	3/3	0.64	0.13	64,64,70,71	0
8	EOH	C	225	3/3	0.64	0.13	50,50,54,60	0
2	PG4	A	202	13/13	0.64	0.13	52,61,76,77	0
5	EDO	D	213	4/4	0.65	0.18	47,51,51,58	0
7	PDO	A	224	5/5	0.65	0.12	70,71,72,72	0
11	ETX	B	234	6/6	0.65	0.14	55,62,69,73	0
9	MOH	A	243	2/2	0.65	0.17	65,65,65,67	0
9	MOH	A	244	2/2	0.65	0.14	62,62,62,70	0
9	MOH	D	244	2/2	0.66	0.17	44,44,44,47	0
13	PGE	B	233	10/10	0.66	0.14	56,63,69,84	0
10	PGO	A	247	5/5	0.66	0.12	62,65,69,77	0
7	PDO	A	219	5/5	0.66	0.10	68,70,76,77	0
8	EOH	C	224	3/3	0.66	0.13	57,57,59,63	0
8	EOH	C	230	3/3	0.67	0.13	68,68,70,74	0
3	PG0	A	204	8/8	0.67	0.17	36,49,55,58	0
8	EOH	A	229	3/3	0.67	0.16	59,59,68,71	0
7	PDO	B	214	5/5	0.68	0.13	50,54,65,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	EOH	B	225	3/3	0.68	0.16	48,48,49,57	0
8	EOH	A	227	3/3	0.68	0.12	48,48,62,67	0
6	GOL	D	222	6/6	0.68	0.12	56,58,65,65	0
12	ETE	B	205	14/14	0.68	0.15	61,69,76,77	0
5	EDO	B	209	4/4	0.68	0.17	63,64,64,65	0
8	EOH	C	226	3/3	0.68	0.14	55,55,56,58	0
8	EOH	A	237	3/3	0.68	0.15	64,64,66,70	0
5	EDO	A	211	4/4	0.68	0.12	67,70,71,73	0
8	EOH	B	216	3/3	0.68	0.16	53,53,56,58	0
3	PG0	D	204	8/8	0.69	0.17	42,49,57,66	0
4	PEG	A	207	7/7	0.69	0.13	63,70,73,74	0
4	PEG	A	208	7/7	0.69	0.11	68,73,78,81	0
14	P33	C	207	22/22	0.69	0.13	44,59,74,77	0
9	MOH	C	237	2/2	0.69	0.13	51,51,51,55	0
8	EOH	A	233	3/3	0.69	0.16	50,50,54,57	0
3	PG0	C	202	8/8	0.70	0.14	49,59,62,68	0
9	MOH	A	245	2/2	0.71	0.15	55,55,55,60	0
3	PG0	B	202	8/8	0.71	0.16	43,57,59,64	0
10	PGO	A	249	5/5	0.71	0.20	42,44,48,48	0
6	GOL	C	218	6/6	0.71	0.11	53,57,63,66	0
5	EDO	C	211	4/4	0.72	0.13	62,70,70,74	0
4	PEG	C	205	7/7	0.72	0.11	55,59,62,67	0
11	ETX	A	251	6/6	0.72	0.12	59,71,74,78	0
9	MOH	A	246	2/2	0.72	0.12	55,55,55,68	0
9	MOH	B	229	2/2	0.72	0.16	65,65,65,65	0
3	PG0	D	203	8/8	0.72	0.13	57,62,63,64	0
3	PG0	A	205	8/8	0.72	0.12	55,61,65,70	0
8	EOH	A	226	3/3	0.73	0.18	49,49,52,55	0
9	MOH	A	241	2/2	0.73	0.21	34,34,34,41	0
10	PGO	A	248	5/5	0.73	0.12	49,50,57,58	0
2	PG4	A	201	13/13	0.73	0.13	55,63,68,69	0
13	PGE	D	248	10/10	0.73	0.10	54,65,76,79	0
10	PGO	B	231	5/5	0.73	0.14	51,60,64,65	0
11	ETX	D	249	6/6	0.73	0.13	60,64,67,70	0
4	PEG	D	207	7/7	0.73	0.11	62,75,81,84	0
8	EOH	D	232	3/3	0.74	0.17	49,49,53,53	0
9	MOH	C	232	2/2	0.74	0.16	45,45,45,48	0
9	MOH	C	233	2/2	0.74	0.23	39,39,39,44	0
9	MOH	C	234	2/2	0.74	0.16	46,46,46,49	0
8	EOH	B	220	3/3	0.74	0.16	54,54,58,59	0
5	EDO	C	213	4/4	0.75	0.12	58,58,59,60	0
4	PEG	B	203	7/7	0.75	0.12	56,60,63,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	PGE	C	240	10/10	0.75	0.12	56,71,77,83	0
8	EOH	A	231	3/3	0.75	0.11	59,59,63,63	0
8	EOH	C	227	3/3	0.75	0.12	53,53,54,61	0
7	PDO	A	222	5/5	0.75	0.13	55,56,60,66	0
8	EOH	C	222	3/3	0.75	0.15	55,55,55,59	0
7	PDO	C	220	5/5	0.76	0.11	53,55,59,60	0
8	EOH	B	215	3/3	0.76	0.14	59,59,59,69	0
8	EOH	A	228	3/3	0.76	0.14	58,58,61,64	0
5	EDO	A	215	4/4	0.76	0.13	54,55,56,65	0
8	EOH	A	230	3/3	0.76	0.12	65,65,72,80	0
10	PGO	D	245	5/5	0.76	0.16	49,51,54,66	0
8	EOH	B	224	3/3	0.76	0.13	54,54,58,61	0
10	PGO	D	247	5/5	0.76	0.11	40,44,49,52	0
8	EOH	B	223	3/3	0.77	0.11	46,46,49,57	0
3	PG0	A	203	8/8	0.77	0.11	45,50,60,63	0
9	MOH	B	227	2/2	0.77	0.14	45,45,45,45	0
5	EDO	D	215	4/4	0.77	0.14	44,46,50,51	0
4	PEG	B	204	7/7	0.77	0.10	61,67,74,76	0
7	PDO	A	225	5/5	0.77	0.14	48,54,56,61	0
5	EDO	A	213	4/4	0.78	0.16	54,55,57,61	0
8	EOH	A	234	3/3	0.78	0.14	50,50,51,61	0
8	EOH	D	235	3/3	0.78	0.14	46,46,46,51	0
13	PGE	C	241	10/10	0.78	0.11	38,51,59,63	0
5	EDO	B	207	4/4	0.78	0.11	56,61,61,67	0
5	EDO	A	212	4/4	0.78	0.11	55,58,60,62	0
7	PDO	A	223	5/5	0.78	0.12	44,45,50,57	0
5	EDO	C	214	4/4	0.78	0.11	52,56,56,56	0
8	EOH	A	236	3/3	0.79	0.20	41,41,45,47	0
6	GOL	A	218	6/6	0.79	0.10	48,50,53,66	0
10	PGO	B	232	5/5	0.79	0.14	44,50,60,61	0
5	EDO	A	210	4/4	0.79	0.14	43,46,46,52	0
7	PDO	B	213	5/5	0.79	0.12	60,64,70,71	0
7	PDO	A	220	5/5	0.79	0.14	46,51,54,55	0
4	PEG	D	206	7/7	0.79	0.27	30,39,50,51	0
7	PDO	C	221	5/5	0.79	0.13	29,34,40,40	0
8	EOH	C	228	3/3	0.79	0.13	49,49,52,55	0
11	ETX	B	235	6/6	0.79	0.11	45,55,56,61	0
7	PDO	D	223	5/5	0.79	0.11	40,41,45,48	0
5	EDO	D	216	4/4	0.79	0.20	44,47,51,54	0
8	EOH	B	222	3/3	0.80	0.18	55,55,59,68	0
9	MOH	D	240	2/2	0.80	0.13	54,54,54,57	0
8	EOH	D	234	3/3	0.80	0.12	45,45,48,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	A	214	4/4	0.81	0.10	63,69,72,73	0
9	MOH	D	238	2/2	0.81	0.12	51,51,51,56	0
3	PG0	C	201	8/8	0.81	0.11	47,51,58,59	0
2	PG4	D	201	13/13	0.81	0.10	41,47,52,56	0
9	MOH	D	241	2/2	0.81	0.13	60,60,60,63	0
10	PGO	C	238	5/5	0.81	0.10	40,44,52,53	0
9	MOH	D	242	2/2	0.81	0.14	45,45,45,48	0
5	EDO	D	218	4/4	0.81	0.13	50,56,60,67	0
8	EOH	D	231	3/3	0.81	0.12	44,44,51,64	0
2	PG4	B	201	13/13	0.82	0.10	54,58,63,66	0
8	EOH	C	231	3/3	0.82	0.12	61,61,63,63	0
8	EOH	D	226	3/3	0.82	0.18	46,46,50,50	0
8	EOH	D	227	3/3	0.82	0.14	46,46,51,63	0
5	EDO	B	208	4/4	0.82	0.12	56,58,62,62	0
8	EOH	B	218	3/3	0.82	0.13	52,52,55,56	0
2	PG4	D	202	13/13	0.82	0.12	30,42,48,53	0
10	PGO	B	230	5/5	0.83	0.12	30,35,41,45	0
8	EOH	D	233	3/3	0.83	0.15	48,48,51,51	0
9	MOH	A	242	2/2	0.83	0.18	29,29,29,34	0
8	EOH	D	228	3/3	0.83	0.17	41,41,48,51	0
4	PEG	D	205	7/7	0.83	0.10	38,45,52,52	0
4	PEG	C	203	7/7	0.84	0.23	35,39,44,50	0
4	PEG	C	204	7/7	0.84	0.15	30,32,36,37	0
8	EOH	D	229	3/3	0.84	0.12	32,32,32,44	0
6	GOL	C	217	6/6	0.84	0.14	42,47,51,59	0
9	MOH	A	239	2/2	0.84	0.13	40,40,40,42	0
5	EDO	D	214	4/4	0.84	0.12	50,51,54,54	0
9	MOH	B	228	2/2	0.84	0.11	47,47,47,54	0
5	EDO	D	211	4/4	0.85	0.11	40,42,47,59	0
8	EOH	B	219	3/3	0.85	0.11	39,39,46,56	0
7	PDO	B	212	5/5	0.85	0.10	40,46,49,51	0
5	EDO	C	212	4/4	0.85	0.13	48,51,57,58	0
9	MOH	A	240	2/2	0.85	0.11	39,39,39,39	0
8	EOH	B	217	3/3	0.86	0.18	30,30,36,42	0
5	EDO	C	209	4/4	0.86	0.12	52,57,57,61	0
15	P6G	D	208	19/19	0.86	0.11	27,47,51,61	0
5	EDO	A	216	4/4	0.86	0.09	47,51,52,56	0
7	PDO	A	221	5/5	0.86	0.14	35,35,38,50	0
8	EOH	D	236	3/3	0.87	0.15	50,50,55,61	0
5	EDO	C	210	4/4	0.87	0.12	37,45,45,46	0
5	EDO	B	211	4/4	0.87	0.15	47,52,52,52	0
8	EOH	C	229	3/3	0.87	0.11	49,49,58,59	0

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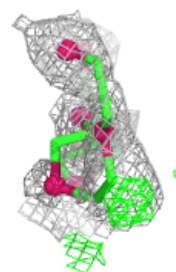
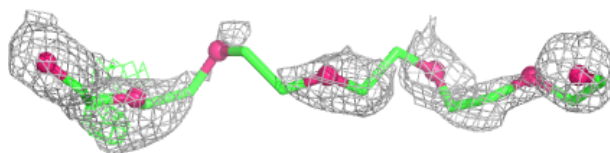
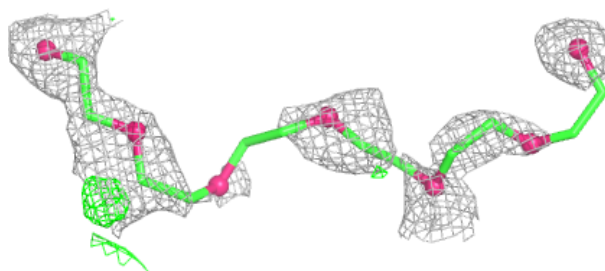
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	A	209	4/4	0.87	0.10	51,55,55,60	0
7	PDO	D	224	5/5	0.87	0.14	21,26,32,35	0
5	EDO	D	217	4/4	0.88	0.18	41,42,43,43	0
5	EDO	C	215	4/4	0.88	0.10	38,48,51,54	0
9	MOH	D	237	2/2	0.88	0.18	35,35,35,41	0
8	EOH	A	235	3/3	0.89	0.10	31,31,38,42	0
8	EOH	C	223	3/3	0.89	0.12	42,42,44,50	0
5	EDO	B	206	4/4	0.89	0.12	36,40,42,42	0
8	EOH	D	225	3/3	0.90	0.09	33,33,35,42	0
5	EDO	D	212	4/4	0.91	0.09	41,43,43,44	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.

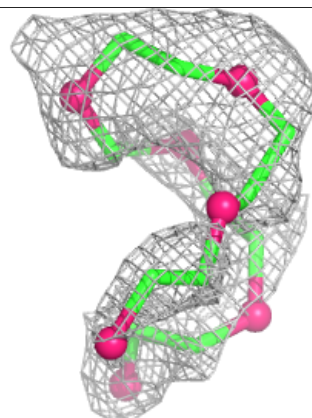
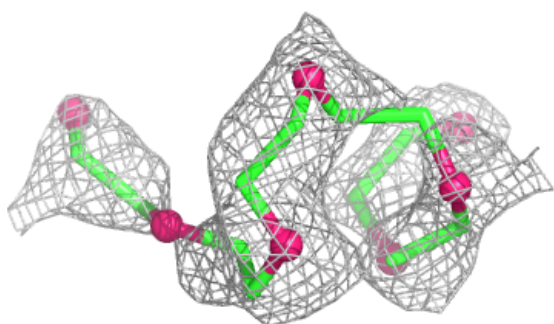
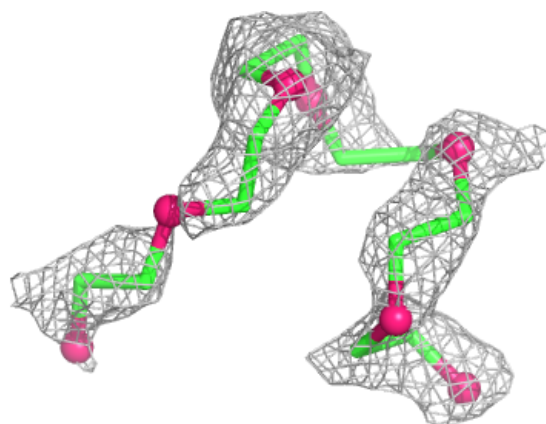
Electron density around P6G D 210:

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

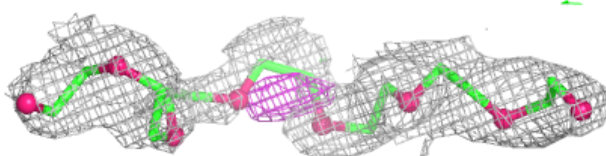
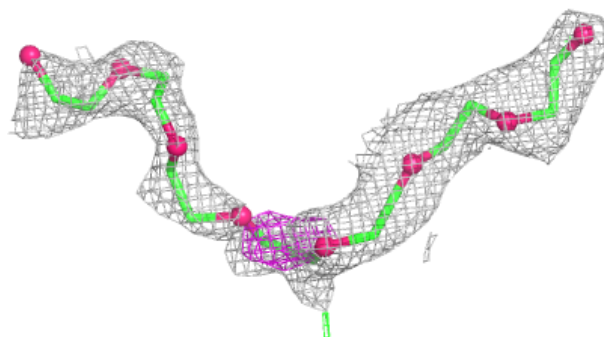


Electron density around P6G D 209:

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

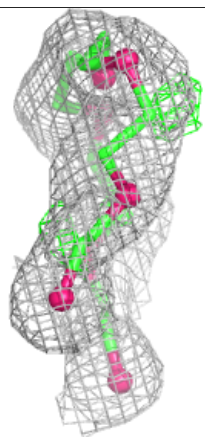
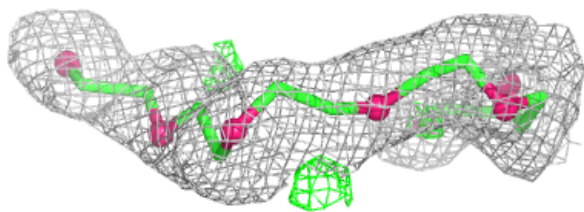
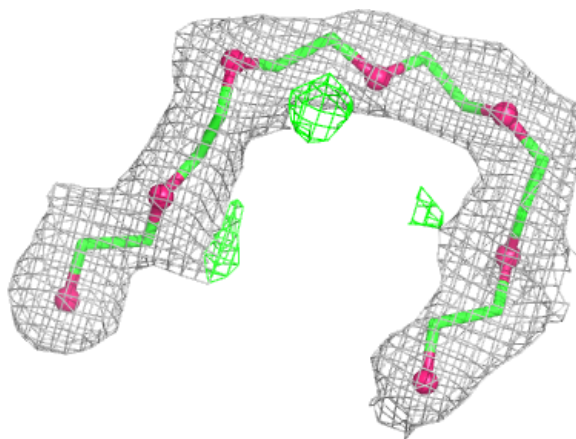
**Electron density around P33 C 207:**

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



Electron density around P6G D 208:

$2mF_o-DF_c$ (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.