



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2024 – 12:24 PM EDT

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 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

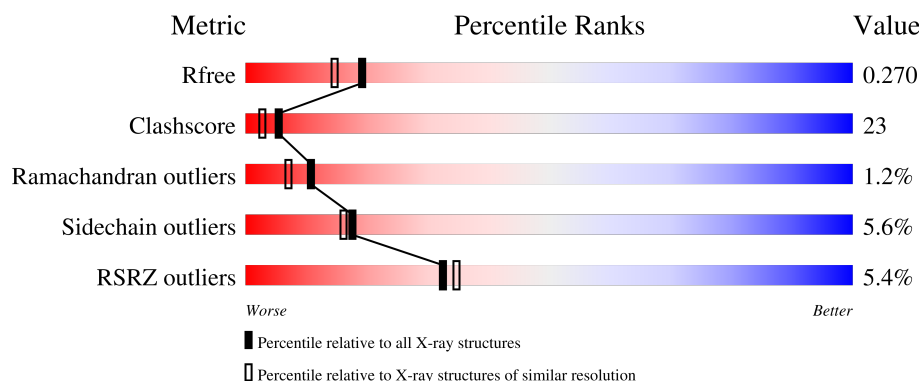
1 Overall quality at a glance

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}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (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	
1	B	176	
1	C	176	
1	D	176	

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:

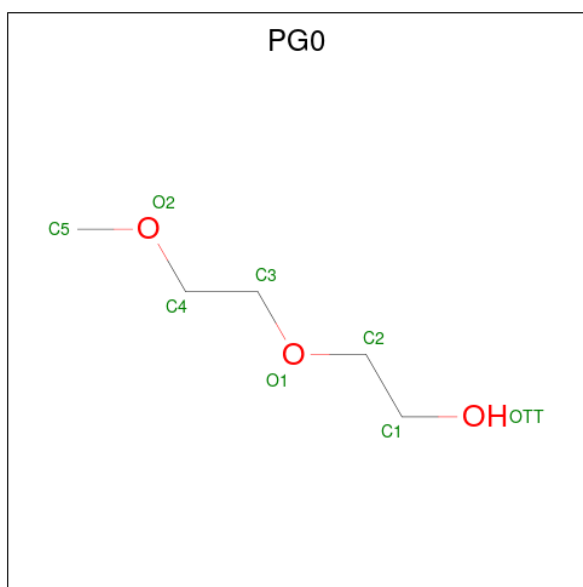
Chain	Residue	Modelled	Actual	Comment	Reference
A	84	ALA	ARG	conflict	UNP P24361
A	147	ALA	ARG	conflict	UNP P24361
B	84	ALA	ARG	conflict	UNP P24361
B	147	ALA	ARG	conflict	UNP P24361
C	84	ALA	ARG	conflict	UNP P24361
C	147	ALA	ARG	conflict	UNP P24361
D	84	ALA	ARG	conflict	UNP P24361
D	147	ALA	ARG	conflict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

- Molecule 2 is TETRAETHYLENE GLYCOL (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	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		
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		

- 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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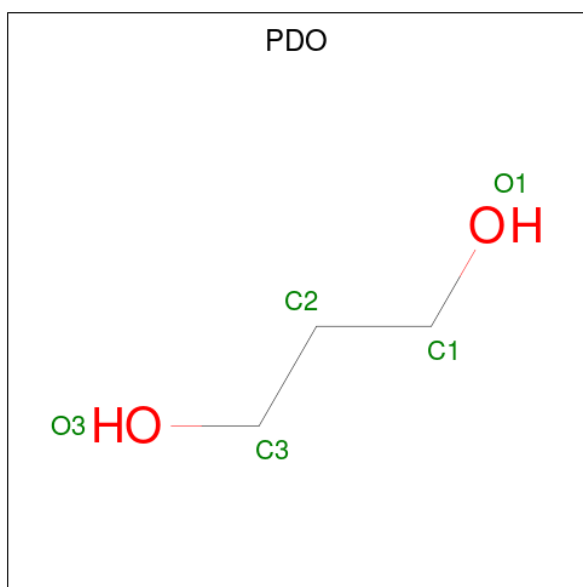
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
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
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 (three-letter code: GOL) (formula: $C_3H_8O_3$).



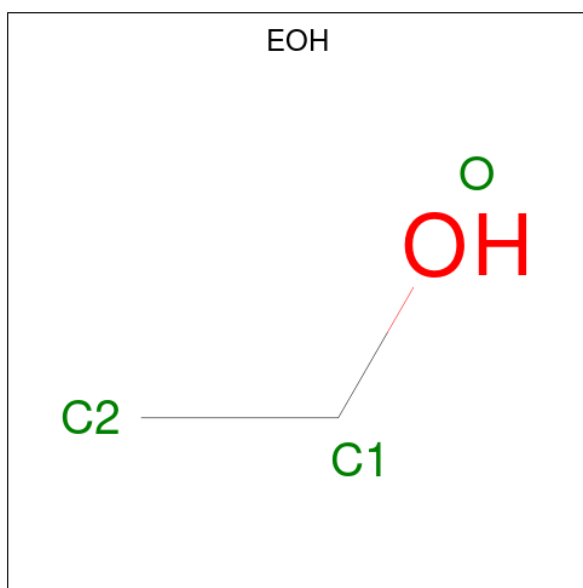
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	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	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 (three-letter code: EOH) (formula: C_2H_6O).



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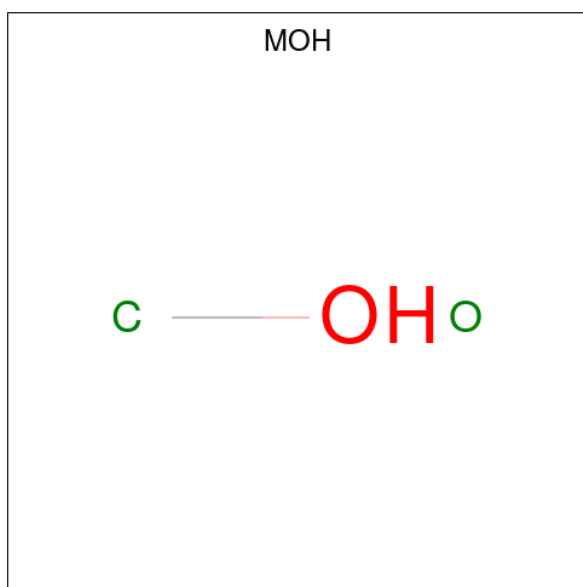
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			3	2	1		
8	B	1	Total	C	O	0	0
			3	2	1		
8	B	1	Total	C	O	0	0
			3	2	1		
8	B	1	Total	C	O	0	0
			3	2	1		
8	B	1	Total	C	O	0	0
			3	2	1		
8	B	1	Total	C	O	0	0
			3	2	1		
8	B	1	Total	C	O	0	0
			3	2	1		
8	B	1	Total	C	O	0	0
			3	2	1		
8	B	1	Total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

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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).



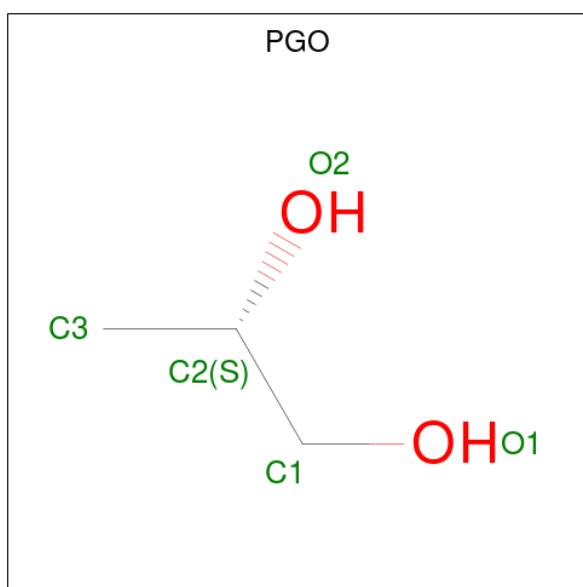
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			2	1	1		
9	A	1	Total	C	O	0	0
			2	1	1		
9	A	1	Total	C	O	0	0
			2	1	1		
9	A	1	Total	C	O	0	0
			2	1	1		
9	A	1	Total	C	O	0	0
			2	1	1		
9	A	1	Total	C	O	0	0
			2	1	1		
9	A	1	Total	C	O	0	0
			2	1	1		
9	B	1	Total	C	O	0	0
			2	1	1		
9	B	1	Total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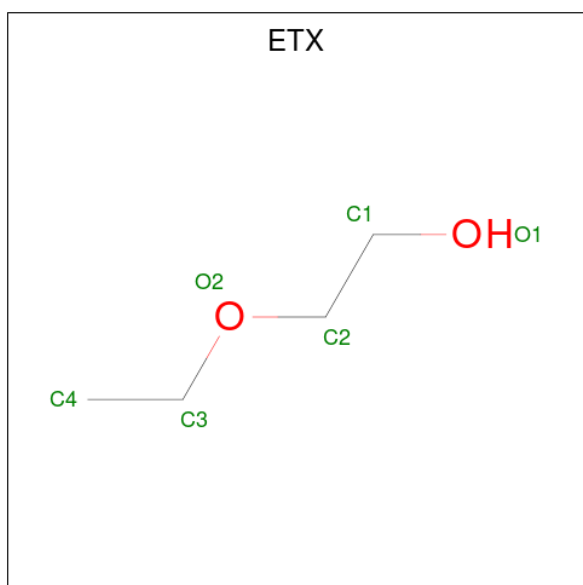
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			2	1	1		
9	C	1	Total	C	O	0	0
			2	1	1		
9	C	1	Total	C	O	0	0
			2	1	1		
9	D	1	Total	C	O	0	0
			2	1	1		
9	D	1	Total	C	O	0	0
			2	1	1		
9	D	1	Total	C	O	0	0
			2	1	1		
9	D	1	Total	C	O	0	0
			2	1	1		
9	D	1	Total	C	O	0	0
			2	1	1		
9	D	1	Total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

- 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: $C_4H_{10}O_2$).



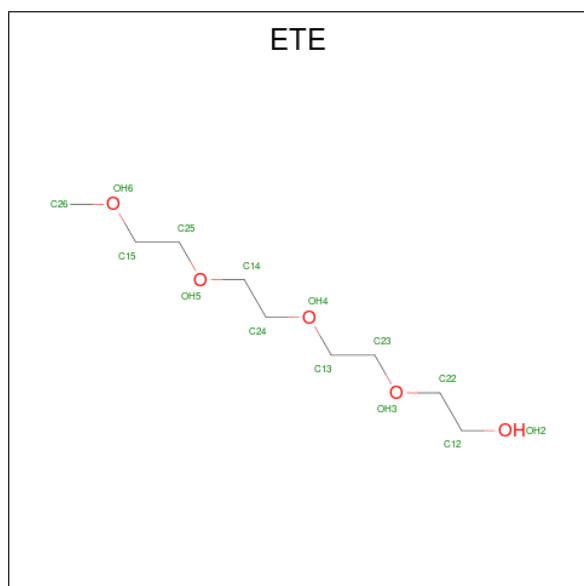
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			6	4	2		
11	A	1	Total	C	O	0	0
			6	4	2		

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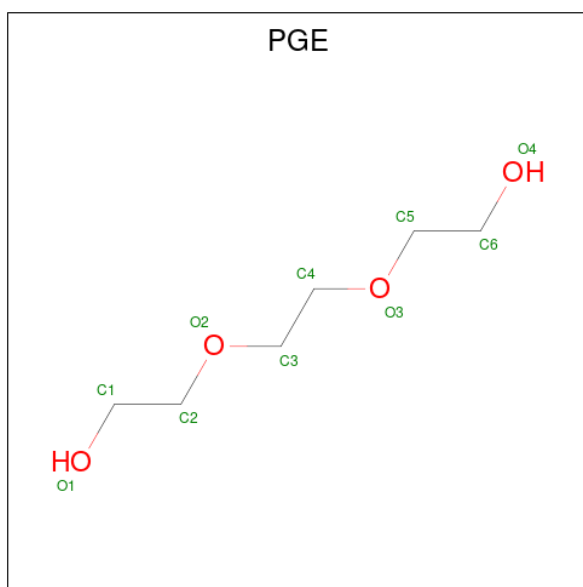
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			6	4	2		
11	B	1	Total	C	O	0	0
			6	4	2		
11	B	1	Total	C	O	0	0
			6	4	2		
11	C	1	Total	C	O	0	0
			6	4	2		
11	D	1	Total	C	O	0	0
			6	4	2		
11	D	1	Total	C	O	0	0
			6	4	2		

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



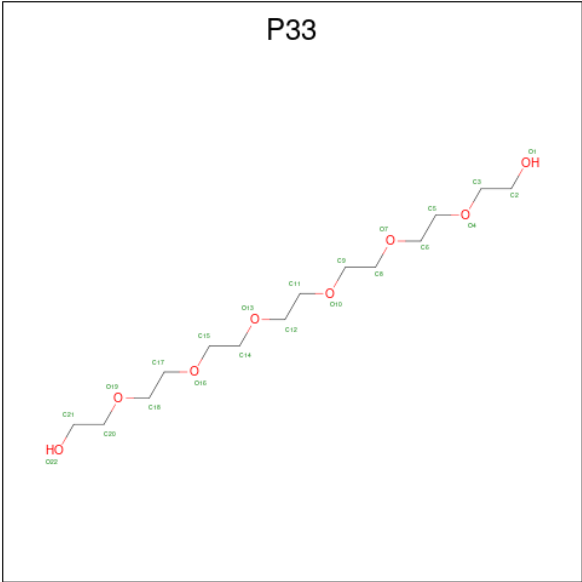
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	C	O	0	0
			14	9	5		
12	C	1	Total	C	O	0	0
			14	9	5		

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



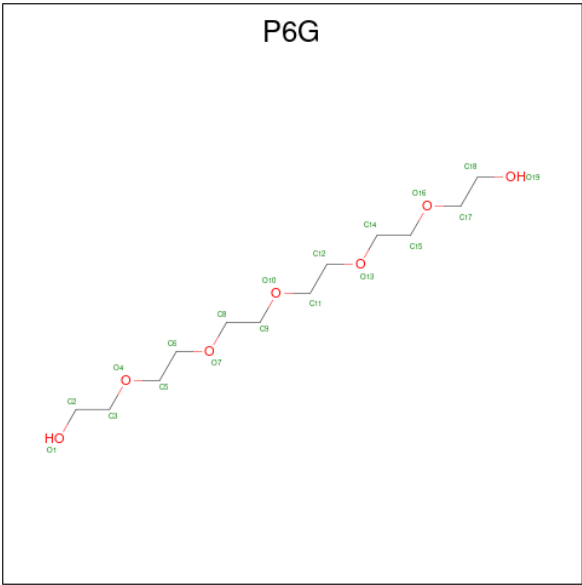
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	B	1	Total	C	O	0	0
			10	6	4		
13	C	1	Total	C	O	0	0
			10	6	4		
13	C	1	Total	C	O	0	0
			10	6	4		
13	C	1	Total	C	O	0	0
			10	6	4		
13	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 14 is 3,6,9,12,15,18-HEXAOSAICOSANE-1,20-DIOL (three-letter code: 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 (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		

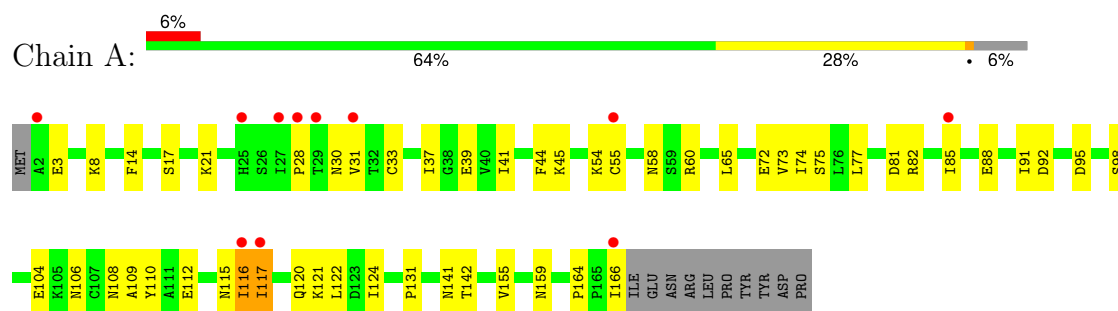
- Molecule 16 is water.

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

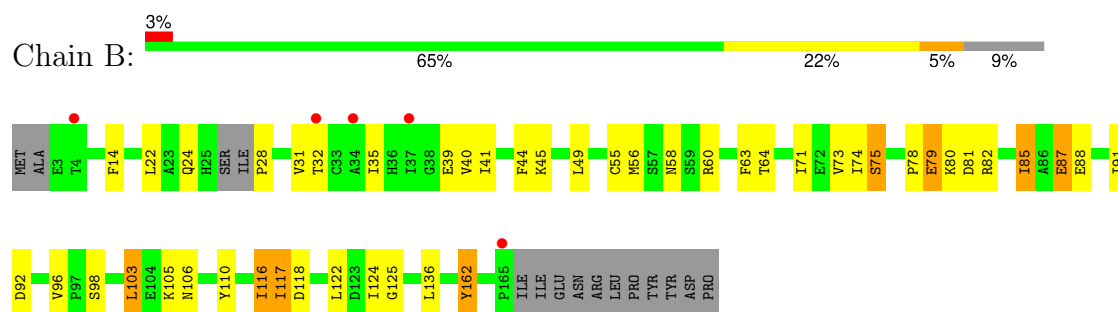
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

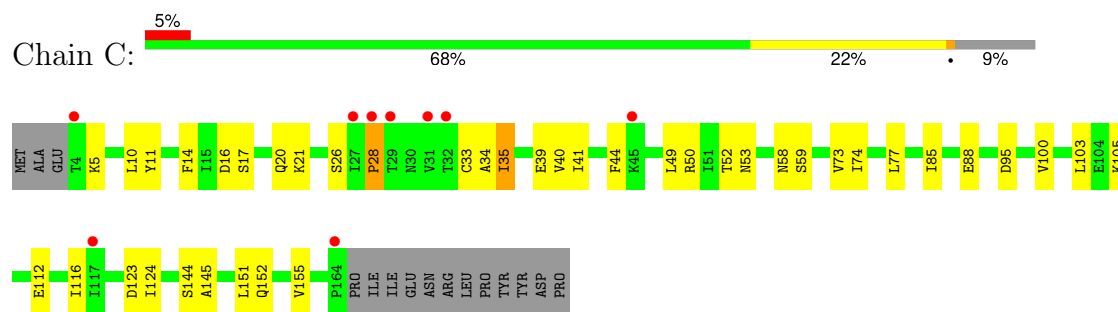
• Molecule 1: Protein F9



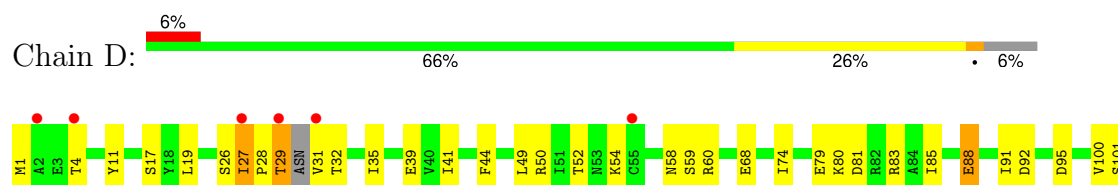
• Molecule 1: Protein F9



• 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 0.227 , 0.270	Depositor DCC
R_{free} test set	35496 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 [i](#)

5.1 Standard geometry [i](#)

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

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
14:C:207:P33:H171	14:C:207:P33:H212	1.38	1.03
15:D:209:P6G:H181	15:D:209:P6G:H142	1.38	1.03
15:D:209:P6G:H51	15:D:209:P6G:H112	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:H12	2:B:201:PG4:H41	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:H151	15:D:209:P6G:C5	2.04	0.87
15:D:209:P6G:H51	15:D:209:P6G:H151	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:H181	15:D:209:P6G:C14	2.02	0.83
14:C:207:P33:H202	14:C:207:P33:C15	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:H51	15:D:209:P6G:C11	2.15	0.74
8:D:230:EOH:H21	11:D:249:ETX:H12	1.69	0.74
14:C:207:P33:H171	14:C:207:P33:C21	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:H22	3:A:206:PG0:O2	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
1:A:41:ILE:HG22	1:C:39:GLU:HG3	1.89	0.55
3:A:206:PG0:H22	3:A:206:PG0:H52	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:H181	15:D:209:P6G:H122	1.92	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
1:D:108:ASN:CG	15:D:208:P6G:H141	2.31	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:H151	15:D:209:P6G:C11	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
1:C:74:ILE:HD11	1:C:85:ILE:HG21	1.95	0.48
4:C:203:PEG:H32	5:C:212:EDO:C1	2.30	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:H151	14:C:207:P33:H182	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:H181	15:D:209:P6G:C12	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:H12	2:B:201:PG4:C4	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:27:ILE:CG2	10:D:246:PGO:H12	2.45	0.42
1:D:146:GLU:CD	1:D:146:GLU:H	2.23	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
1:D:74:ILE:HD12	1:D:74:ILE:HA	1.89	0.42
8:D:230:EOH:H11	11:D:249:ETX:H12	2.00	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:B:45:LYS:O	1:D:52:THR:HA	2.21	0.41
1:D:27:ILE:HG23	10:D:246:PGO:C1	2.45	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:H21	14:C:207:P33:H52	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	11	7
1	B	157/176 (89%)	144 (92%)	9 (6%)	4 (2%)	4	2
1	C	160/176 (91%)	149 (93%)	10 (6%)	1 (1%)	22	19
1	D	163/176 (93%)	153 (94%)	9 (6%)	1 (1%)	22	19
All	All	643/704 (91%)	597 (93%)	38 (6%)	8 (1%)	11	7

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 ⓘ

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%)	24	24
1	B	132/157 (84%)	120 (91%)	12 (9%)	7	5
1	C	134/157 (85%)	129 (96%)	5 (4%)	29	31
1	D	141/157 (90%)	134 (95%)	7 (5%)	20	20
All	All	542/628 (86%)	512 (94%)	30 (6%)	17	16

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

Sometimes 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 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
8	EOH	A	237	-	2,2,2	0.72	0	1,1,1	0.74	0
3	PG0	A	203	-	7,7,7	0.79	0	6,6,6	0.71	0
8	EOH	B	225	-	2,2,2	0.63	0	1,1,1	0.44	0
5	EDO	D	219	-	3,3,3	0.43	0	2,2,2	0.38	0
13	PGE	C	240	-	9,9,9	0.45	0	8,8,8	0.29	0
7	PDO	C	221	-	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
4	PEG	C	204	-	6,6,6	0.43	0	5,5,5	0.30	0
10	PGO	D	245	-	4,4,4	1.23	0	4,4,4	1.54	1 (25%)
8	EOH	C	224	-	2,2,2	0.39	0	1,1,1	0.39	0
4	PEG	C	205	-	6,6,6	0.65	0	5,5,5	2.40	3 (60%)
11	ETX	B	234	-	5,5,5	0.32	0	4,4,4	0.81	0
8	EOH	A	238	-	2,2,2	0.16	0	1,1,1	0.28	0
6	GOL	C	217	-	5,5,5	1.33	1 (20%)	5,5,5	1.38	1 (20%)
15	P6G	D	210	-	18,18,18	0.83	0	17,17,17	1.63	4 (23%)
9	MOH	D	243	-	1,1,1	0.08	0	-		
5	EDO	B	211	-	3,3,3	0.84	0	2,2,2	0.42	0
9	MOH	A	246	-	1,1,1	0.08	0	-		
9	MOH	B	227	-	1,1,1	0.08	0	-		
3	PG0	D	204	-	7,7,7	0.44	0	6,6,6	0.26	0
4	PEG	A	207	-	6,6,6	0.54	0	5,5,5	2.05	2 (40%)
2	PG4	D	201	-	12,12,12	1.34	2 (16%)	11,11,11	1.62	2 (18%)
5	EDO	A	209	-	3,3,3	0.43	0	2,2,2	0.38	0
9	MOH	D	237	-	1,1,1	0.08	0	-		
8	EOH	D	230	-	2,2,2	0.40	0	1,1,1	0.39	0
7	PDO	A	224	-	4,4,4	0.32	0	3,3,3	0.35	0
5	EDO	B	210	-	3,3,3	0.70	0	2,2,2	1.03	0
3	PG0	D	203	-	7,7,7	0.44	0	6,6,6	0.26	0
5	EDO	D	220	-	3,3,3	0.30	0	2,2,2	0.61	0
9	MOH	C	234	-	1,1,1	0.07	0	-		
5	EDO	D	217	-	3,3,3	0.90	0	2,2,2	0.71	0
5	EDO	A	214	-	3,3,3	0.37	0	2,2,2	0.81	0
11	ETX	B	236	-	5,5,5	0.53	0	4,4,4	1.21	1 (25%)
4	PEG	D	205	-	6,6,6	0.44	0	5,5,5	0.31	0
7	PDO	A	225	-	4,4,4	0.97	0	3,3,3	0.84	0
9	MOH	D	240	-	1,1,1	0.08	0	-		
8	EOH	C	230	-	2,2,2	0.39	0	1,1,1	0.39	0
5	EDO	A	210	-	3,3,3	0.42	0	2,2,2	0.38	0
8	EOH	A	236	-	2,2,2	0.56	0	1,1,1	0.14	0
9	MOH	A	242	-	1,1,1	0.07	0	-		
8	EOH	D	227	-	2,2,2	0.40	0	1,1,1	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	PGO	C	238	-	4,4,4	1.17	0	4,4,4	1.10	0
10	PGO	D	247	-	4,4,4	1.42	1 (25%)	4,4,4	1.57	2 (50%)
8	EOH	D	233	-	2,2,2	0.39	0	1,1,1	0.39	0
8	EOH	D	231	-	2,2,2	0.40	0	1,1,1	0.39	0
4	PEG	D	207	-	6,6,6	0.48	0	5,5,5	0.91	0
7	PDO	B	212	-	4,4,4	0.32	0	3,3,3	0.35	0
9	MOH	C	237	-	1,1,1	0.12	0	-		
4	PEG	D	206	-	6,6,6	0.43	0	5,5,5	0.31	0
5	EDO	C	213	-	3,3,3	0.42	0	2,2,2	0.38	0
8	EOH	D	232	-	2,2,2	0.39	0	1,1,1	0.38	0
11	ETX	D	250	-	5,5,5	0.65	0	4,4,4	0.83	0
9	MOH	A	244	-	1,1,1	0.09	0	-		
5	EDO	C	215	-	3,3,3	1.46	1 (33%)	2,2,2	0.41	0
5	EDO	D	221	-	3,3,3	0.43	0	2,2,2	0.39	0
9	MOH	A	240	-	1,1,1	0.08	0	-		
5	EDO	B	206	-	3,3,3	0.42	0	2,2,2	0.38	0
5	EDO	D	214	-	3,3,3	0.57	0	2,2,2	0.44	0
5	EDO	C	214	-	3,3,3	1.02	0	2,2,2	1.15	0
11	ETX	D	249	-	5,5,5	0.41	0	4,4,4	0.58	0
5	EDO	D	218	-	3,3,3	1.22	1 (33%)	2,2,2	0.56	0
2	PG4	A	201	-	12,12,12	0.56	0	11,11,11	0.45	0
8	EOH	B	222	-	2,2,2	0.40	0	1,1,1	0.39	0
8	EOH	A	231	-	2,2,2	0.40	0	1,1,1	0.39	0
8	EOH	A	230	-	2,2,2	0.40	0	1,1,1	0.39	0
9	MOH	D	242	-	1,1,1	0.08	0	-		
8	EOH	C	225	-	2,2,2	0.40	0	1,1,1	0.39	0
8	EOH	B	220	-	2,2,2	0.40	0	1,1,1	0.39	0
8	EOH	B	224	-	2,2,2	0.50	0	1,1,1	0.43	0
10	PGO	B	231	-	4,4,4	0.65	0	4,4,4	0.74	0
14	P33	C	207	-	21,21,21	0.48	0	20,20,20	0.31	0
10	PGO	B	232	-	4,4,4	0.60	0	4,4,4	0.79	0
5	EDO	A	213	-	3,3,3	0.57	0	2,2,2	0.14	0
8	EOH	C	228	-	2,2,2	0.39	0	1,1,1	0.39	0
8	EOH	C	223	-	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	212	-	3,3,3	0.39	0	2,2,2	0.52	0
5	EDO	D	211	-	3,3,3	0.46	0	2,2,2	0.39	0
11	ETX	C	242	-	5,5,5	0.43	0	4,4,4	0.31	0
9	MOH	C	236	-	1,1,1	0.01	0	-		
3	PG0	B	202	-	7,7,7	0.45	0	6,6,6	0.26	0
7	PDO	B	213	-	4,4,4	0.32	0	3,3,3	0.35	0
9	MOH	B	228	-	1,1,1	0.09	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	EOH	D	235	-	2,2,2	0.59	0	1,1,1	0.86	0
8	EOH	C	226	-	2,2,2	0.50	0	1,1,1	0.39	0
5	EDO	A	212	-	3,3,3	0.42	0	2,2,2	0.38	0
4	PEG	B	204	-	6,6,6	0.31	0	5,5,5	1.34	1 (20%)
8	EOH	B	219	-	2,2,2	0.39	0	1,1,1	0.39	0
8	EOH	A	226	-	2,2,2	0.07	0	1,1,1	0.12	0
7	PDO	A	219	-	4,4,4	0.61	0	3,3,3	2.10	1 (33%)
5	EDO	D	213	-	3,3,3	0.41	0	2,2,2	0.50	0
8	EOH	B	216	-	2,2,2	0.40	0	1,1,1	0.39	0
5	EDO	B	208	-	3,3,3	0.32	0	2,2,2	0.19	0
7	PDO	B	214	-	4,4,4	0.42	0	3,3,3	1.00	0
6	GOL	D	222	-	5,5,5	1.55	1 (20%)	5,5,5	0.82	0
8	EOH	D	229	-	2,2,2	0.39	0	1,1,1	0.39	0
15	P6G	D	208	-	18,18,18	0.46	0	17,17,17	0.26	0
13	PGE	C	239	-	9,9,9	0.45	0	8,8,8	0.29	0
9	MOH	C	232	-	1,1,1	0.21	0	-		
6	GOL	C	219	-	5,5,5	1.17	0	5,5,5	2.33	3 (60%)
13	PGE	C	241	-	9,9,9	1.28	2 (22%)	8,8,8	2.10	2 (25%)
15	P6G	D	209	-	18,18,18	0.56	0	17,17,17	0.79	1 (5%)
8	EOH	B	215	-	2,2,2	0.39	0	1,1,1	0.39	0
5	EDO	C	209	-	3,3,3	1.18	0	2,2,2	1.34	0
5	EDO	C	211	-	3,3,3	0.43	0	2,2,2	0.38	0
8	EOH	B	218	-	2,2,2	0.40	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	D	246	-	4,4,4	0.65	0	4,4,4	0.74	0
8	EOH	B	217	-	2,2,2	0.39	0	1,1,1	0.39	0
7	PDO	A	221	-	4,4,4	0.32	0	3,3,3	0.35	0
8	EOH	C	229	-	2,2,2	0.40	0	1,1,1	0.39	0
5	EDO	A	211	-	3,3,3	0.43	0	2,2,2	0.39	0
4	PEG	C	206	-	6,6,6	0.61	0	5,5,5	1.23	0
8	EOH	A	229	-	2,2,2	0.20	0	1,1,1	0.57	0
5	EDO	A	216	-	3,3,3	0.82	0	2,2,2	0.74	0
5	EDO	B	207	-	3,3,3	0.52	0	2,2,2	1.10	0
8	EOH	A	232	-	2,2,2	0.65	0	1,1,1	0.87	0
8	EOH	C	227	-	2,2,2	0.39	0	1,1,1	0.39	0
8	EOH	D	228	-	2,2,2	0.40	0	1,1,1	0.39	0
11	ETX	A	251	-	5,5,5	0.82	0	4,4,4	1.60	1 (25%)
6	GOL	C	216	-	5,5,5	1.02	0	5,5,5	1.04	0
3	PG0	A	205	-	7,7,7	0.34	0	6,6,6	1.42	2 (33%)
10	PGO	A	247	-	4,4,4	0.60	0	4,4,4	1.21	0
9	MOH	D	238	-	1,1,1	0.09	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	EOH	D	236	-	2,2,2	0.39	0	1,1,1	0.39	0
9	MOH	D	239	-	1,1,1	0.11	0	-		
9	MOH	A	239	-	1,1,1	0.08	0	-		
11	ETX	A	250	-	5,5,5	0.43	0	4,4,4	0.30	0
6	GOL	A	218	-	5,5,5	1.45	1 (20%)	5,5,5	2.77	4 (80%)
9	MOH	D	241	-	1,1,1	0.06	0	-		
11	ETX	B	235	-	5,5,5	0.44	0	4,4,4	0.30	0
2	PG4	B	201	-	12,12,12	0.96	0	11,11,11	1.41	1 (9%)
13	PGE	B	233	-	9,9,9	0.44	0	8,8,8	0.29	0
2	PG4	D	202	-	12,12,12	0.45	0	11,11,11	0.28	0
7	PDO	C	220	-	4,4,4	0.32	0	3,3,3	0.35	0
8	EOH	A	228	-	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	216	-	3,3,3	0.43	0	2,2,2	0.38	0
9	MOH	D	244	-	1,1,1	0.33	0	-		
7	PDO	D	224	-	4,4,4	0.31	0	3,3,3	0.35	0
7	PDO	A	220	-	4,4,4	0.32	0	3,3,3	0.35	0
8	EOH	A	227	-	2,2,2	0.39	0	1,1,1	0.39	0
4	PEG	A	208	-	6,6,6	0.61	0	5,5,5	1.12	1 (20%)
7	PDO	D	223	-	4,4,4	0.32	0	3,3,3	0.35	0
8	EOH	A	233	-	2,2,2	0.22	0	1,1,1	0.40	0
8	EOH	D	225	-	2,2,2	0.44	0	1,1,1	0.28	0
10	PGO	A	248	-	4,4,4	0.79	0	4,4,4	0.87	0
12	ETE	C	208	-	13,13,13	0.68	0	12,12,12	1.36	3 (25%)
8	EOH	A	235	-	2,2,2	0.40	0	1,1,1	0.39	0
4	PEG	B	203	-	6,6,6	0.44	0	5,5,5	0.31	0
9	MOH	A	241	-	1,1,1	0.08	0	-		
7	PDO	A	222	-	4,4,4	0.32	0	3,3,3	0.35	0
9	MOH	C	235	-	1,1,1	0.09	0	-		
8	EOH	B	221	-	2,2,2	0.40	0	1,1,1	0.66	0
8	EOH	B	223	-	2,2,2	0.39	0	1,1,1	0.39	0
9	MOH	A	245	-	1,1,1	0.08	0	-		
5	EDO	C	212	-	3,3,3	0.42	0	2,2,2	0.39	0
5	EDO	C	210	-	3,3,3	0.43	0	2,2,2	0.39	0
6	GOL	C	218	-	5,5,5	1.70	1 (20%)	5,5,5	2.53	2 (40%)
3	PG0	C	202	-	7,7,7	0.76	0	6,6,6	0.83	0
8	EOH	D	234	-	2,2,2	0.57	0	1,1,1	0.27	0
3	PG0	A	206	-	7,7,7	1.08	1 (14%)	6,6,6	1.90	3 (50%)
5	EDO	A	215	-	3,3,3	0.42	0	2,2,2	0.38	0
2	PG4	A	202	-	12,12,12	0.59	0	11,11,11	1.24	3 (27%)
8	EOH	C	222	-	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
5	EDO	D	215	-	3,3,3	0.43	0	2,2,2	0.38	0
7	PDO	A	223	-	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
8	EOH	B	226	-	2,2,2	0.37	0	1,1,1	0.17	0
9	MOH	A	243	-	1,1,1	0.12	0	-		
9	MOH	B	229	-	1,1,1	0.07	0	-		
5	EDO	B	209	-	3,3,3	0.47	0	2,2,2	0.16	0
9	MOH	C	233	-	1,1,1	0.08	0	-		
10	PGO	B	230	-	4,4,4	3.00	1 (25%)	4,4,4	1.73	2 (50%)
13	PGE	D	248	-	9,9,9	0.45	0	8,8,8	0.28	0
3	PG0	C	201	-	7,7,7	0.57	0	6,6,6	1.59	1 (16%)
8	EOH	C	231	-	2,2,2	0.39	0	1,1,1	0.39	0
3	PG0	A	204	-	7,7,7	0.45	0	6,6,6	0.26	0
10	PGO	A	249	-	4,4,4	0.70	0	4,4,4	1.90	2 (50%)

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
3	PG0	A	203	-	-	3/5/5/5	-
5	EDO	D	219	-	-	1/1/1/1	-
13	PGE	C	240	-	-	3/7/7/7	-
7	PDO	C	221	-	-	1/2/2/2	-
4	PEG	C	204	-	-	3/4/4/4	-
10	PGO	D	245	-	-	1/2/2/2	-
4	PEG	C	205	-	-	3/4/4/4	-
11	ETX	B	234	-	-	2/3/3/3	-
6	GOL	C	217	-	-	4/4/4/4	-
15	P6G	D	210	-	-	10/16/16/16	-
5	EDO	B	211	-	-	0/1/1/1	-
3	PG0	D	204	-	-	3/5/5/5	-
4	PEG	A	207	-	-	4/4/4/4	-
2	PG4	D	201	-	-	6/10/10/10	-
5	EDO	A	209	-	-	0/1/1/1	-
7	PDO	A	224	-	-	2/2/2/2	-
5	EDO	B	210	-	-	1/1/1/1	-
3	PG0	D	203	-	-	1/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	D	220	-	-	1/1/1/1	-
5	EDO	D	217	-	-	0/1/1/1	-
5	EDO	A	214	-	-	1/1/1/1	-
11	ETX	B	236	-	-	2/3/3/3	-
4	PEG	D	205	-	-	2/4/4/4	-
7	PDO	A	225	-	-	1/2/2/2	-
5	EDO	A	210	-	-	1/1/1/1	-
10	PGO	C	238	-	-	0/2/2/2	-
10	PGO	D	247	-	-	2/2/2/2	-
4	PEG	D	207	-	-	3/4/4/4	-
7	PDO	B	212	-	-	1/2/2/2	-
4	PEG	D	206	-	-	4/4/4/4	-
5	EDO	C	213	-	-	1/1/1/1	-
11	ETX	D	250	-	-	2/3/3/3	-
5	EDO	C	215	-	-	1/1/1/1	-
5	EDO	D	221	-	-	1/1/1/1	-
5	EDO	B	206	-	-	1/1/1/1	-
5	EDO	D	214	-	-	0/1/1/1	-
5	EDO	C	214	-	-	0/1/1/1	-
11	ETX	D	249	-	-	2/3/3/3	-
5	EDO	D	218	-	-	1/1/1/1	-
2	PG4	A	201	-	-	3/10/10/10	-
10	PGO	B	231	-	-	2/2/2/2	-
14	P33	C	207	-	-	11/19/19/19	-
10	PGO	B	232	-	-	2/2/2/2	-
5	EDO	A	213	-	-	1/1/1/1	-
12	ETE	B	205	-	-	7/11/11/11	-
5	EDO	D	212	-	-	1/1/1/1	-
5	EDO	D	211	-	-	1/1/1/1	-
11	ETX	C	242	-	-	3/3/3/3	-
3	PG0	B	202	-	-	1/5/5/5	-
7	PDO	B	213	-	-	1/2/2/2	-
5	EDO	A	212	-	-	0/1/1/1	-
4	PEG	B	204	-	-	2/4/4/4	-
7	PDO	A	219	-	-	1/2/2/2	-
5	EDO	D	213	-	-	0/1/1/1	-
5	EDO	B	208	-	-	1/1/1/1	-
7	PDO	B	214	-	-	1/2/2/2	-
6	GOL	D	222	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	P6G	D	208	-	-	10/16/16/16	-
13	PGE	C	239	-	-	4/7/7/7	-
6	GOL	C	219	-	-	4/4/4/4	-
13	PGE	C	241	-	-	4/7/7/7	-
15	P6G	D	209	-	-	7/16/16/16	-
5	EDO	C	209	-	-	1/1/1/1	-
5	EDO	C	211	-	-	1/1/1/1	-
5	EDO	A	217	-	-	1/1/1/1	-
10	PGO	D	246	-	-	0/2/2/2	-
7	PDO	A	221	-	-	1/2/2/2	-
5	EDO	A	211	-	-	1/1/1/1	-
4	PEG	C	206	-	-	2/4/4/4	-
5	EDO	A	216	-	-	1/1/1/1	-
5	EDO	B	207	-	-	1/1/1/1	-
11	ETX	A	251	-	-	2/3/3/3	-
6	GOL	C	216	-	-	2/4/4/4	-
3	PG0	A	205	-	-	3/5/5/5	-
10	PGO	A	247	-	-	2/2/2/2	-
11	ETX	A	250	-	-	2/3/3/3	-
6	GOL	A	218	-	-	4/4/4/4	-
11	ETX	B	235	-	-	1/3/3/3	-
2	PG4	B	201	-	-	5/10/10/10	-
13	PGE	B	233	-	-	3/7/7/7	-
2	PG4	D	202	-	-	1/10/10/10	-
7	PDO	C	220	-	-	2/2/2/2	-
5	EDO	D	216	-	-	1/1/1/1	-
7	PDO	D	224	-	-	1/2/2/2	-
7	PDO	A	220	-	-	1/2/2/2	-
4	PEG	A	208	-	-	3/4/4/4	-
7	PDO	D	223	-	-	1/2/2/2	-
10	PGO	A	248	-	-	2/2/2/2	-
12	ETE	C	208	-	-	6/11/11/11	-
4	PEG	B	203	-	-	3/4/4/4	-
7	PDO	A	222	-	-	2/2/2/2	-
5	EDO	C	212	-	-	1/1/1/1	-
5	EDO	C	210	-	-	1/1/1/1	-
6	GOL	C	218	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PG0	C	202	-	-	4/5/5/5	-
3	PG0	A	206	-	-	2/5/5/5	-
5	EDO	A	215	-	-	0/1/1/1	-
2	PG4	A	202	-	-	7/10/10/10	-
5	EDO	D	215	-	-	1/1/1/1	-
7	PDO	A	223	-	-	1/2/2/2	-
4	PEG	C	203	-	-	1/4/4/4	-
10	PGO	B	230	-	1/1/1/1	1/2/2/2	-
5	EDO	B	209	-	-	1/1/1/1	-
13	PGE	D	248	-	-	6/7/7/7	-
3	PG0	C	201	-	-	0/5/5/5	-
3	PG0	A	204	-	-	4/5/5/5	-
10	PGO	A	249	-	-	2/2/2/2	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	230	PGO	O2-C2	-5.84	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
2	D	201	PG4	O4-C6	-2.36	1.31	1.42
3	A	206	PG0	O1-C3	-2.35	1.31	1.42
10	D	247	PGO	O1-C1	-2.35	1.32	1.42
13	C	241	PGE	O1-C1	-2.34	1.30	1.42
2	D	201	PG4	O3-C5	-2.31	1.32	1.42
13	C	241	PGE	O2-C2	-2.19	1.32	1.42
5	C	215	EDO	O1-C1	-2.05	1.31	1.42
5	D	218	EDO	O1-C1	-2.04	1.31	1.42

All (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
3	C	201	PG0	O1-C2-C1	3.39	125.04	110.11
7	A	219	PDO	O3-C3-C2	-3.33	90.31	111.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	201	PG4	C5-O3-C4	-3.31	98.79	113.26
2	B	201	PG4	O4-C7-C8	3.21	124.27	110.11
6	A	218	GOL	O2-C2-C3	-3.18	96.01	109.18
6	C	219	GOL	O2-C2-C3	3.14	122.20	109.18
6	C	218	GOL	O3-C3-C2	-3.14	96.26	110.38
4	C	205	PEG	C3-O2-C2	3.06	126.66	113.26
6	C	219	GOL	O3-C3-C2	3.02	123.95	110.38
13	C	241	PGE	O2-C2-C1	3.00	123.33	110.11
4	C	205	PEG	O2-C3-C4	-2.98	96.98	110.11
10	A	249	PGO	O1-C1-C2	2.95	130.16	114.54
12	B	205	ETE	C23-OH3-C22	2.90	125.94	113.26
3	A	206	PG0	O1-C2-C1	2.86	122.71	110.11
12	B	205	ETE	OH5-C14-C24	2.75	122.89	110.35
3	A	206	PG0	C2-O1-C3	2.73	125.19	113.26
6	A	218	GOL	O2-C2-C1	2.73	120.46	109.18
15	D	210	P6G	O7-C8-C9	2.68	122.59	110.35
11	A	251	ETX	O1-C1-C2	-2.61	96.48	111.82
4	A	207	PEG	O2-C3-C4	2.58	121.48	110.11
4	C	205	PEG	O1-C1-C2	-2.57	96.71	111.82
3	A	205	PG0	OTT-C1-C2	2.55	126.84	111.82
10	D	245	PGO	O2-C2-C3	-2.47	98.81	109.45
12	C	208	ETE	OH5-C14-C24	2.47	121.62	110.35
6	C	219	GOL	C3-C2-C1	-2.44	102.83	111.80
10	B	230	PGO	C3-C2-C1	2.40	120.68	110.80
11	B	236	ETX	C3-O2-C2	2.35	121.31	113.06
3	A	206	PG0	O1-C3-C4	-2.34	99.70	110.35
15	D	210	P6G	C14-O13-C12	-2.31	103.14	113.26
10	A	249	PGO	C3-C2-C1	-2.29	101.37	110.80
6	C	217	GOL	O3-C3-C2	2.28	120.64	110.38
4	B	204	PEG	O2-C3-C4	-2.26	100.16	110.11
2	A	202	PG4	O4-C6-C5	2.25	120.61	110.35
4	A	208	PEG	C3-O2-C2	2.24	123.07	113.26
15	D	210	P6G	O13-C14-C15	2.22	120.49	110.35
2	A	202	PG4	C7-O4-C6	2.19	122.83	113.26
12	C	208	ETE	OH3-C22-C12	2.16	119.63	110.11
15	D	209	P6G	O16-C17-C18	-2.15	100.64	110.11
10	D	247	PGO	C3-C2-C1	2.12	119.52	110.80
10	D	247	PGO	O2-C2-C1	-2.11	104.64	114.99
3	A	205	PG0	O1-C3-C4	2.06	119.73	110.35
12	C	208	ETE	OH4-C13-C23	-2.05	101.03	110.35
2	D	201	PG4	O2-C2-C1	2.04	119.10	110.11
6	A	218	GOL	O3-C3-C2	2.01	119.44	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	230	PGO	O2-C2-C3	2.01	118.09	109.45
2	A	202	PG4	C3-O2-C2	-2.00	104.49	113.26

All (1) chirality outliers are listed below:

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
6	C	218	GOL	C1-C2-C3-O3
6	C	218	GOL	O2-C2-C3-O3
6	C	219	GOL	O1-C1-C2-C3
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	222	PDO	O1-C1-C2-C3
7	A	223	PDO	O1-C1-C2-C3
7	A	224	PDO	O1-C1-C2-C3
7	A	224	PDO	C1-C2-C3-O3
7	A	225	PDO	O1-C1-C2-C3
7	B	212	PDO	O1-C1-C2-C3
7	B	214	PDO	O1-C1-C2-C3
7	C	220	PDO	O1-C1-C2-C3
7	D	224	PDO	O1-C1-C2-C3
10	A	247	PGO	O1-C1-C2-C3
10	A	248	PGO	O1-C1-C2-C3
10	A	248	PGO	O1-C1-C2-O2
10	B	230	PGO	O1-C1-C2-O2
10	B	232	PGO	O1-C1-C2-O2
10	D	247	PGO	O1-C1-C2-C3
2	A	202	PG4	C5-C6-O4-C7
2	B	201	PG4	C1-C2-O2-C3
13	C	239	PGE	C1-C2-O2-C3
14	C	207	P33	C17-C18-O19-C20
14	C	207	P33	C8-C9-O10-C11
13	C	240	PGE	C4-C3-O2-C2
14	C	207	P33	C18-C17-O16-C15
3	A	203	PG0	O1-C3-C4-O2

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

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Mol	Chain	Res	Type	Atoms
4	D	206	PEG	O1-C1-C2-O2
4	D	207	PEG	O1-C1-C2-O2
12	B	205	ETE	OH2-C12-C22-OH3
13	B	233	PGE	O1-C1-C2-O2
4	D	207	PEG	C4-C3-O2-C2
13	C	239	PGE	O2-C3-C4-O3
15	D	209	P6G	O4-C5-C6-O7
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	C	218	GOL	O1-C1-C2-O2
6	D	222	GOL	O2-C2-C3-O3
15	D	209	P6G	O7-C8-C9-O10
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	D	221	EDO	O1-C1-C2-O2
4	A	207	PEG	O1-C1-C2-O2
15	D	210	P6G	C11-C12-O13-C14
12	C	208	ETE	OH5-C14-C24-OH4
4	B	203	PEG	O2-C3-C4-O4
10	A	247	PGO	O1-C1-C2-O2
10	A	249	PGO	O1-C1-C2-O2
10	D	247	PGO	O1-C1-C2-O2
3	A	205	PG0	O1-C3-C4-O2
7	A	220	PDO	O1-C1-C2-C3
7	A	222	PDO	C1-C2-C3-O3
7	C	220	PDO	C1-C2-C3-O3
5	A	210	EDO	O1-C1-C2-O2
5	A	211	EDO	O1-C1-C2-O2
5	A	216	EDO	O1-C1-C2-O2
5	B	206	EDO	O1-C1-C2-O2
5	B	208	EDO	O1-C1-C2-O2
5	C	209	EDO	O1-C1-C2-O2
5	C	210	EDO	O1-C1-C2-O2
5	C	212	EDO	O1-C1-C2-O2
5	C	215	EDO	O1-C1-C2-O2
5	D	219	EDO	O1-C1-C2-O2
2	A	201	PG4	O3-C5-C6-O4
11	D	249	ETX	C4-C3-O2-C2
11	D	249	ETX	O1-C1-C2-O2
15	D	209	P6G	O1-C2-C3-O4

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Mol	Chain	Res	Type	Atoms
6	C	219	GOL	O2-C2-C3-O3
4	C	205	PEG	C1-C2-O2-C3
3	C	202	PG0	OTT-C1-C2-O1
15	D	208	P6G	O16-C17-C18-O19
5	A	214	EDO	O1-C1-C2-O2
5	B	209	EDO	O1-C1-C2-O2
10	A	249	PGO	O1-C1-C2-C3
10	B	231	PGO	O1-C1-C2-C3
3	A	206	PG0	C3-C4-O2-C5
3	A	204	PG0	C3-C4-O2-C5
15	D	209	P6G	C5-C6-O7-C8
15	D	210	P6G	C8-C9-O10-C11
15	D	208	P6G	C18-C17-O16-C15
15	D	210	P6G	C9-C8-O7-C6
2	D	201	PG4	C5-C6-O4-C7
14	C	207	P33	C15-C14-O13-C12
3	A	203	PG0	C1-C2-O1-C3
4	A	208	PEG	C4-C3-O2-C2
11	B	236	ETX	C4-C3-O2-C2
12	B	205	ETE	C24-C14-OH5-C25
15	D	208	P6G	C12-C11-O10-C9
12	C	208	ETE	C13-C23-OH3-C22
15	D	210	P6G	C14-C15-O16-C17
2	D	201	PG4	O4-C7-C8-O5
4	A	207	PEG	O2-C3-C4-O4
4	C	206	PEG	O2-C3-C4-O4
13	C	241	PGE	O1-C1-C2-O2
13	C	241	PGE	O3-C5-C6-O4
15	D	210	P6G	C12-C11-O10-C9
2	A	201	PG4	C3-C4-O3-C5
11	B	234	ETX	C4-C3-O2-C2
3	C	202	PG0	C1-C2-O1-C3
11	B	234	ETX	C1-C2-O2-C3
2	A	202	PG4	C1-C2-O2-C3
3	D	204	PG0	C4-C3-O1-C2
5	D	211	EDO	O1-C1-C2-O2
14	C	207	P33	C6-C5-O4-C3
13	D	248	PGE	C1-C2-O2-C3
4	D	205	PEG	O1-C1-C2-O2
13	B	233	PGE	C3-C4-O3-C5
2	D	201	PG4	C8-C7-O4-C6
11	C	242	ETX	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
13	D	248	PGE	C4-C3-O2-C2
2	D	201	PG4	C6-C5-O3-C4
13	D	248	PGE	C3-C4-O3-C5
4	D	206	PEG	C1-C2-O2-C3
15	D	208	P6G	C11-C12-O13-C14
4	B	203	PEG	O1-C1-C2-O2
13	C	239	PGE	C4-C3-O2-C2
4	C	206	PEG	C4-C3-O2-C2
10	B	231	PGO	O1-C1-C2-O2
10	D	245	PGO	O1-C1-C2-O2
4	C	203	PEG	C4-C3-O2-C2
3	D	204	PG0	C1-C2-O1-C3
2	A	201	PG4	C1-C2-O2-C3
12	C	208	ETE	C15-C25-OH5-C14
13	C	240	PGE	C6-C5-O3-C4
13	C	239	PGE	O1-C1-C2-O2
15	D	208	P6G	C15-C14-O13-C12
15	D	209	P6G	C8-C9-O10-C11
11	C	242	ETX	O1-C1-C2-O2
2	A	202	PG4	C4-C3-O2-C2
3	D	203	PG0	C4-C3-O1-C2
2	B	201	PG4	C4-C3-O2-C2
15	D	208	P6G	C2-C3-O4-C5
15	D	210	P6G	O4-C5-C6-O7
11	A	251	ETX	O1-C1-C2-O2
12	C	208	ETE	C14-C24-OH4-C13
3	D	204	PG0	C3-C4-O2-C5
3	A	204	PG0	OTT-C1-C2-O1
4	A	208	PEG	C1-C2-O2-C3
11	C	242	ETX	C1-C2-O2-C3
3	C	202	PG0	C4-C3-O1-C2
5	D	216	EDO	O1-C1-C2-O2
5	D	220	EDO	O1-C1-C2-O2
11	A	251	ETX	C1-C2-O2-C3
4	A	207	PEG	C4-C3-O2-C2
2	B	201	PG4	C5-C6-O4-C7
4	B	203	PEG	C4-C3-O2-C2
12	B	205	ETE	C25-C15-OH6-C26
3	A	205	PG0	OTT-C1-C2-O1
13	D	248	PGE	C6-C5-O3-C4
6	C	217	GOL	O1-C1-C2-C3
3	A	205	PG0	C3-C4-O2-C5

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Mol	Chain	Res	Type	Atoms
5	B	207	EDO	O1-C1-C2-O2
6	D	222	GOL	O1-C1-C2-O2
10	B	232	PGO	O1-C1-C2-C3
13	C	241	PGE	C6-C5-O3-C4
14	C	207	P33	C12-C11-O10-C9
7	B	213	PDO	C1-C2-C3-O3
7	C	221	PDO	C1-C2-C3-O3
7	D	223	PDO	O1-C1-C2-C3
11	A	250	ETX	C4-C3-O2-C2
11	A	250	ETX	C1-C2-O2-C3
5	A	213	EDO	O1-C1-C2-O2
5	D	212	EDO	O1-C1-C2-O2
12	B	205	ETE	C15-C25-OH5-C14
3	A	203	PG0	C3-C4-O2-C5
4	D	206	PEG	C4-C3-O2-C2
6	C	217	GOL	O1-C1-C2-O2
5	C	213	EDO	O1-C1-C2-O2
5	D	215	EDO	O1-C1-C2-O2
5	D	218	EDO	O1-C1-C2-O2
2	A	202	PG4	C3-C4-O3-C5
4	D	207	PEG	C1-C2-O2-C3
11	D	250	ETX	C4-C3-O2-C2
2	D	202	PG4	O4-C7-C8-O5
12	C	208	ETE	C25-C15-OH6-C26
4	C	204	PEG	C1-C2-O2-C3
4	D	205	PEG	C4-C3-O2-C2
3	A	204	PG0	C1-C2-O1-C3
13	D	248	PGE	O2-C3-C4-O3
11	B	235	ETX	C4-C3-O2-C2
15	D	210	P6G	C15-C14-O13-C12
4	A	207	PEG	C1-C2-O2-C3
2	B	201	PG4	O2-C3-C4-O3
12	B	205	ETE	C12-C22-OH3-C23
15	D	210	P6G	C18-C17-O16-C15
15	D	208	P6G	C5-C6-O7-C8
5	B	210	EDO	O1-C1-C2-O2
2	A	202	PG4	C8-C7-O4-C6
3	A	204	PG0	O1-C3-C4-O2

There are no ring outliers.

85 monomers are involved in 213 short contacts:

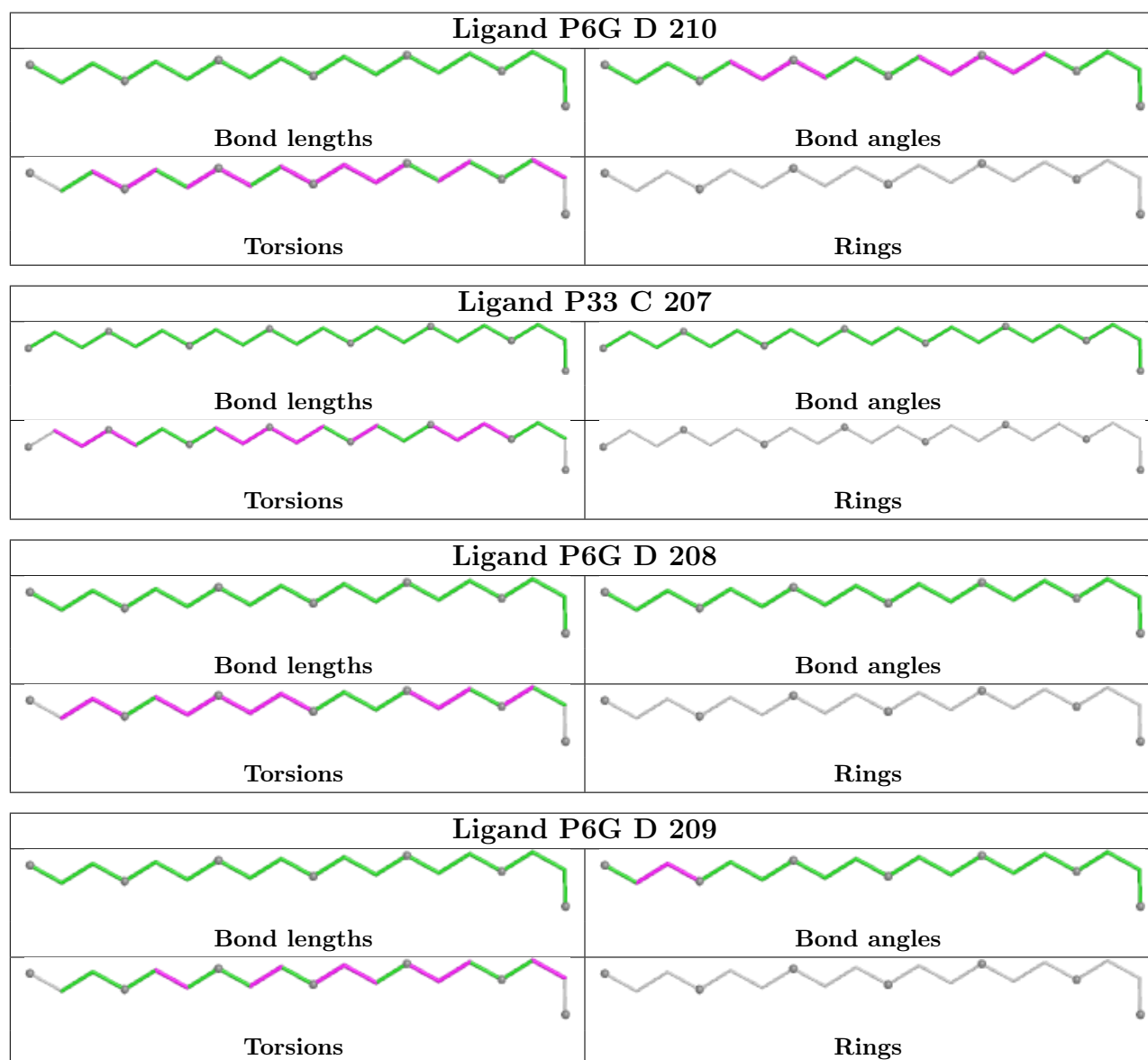
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	203	PG0	3	0
13	C	240	PGE	1	0
7	C	221	PDO	1	0
4	C	204	PEG	1	0
10	D	245	PGO	4	0
8	C	224	EOH	1	0
4	C	205	PEG	4	0
11	B	234	ETX	2	0
6	C	217	GOL	1	0
15	D	210	P6G	5	0
3	D	204	PG0	5	0
4	A	207	PEG	4	0
2	D	201	PG4	4	0
5	A	209	EDO	2	0
9	D	237	MOH	1	0
8	D	230	EOH	11	0
3	D	203	PG0	4	0
5	D	220	EDO	1	0
5	A	214	EDO	1	0
11	B	236	ETX	1	0
4	D	205	PEG	6	0
5	A	210	EDO	1	0
8	A	236	EOH	2	0
7	B	212	PDO	1	0
4	D	206	PEG	6	0
11	D	250	ETX	6	0
5	C	215	EDO	1	0
5	B	206	EDO	1	0
5	C	214	EDO	1	0
11	D	249	ETX	12	0
8	A	231	EOH	1	0
8	A	230	EOH	1	0
8	C	225	EOH	4	0
8	B	220	EOH	2	0
14	C	207	P33	14	0
12	B	205	ETE	4	0
5	D	212	EDO	2	0
3	B	202	PG0	2	0
8	C	226	EOH	3	0
5	A	212	EDO	1	0
8	A	226	EOH	2	0
7	A	219	PDO	3	0
6	D	222	GOL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	D	208	P6G	2	0
13	C	239	PGE	5	0
6	C	219	GOL	1	0
13	C	241	PGE	2	0
15	D	209	P6G	15	0
5	C	209	EDO	1	0
10	D	246	PGO	5	0
8	B	217	EOH	2	0
7	A	221	PDO	7	0
5	A	216	EDO	2	0
5	B	207	EDO	3	0
8	A	232	EOH	1	0
8	C	227	EOH	1	0
3	A	205	PG0	1	0
10	A	247	PGO	10	0
9	D	239	MOH	1	0
11	A	250	ETX	8	0
2	B	201	PG4	2	0
13	B	233	PGE	3	0
2	D	202	PG4	9	0
7	D	224	PDO	11	0
7	A	220	PDO	2	0
8	D	225	EOH	1	0
12	C	208	ETE	1	0
7	A	222	PDO	1	0
8	B	223	EOH	2	0
5	C	212	EDO	2	0
5	C	210	EDO	1	0
3	C	202	PG0	5	0
3	A	206	PG0	5	0
2	A	202	PG4	1	0
8	C	222	EOH	1	0
4	C	203	PEG	8	0
8	B	226	EOH	1	0
9	B	229	MOH	2	0
5	B	209	EDO	1	0
10	B	230	PGO	2	0
13	D	248	PGE	1	0
3	C	201	PG0	3	0
8	C	231	EOH	1	0
3	A	204	PG0	7	0
10	A	249	PGO	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	0.50	11 (6%) 25 27	23, 38, 71, 84	0
1	B	161/176 (91%)	0.38	5 (3%) 51 53	22, 38, 62, 76	0
1	C	161/176 (91%)	0.29	9 (5%) 31 33	21, 33, 56, 83	1 (0%)
1	D	166/176 (94%)	0.39	10 (6%) 29 31	21, 36, 63, 91	1 (0%)
All	All	653/704 (92%)	0.39	35 (5%) 32 35	21, 36, 64, 91	2 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	29	THR	5.2
1	A	2	ALA	4.1
1	D	166	ILE	3.2
1	D	4	THR	3.2
1	A	116	ILE	3.1
1	C	32	THR	3.0
1	C	28	PRO	3.0
1	C	27	ILE	3.0
1	A	117	ILE	2.9
1	D	167	ILE	2.9
1	C	164	PRO	2.8
1	D	27	ILE	2.7
1	D	2	ALA	2.6
1	B	34	ALA	2.6
1	A	55	CYS	2.6
1	D	29	THR	2.6
1	B	165	PRO	2.6
1	D	31	VAL	2.5
1	C	117	ILE	2.4
1	A	166	ILE	2.4
1	B	32	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	45	LYS	2.4
1	B	37	ILE	2.4
1	D	55	CYS	2.3
1	D	162	TYR	2.3
1	C	4	THR	2.3
1	A	28	PRO	2.3
1	C	31	VAL	2.2
1	A	29	THR	2.2
1	A	85	ILE	2.1
1	D	132	GLY	2.1
1	A	31	VAL	2.1
1	B	4	THR	2.1
1	A	25	HIS	2.0
1	A	27	ILE	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 monosaccharides 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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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
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

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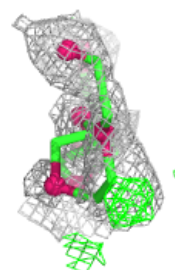
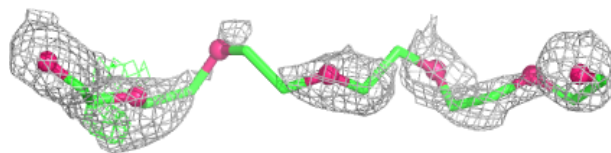
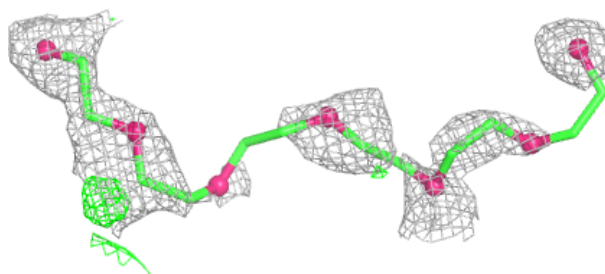
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	EOH	D	225	3/3	0.90	0.09	33,33,35,42	0
5	EDO	D	212	4/4	0.91	0.09	41,43,43,44	0

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.

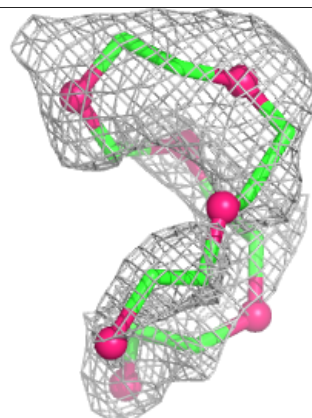
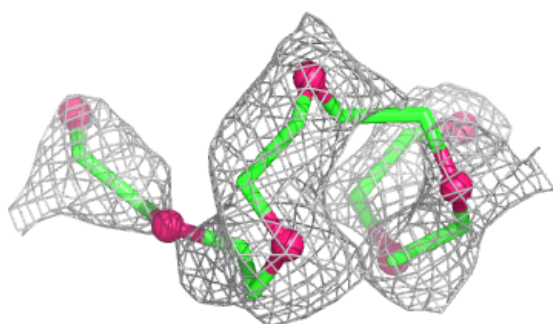
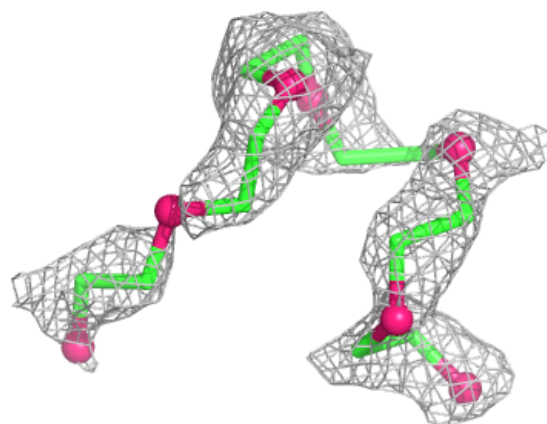
Electron density around P6G D 210:

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

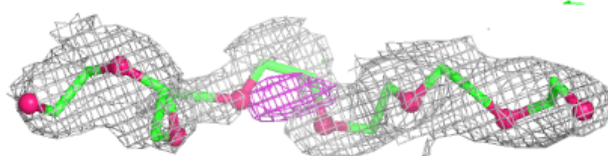
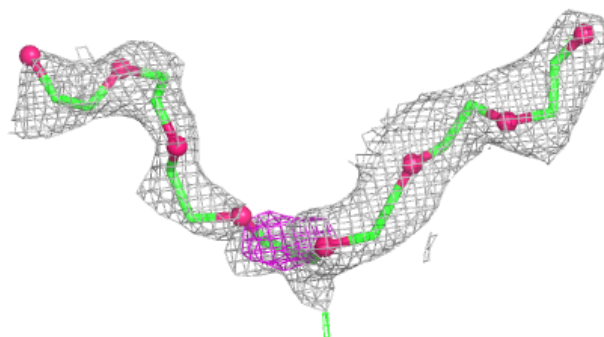


Electron density around P6G D 209:

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

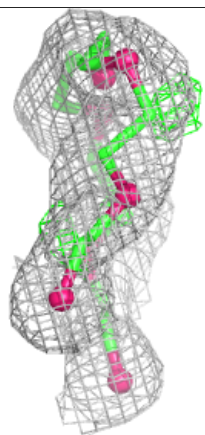
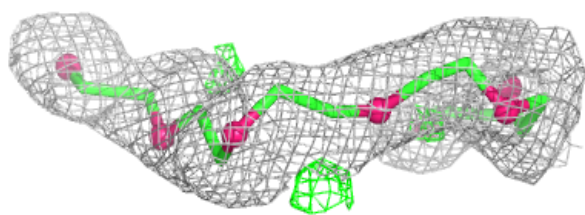
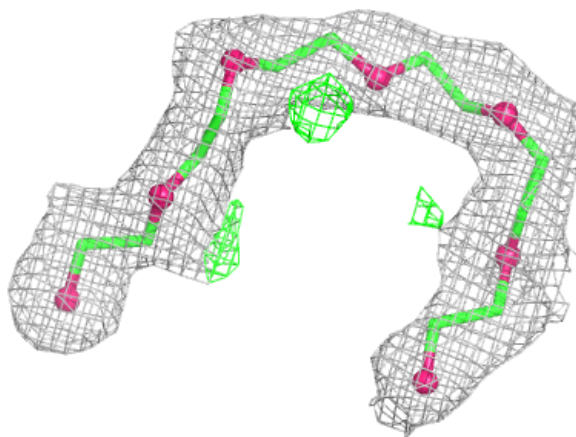
**Electron density around P33 C 207:**

$2mF_o-DF_c$ (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.