



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:02 PM UTC

PDB ID : 8VRI / pdb_00008vri
Title : E. coli peptidyl-prolyl cis-trans isomerase containing difluoro-leucines
Authors : Frkic, R.L.; Jackson, C.J.
Deposited on : 2024-01-22
Resolution : 1.65 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

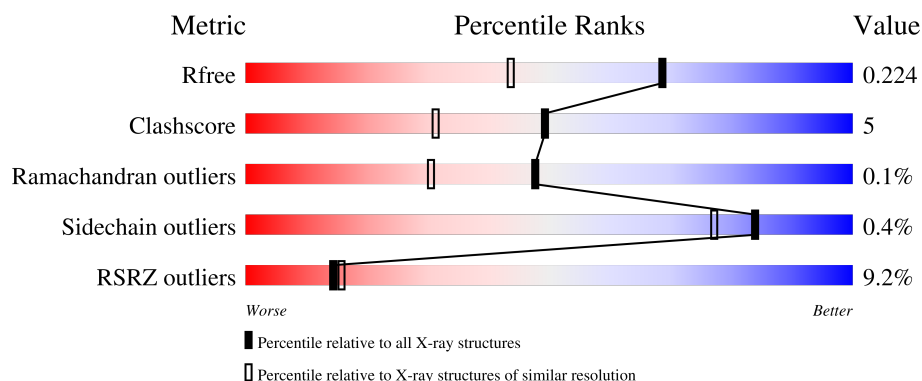
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	170	0% 90% 9% .
1	B	170	0% 88% 12% .
2	C	170	2% 88% 8% ..
2	D	170	2% 84% 12% .
2	E	170	39% 86% 9% ..

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
5	EDO	D	207	-	-	X	-
6	PG4	B	204	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7798 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 Peptidyl-prolyl cis-trans isomerase B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	170	Total	C	F	N	O	S	0	11	0
			1445	901	12	253	271	8			
1	B	170	Total	C	F	N	O	S	0	9	0
			1422	889	12	247	266	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	165	HIS	-	expression tag	UNP P23869
A	166	HIS	-	expression tag	UNP P23869
A	167	HIS	-	expression tag	UNP P23869
A	168	HIS	-	expression tag	UNP P23869
A	169	HIS	-	expression tag	UNP P23869
A	170	HIS	-	expression tag	UNP P23869
B	165	HIS	-	expression tag	UNP P23869
B	166	HIS	-	expression tag	UNP P23869
B	167	HIS	-	expression tag	UNP P23869
B	168	HIS	-	expression tag	UNP P23869
B	169	HIS	-	expression tag	UNP P23869
B	170	HIS	-	expression tag	UNP P23869

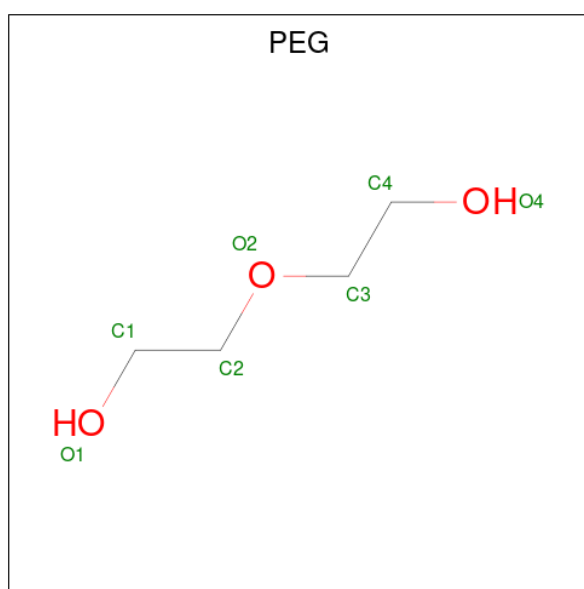
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	164	Total	C	F	N	O	S	0	4	0
			1318	823	10	226	250	9			
2	D	164	Total	C	F	N	O	S	0	3	0
			1310	819	10	222	250	9			
2	E	163	Total	C	F	N	O	S	0	0	0
			1273	796	10	218	242	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	165	HIS	-	expression tag	UNP P23869
C	166	HIS	-	expression tag	UNP P23869
C	167	HIS	-	expression tag	UNP P23869
C	168	HIS	-	expression tag	UNP P23869
C	169	HIS	-	expression tag	UNP P23869
C	170	HIS	-	expression tag	UNP P23869
D	165	HIS	-	expression tag	UNP P23869
D	166	HIS	-	expression tag	UNP P23869
D	167	HIS	-	expression tag	UNP P23869
D	168	HIS	-	expression tag	UNP P23869
D	169	HIS	-	expression tag	UNP P23869
D	170	HIS	-	expression tag	UNP P23869
E	165	HIS	-	expression tag	UNP P23869
E	166	HIS	-	expression tag	UNP P23869
E	167	HIS	-	expression tag	UNP P23869
E	168	HIS	-	expression tag	UNP P23869
E	169	HIS	-	expression tag	UNP P23869
E	170	HIS	-	expression tag	UNP P23869

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



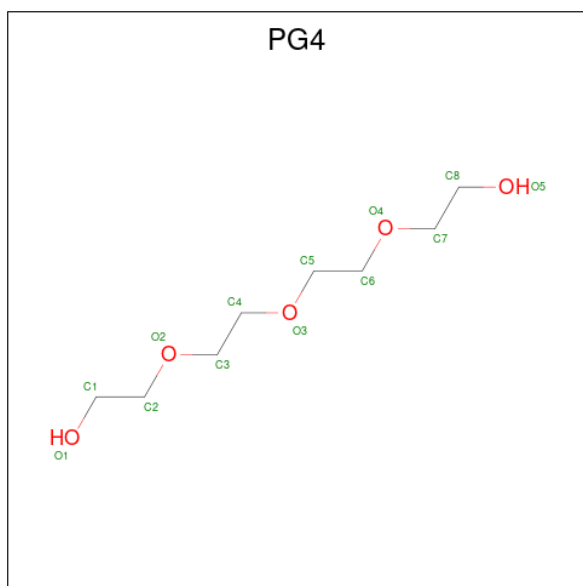
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

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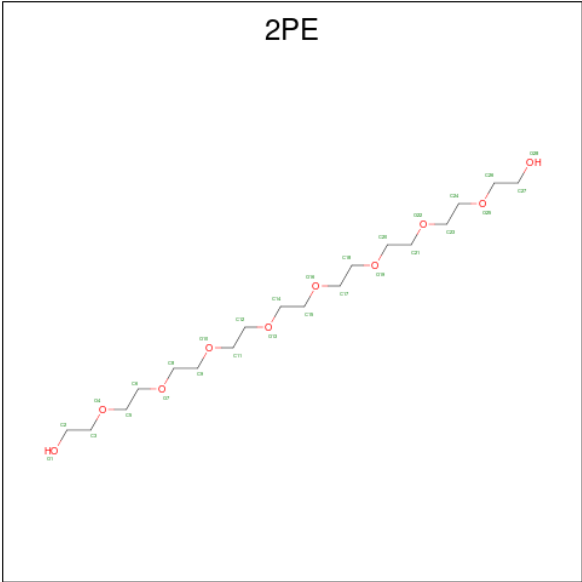
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is NONAETHYLENE GLYCOL (CCD ID: 2PE) (formula: $C_{18}H_{38}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			28	18	10		
7	D	1	Total	C	O	0	0
			28	18	10		

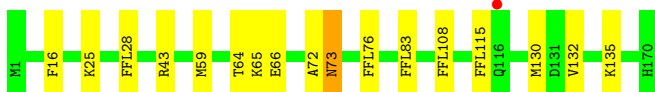
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	206	Total	O	0	0
			206	206		
8	B	199	Total	O	0	0
			199	199		
8	C	209	Total	O	0	0
			209	209		
8	D	183	Total	O	0	0
			183	183		
8	E	96	Total	O	0	0
			96	96		

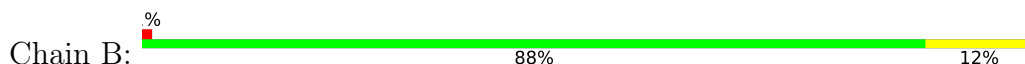
3 Residue-property plots

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.

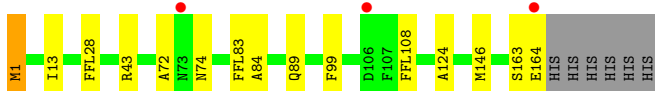
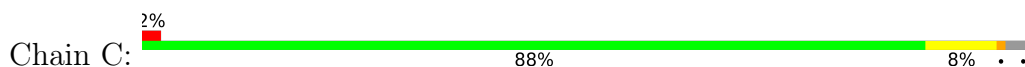
- Molecule 1: Peptidyl-prolyl cis-trans isomerase B



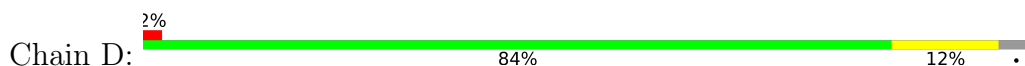
- Molecule 1: Peptidyl-prolyl cis-trans isomerase B



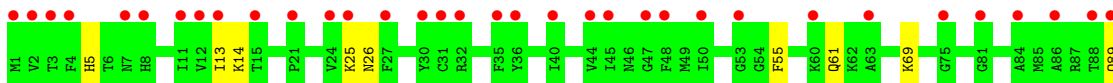
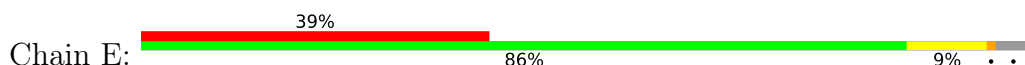
- Molecule 2: Peptidyl-prolyl cis-trans isomerase B

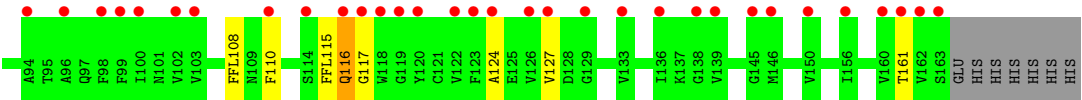


- Molecule 2: Peptidyl-prolyl cis-trans isomerase B



- Molecule 2: Peptidyl-prolyl cis-trans isomerase B





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.66Å 83.44Å 122.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.12 – 1.65 24.12 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.6 (24.12-1.65) 99.5 (24.12-1.65)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 1.65Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.183 , 0.224 0.183 , 0.224	Depositor DCC
R_{free} test set	4920 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	15.0	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7798	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% of the height of the origin peak. No significant pseudotranslation is detected.*

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: FFL, EDO, PEG, PG4, 2PE, FME, PGE

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	0.54	0/1404	0.71	0/1886
1	B	0.55	0/1387	0.70	0/1865
2	C	0.55	0/1289	0.72	0/1729
2	D	0.53	0/1281	0.73	0/1719
2	E	0.36	0/1244	0.53	0/1671
All	All	0.51	0/6605	0.68	0/8870

There are no bond length outliers.

There are no bond angle outliers.

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	1445	0	1299	14	0
1	B	1422	0	1279	15	0
2	C	1318	0	1215	10	0
2	D	1310	0	1204	16	0
2	E	1273	0	1166	10	0
3	A	7	0	10	2	0
3	B	7	0	10	0	0
4	A	10	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	4	0	6	1	0
5	B	12	0	18	2	0
5	C	4	0	6	1	0
5	D	24	0	36	6	0
6	B	13	0	18	7	0
7	C	28	0	38	5	0
7	D	28	0	38	5	0
8	A	206	0	0	4	0
8	B	199	0	0	4	0
8	C	209	0	0	2	0
8	D	183	0	0	3	0
8	E	96	0	0	0	0
All	All	7798	0	6357	72	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 5.

The worst 5 of 72 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:THR:H	3:A:201:PEG:H12	1.32	0.95
2:D:43:ARG:HH12	7:D:203:2PE:H262	1.56	0.70
1:B:103:VAL:HA	5:B:202:EDO:H21	1.75	0.69
2:E:14:LYS:HE3	2:E:127:VAL:HG11	1.74	0.69
2:C:43:ARG:HH12	7:C:201:2PE:H271	1.59	0.68

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	173/170 (102%)	164 (95%)	9 (5%)	0	100	100
1	B	171/170 (101%)	164 (96%)	7 (4%)	0	100	100
2	C	160/170 (94%)	152 (95%)	8 (5%)	0	100	100
2	D	159/170 (94%)	151 (95%)	8 (5%)	0	100	100
2	E	156/170 (92%)	146 (94%)	9 (6%)	1 (1%)	21	8
All	All	819/850 (96%)	777 (95%)	41 (5%)	1 (0%)	48	30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	116	GLN

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	148/138 (107%)	146 (99%)	2 (1%)	59	39
1	B	146/138 (106%)	146 (100%)	0	100	100
2	C	137/139 (99%)	135 (98%)	2 (2%)	57	37
2	D	136/139 (98%)	135 (99%)	1 (1%)	76	64
2	E	131/139 (94%)	131 (100%)	0	100	100
All	All	698/693 (101%)	693 (99%)	5 (1%)	84	64

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73[A]	ASN
1	A	73[B]	ASN
2	C	1[A]	MET
2	C	1[B]	MET
2	D	135	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15

such sidechains are listed below:

Mol	Chain	Res	Type
2	C	101	ASN
2	E	101	ASN
2	C	105	ASN
2	E	105	ASN
2	D	105	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

29 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FFL	E	115	2	5,9,10	0.47	0	6,10,12	2.22	3 (50%)
2	FFL	D	115	2	5,9,10	0.29	0	6,10,12	0.92	1 (16%)
2	FFL	D	28	2	5,9,10	0.81	0	6,10,12	1.32	1 (16%)
2	FFL	D	108	2	5,9,10	0.54	0	6,10,12	1.17	1 (16%)
2	FFL	E	76	2	5,9,10	0.46	0	6,10,12	0.76	0
2	FFL	C	83	2	5,9,10	0.62	0	6,10,12	1.83	1 (16%)
2	FFL	E	108	2	5,9,10	0.34	0	6,10,12	1.55	2 (33%)
2	FFL	E	83	2	5,9,10	0.37	0	6,10,12	0.82	0
2	FFL	E	28	2	5,9,10	0.35	0	6,10,12	0.89	0
1	FFL	B	108	1	5,9,10	0.31	0	6,10,12	2.25	3 (50%)
1	FFL	A	108	1	5,9,10	0.39	0	6,10,12	2.74	2 (33%)
1	FFL	A	83	1	5,9,10	0.53	0	6,10,12	1.95	1 (16%)
2	FFL	C	108	2	5,9,10	0.48	0	6,10,12	1.94	3 (50%)
1	FME	B	1	1	8,9,10	1.60	1 (12%)	8,9,11	1.32	1 (12%)
2	FFL	D	76	2	5,9,10	0.46	0	6,10,12	1.02	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FFL	B	76	1	5,9,10	0.41	0	6,10,12	2.12	1 (16%)
1	FFL	A	76	1	5,9,10	0.53	0	6,10,12	1.93	2 (33%)
1	FFL	A	28[A]	1	5,9,10	0.27	0	6,10,12	1.31	1 (16%)
1	FFL	B	28[A]	-	5,9,10	0.37	0	6,10,12	1.96	1 (16%)
1	FFL	B	83	1	5,9,10	0.79	0	6,10,12	1.39	1 (16%)
2	FFL	C	76	2	5,9,10	0.29	0	6,10,12	1.01	0
2	FFL	C	115	2	5,9,10	0.33	0	6,10,12	0.47	0
1	FFL	A	28[B]	1	5,9,10	0.35	0	6,10,12	1.68	2 (33%)
1	FME	A	1	1	8,9,10	1.09	0	8,9,11	0.83	0
1	FFL	B	28[B]	-	5,9,10	0.37	0	6,10,12	1.39	1 (16%)
1	FFL	B	115	1	5,9,10	0.37	0	6,10,12	1.03	0
2	FFL	C	28	2	5,9,10	0.48	0	6,10,12	1.48	2 (33%)
2	FFL	D	83	2	5,9,10	0.42	0	6,10,12	1.61	1 (16%)
1	FFL	A	115	1	5,9,10	0.38	0	6,10,12	3.55	1 (16%)

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
2	FFL	E	115	2	-	6/9/10/12	-
2	FFL	D	115	2	-	6/9/10/12	-
2	FFL	D	28	2	-	3/9/10/12	-
2	FFL	D	108	2	-	1/9/10/12	-
2	FFL	E	76	2	-	0/9/10/12	-
2	FFL	C	83	2	-	0/9/10/12	-
2	FFL	E	108	2	-	4/9/10/12	-
2	FFL	E	83	2	-	4/9/10/12	-
2	FFL	E	28	2	-	2/9/10/12	-
1	FFL	B	108	1	-	0/9/10/12	-
1	FFL	A	108	1	-	0/9/10/12	-
1	FFL	A	83	1	-	0/9/10/12	-
2	FFL	C	108	2	-	0/9/10/12	-
1	FME	B	1	1	-	2/7/9/11	-
2	FFL	D	76	2	-	2/9/10/12	-
1	FFL	B	76	1	-	1/9/10/12	-
1	FFL	A	76	1	-	2/9/10/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FFL	A	28[A]	1	-	0/9/10/12	-
1	FFL	B	28[A]	-	-	2/9/10/12	-
1	FFL	B	83	1	-	0/9/10/12	-
2	FFL	C	76	2	-	4/9/10/12	-
2	FFL	C	115	2	-	3/9/10/12	-
1	FFL	A	28[B]	1	-	0/9/10/12	-
1	FME	A	1	1	-	1/7/9/11	-
1	FFL	B	28[B]	-	-	3/9/10/12	-
1	FFL	B	115	1	-	5/9/10/12	-
2	FFL	C	28	2	-	2/9/10/12	-
2	FFL	D	83	2	-	0/9/10/12	-
1	FFL	A	115	1	-	5/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	FME	CA-N	-3.54	1.41	1.46

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	FFL	CG-CB-CA	-8.22	103.46	114.52
1	A	108	FFL	CD1-CG-CD2	-4.93	102.23	110.96
1	B	28[A]	FFL	CG-CB-CA	-4.37	108.64	114.52
1	B	76	FFL	CB-CG-CD1	-4.30	100.26	111.18
1	A	108	FFL	CB-CA-C	-3.91	104.97	110.99

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	76	FFL	F1-CD1-CG-CD2
1	A	115	FFL	CA-CB-CG-CD1
1	A	115	FFL	CA-CB-CG-CD2
1	A	115	FFL	F1-CD1-CG-CB
1	A	115	FFL	F1-CD1-CG-CD2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

17 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	EDO	D	202	-	3,3,3	0.53	0	2,2,2	0.17	0
5	EDO	D	207	-	3,3,3	0.45	0	2,2,2	0.37	0
5	EDO	D	205	-	3,3,3	0.45	0	2,2,2	0.42	0
5	EDO	B	201	-	3,3,3	0.43	0	2,2,2	0.65	0
5	EDO	A	203	-	3,3,3	0.51	0	2,2,2	0.64	0
6	PG4	B	204	-	12,12,12	0.33	0	11,11,11	1.06	1 (9%)
4	PGE	A	202	-	9,9,9	0.37	0	8,8,8	0.62	0
5	EDO	B	202	-	3,3,3	0.39	0	2,2,2	0.22	0
3	PEG	B	203	-	6,6,6	0.20	0	5,5,5	0.04	0
5	EDO	C	202	-	3,3,3	0.38	0	2,2,2	0.89	0
7	2PE	C	201	-	27,27,27	0.23	0	26,26,26	0.24	0
5	EDO	D	204	-	3,3,3	0.58	0	2,2,2	0.09	0
3	PEG	A	201	-	6,6,6	0.27	0	5,5,5	0.14	0
7	2PE	D	203	-	27,27,27	0.18	0	26,26,26	0.42	0
5	EDO	D	201	-	3,3,3	0.51	0	2,2,2	0.27	0
5	EDO	B	205	-	3,3,3	0.50	0	2,2,2	0.60	0
5	EDO	D	206	-	3,3,3	0.49	0	2,2,2	0.24	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	D	202	-	-	0/1/1/1	-
5	EDO	D	207	-	-	1/1/1/1	-
5	EDO	D	205	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	201	-	-	0/1/1/1	-
5	EDO	A	203	-	-	1/1/1/1	-
6	PG4	B	204	-	-	5/10/10/10	-
4	PGE	A	202	-	-	3/7/7/7	-
5	EDO	B	202	-	-	1/1/1/1	-
3	PEG	B	203	-	-	1/4/4/4	-
5	EDO	C	202	-	-	0/1/1/1	-
7	2PE	C	201	-	-	13/25/25/25	-
5	EDO	D	204	-	-	1/1/1/1	-
3	PEG	A	201	-	-	4/4/4/4	-
7	2PE	D	203	-	-	14/25/25/25	-
5	EDO	D	201	-	-	1/1/1/1	-
5	EDO	B	205	-	-	1/1/1/1	-
5	EDO	D	206	-	-	1/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	204	PG4	C5-O3-C4	-2.55	102.08	113.26

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	201	2PE	C24-C23-O22-C21
7	C	201	2PE	C27-C26-O25-C24
7	C	201	2PE	O7-C8-C9-O10
7	C	201	2PE	O10-C11-C12-O13
7	C	201	2PE	O22-C23-C24-O25

There are no ring outliers.

12 monomers are involved in 30 short contacts:

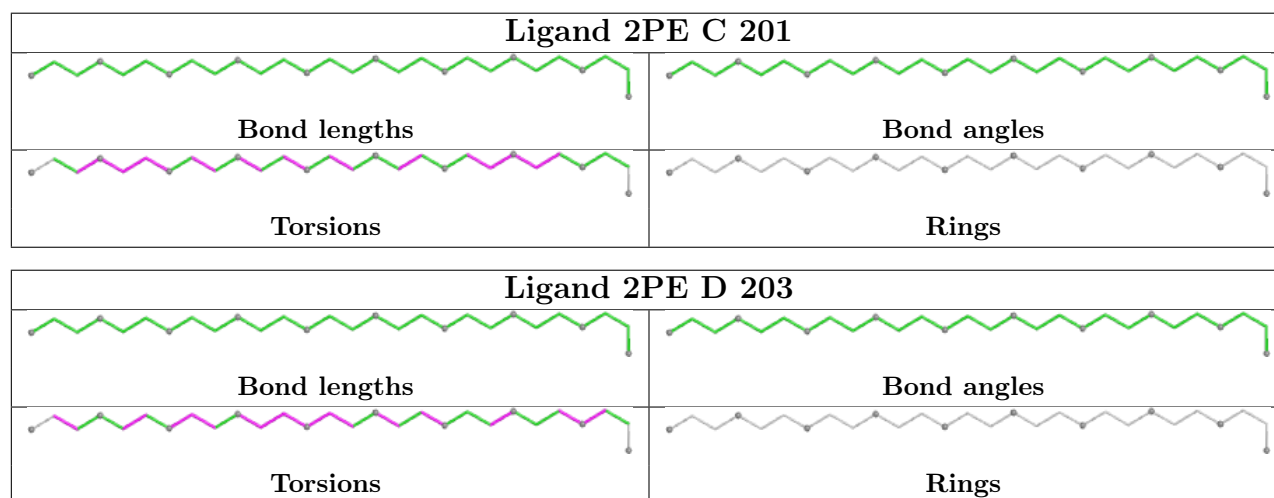
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	202	EDO	1	0
5	D	207	EDO	4	0
5	A	203	EDO	1	0
6	B	204	PG4	7	0
4	A	202	PGE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	202	EDO	1	0
5	C	202	EDO	1	0
7	C	201	2PE	5	0
3	A	201	PEG	2	0
7	D	203	2PE	5	0
5	D	201	EDO	1	0
5	B	205	EDO	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	164/170 (96%)	-0.44	1 (0%) 85 90	7, 15, 29, 53	10 (6%)
1	B	164/170 (96%)	-0.39	1 (0%) 85 90	6, 15, 34, 56	8 (4%)
2	C	159/170 (93%)	-0.39	3 (1%) 66 71	6, 16, 31, 77	4 (2%)
2	D	159/170 (93%)	-0.26	3 (1%) 66 71	8, 18, 39, 65	3 (1%)
2	E	158/170 (92%)	1.84	66 (41%) 0 0	33, 47, 63, 83	0
All	All	804/850 (94%)	0.06	74 (9%) 14 16	6, 18, 53, 83	25 (3%)

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	116	GLN	4.3
2	E	127	VAL	3.6
2	E	162	VAL	3.6
2	E	120	TYR	3.5
1	B	169	HIS	3.4

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FFL	E	115	10/11	0.39	0.28	98,103,118,119	0
2	FFL	E	28	10/11	0.75	0.15	45,51,65,67	0
1	FFL	B	115	10/11	0.76	0.17	50,57,64,78	0
2	FFL	D	115	10/11	0.77	0.14	52,64,79,81	0
2	FFL	E	76	10/11	0.81	0.13	46,50,59,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FFL	E	108	10/11	0.82	0.12	36,45,48,52	0
2	FFL	C	115	10/11	0.87	0.14	37,46,72,78	0
2	FFL	E	83	10/11	0.87	0.12	35,36,38,42	0
1	FFL	A	115	10/11	0.89	0.14	21,26,42,43	0
1	FME	B	1	10/11	0.90	0.11	14,24,31,51	0
1	FFL	B	108	10/11	0.91	0.07	12,15,23,25	0
1	FFL	A	28[A]	10/11	0.91	0.08	11,13,20,21	10
1	FFL	A	28[B]	10/11	0.91	0.08	11,13,20,22	10
2	FFL	D	76	10/11	0.92	0.09	22,28,40,47	0
2	FFL	D	108	10/11	0.92	0.09	22,27,32,42	0
1	FFL	A	108	10/11	0.93	0.07	10,13,19,23	0
2	FFL	C	76	10/11	0.94	0.08	19,21,37,39	0
2	FFL	C	108	10/11	0.94	0.07	17,21,27,40	0
1	FFL	A	76	10/11	0.94	0.07	13,14,27,27	0
2	FFL	D	28	10/11	0.94	0.09	13,20,36,36	0
1	FFL	B	76	10/11	0.94	0.08	16,20,32,34	0
2	FFL	C	28	10/11	0.94	0.09	14,15,35,36	0
1	FFL	A	83	10/11	0.95	0.06	7,10,17,20	0
2	FFL	C	83	10/11	0.96	0.06	8,10,14,19	0
1	FME	A	1	10/11	0.96	0.07	13,16,32,32	0
1	FFL	B	83	10/11	0.96	0.06	9,10,15,19	0
1	FFL	B	28[A]	10/11	0.97	0.06	12,15,24,32	7
1	FFL	B	28[B]	10/11	0.97	0.06	12,15,21,24	7
2	FFL	D	83	10/11	0.98	0.04	11,13,20,21	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	B	205	4/4	0.66	0.19	31,35,51,73	0
5	EDO	A	203	4/4	0.69	0.17	27,27,30,43	4
3	PEG	B	203	7/7	0.76	0.14	36,41,49,52	0
3	PEG	A	201	7/7	0.78	0.12	19,31,37,39	7

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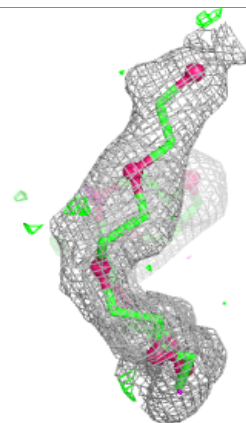
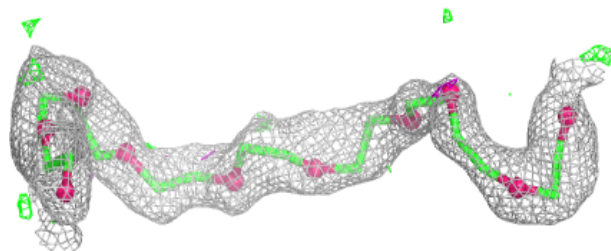
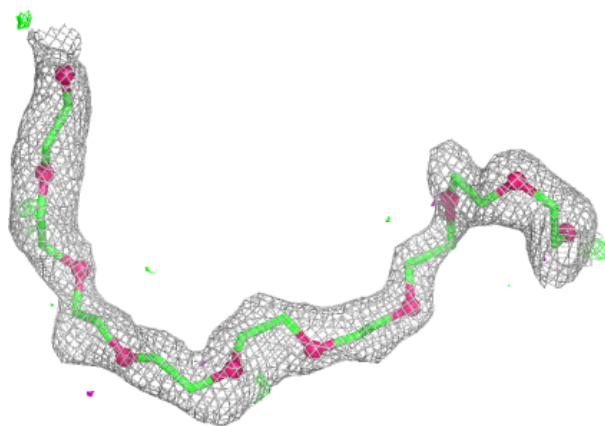
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	D	206	4/4	0.80	0.17	33,38,40,49	0
7	2PE	C	201	28/28	0.80	0.13	24,36,43,47	0
6	PG4	B	204	13/13	0.82	0.13	20,31,43,45	0
5	EDO	D	205	4/4	0.83	0.13	32,36,39,45	0
5	EDO	D	207	4/4	0.83	0.16	28,33,34,38	0
5	EDO	B	201	4/4	0.84	0.13	34,35,36,38	0
5	EDO	B	202	4/4	0.84	0.13	20,27,27,31	4
5	EDO	D	201	4/4	0.85	0.20	25,27,34,38	0
7	2PE	D	203	28/28	0.85	0.11	24,35,40,44	0
5	EDO	C	202	4/4	0.86	0.19	27,32,36,50	0
4	PGE	A	202	10/10	0.86	0.12	16,27,39,44	0
5	EDO	D	202	4/4	0.91	0.15	19,20,31,45	0
5	EDO	D	204	4/4	0.91	0.20	20,32,37,43	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.

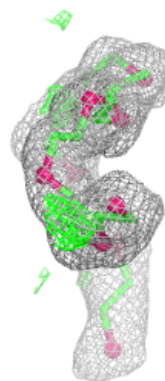
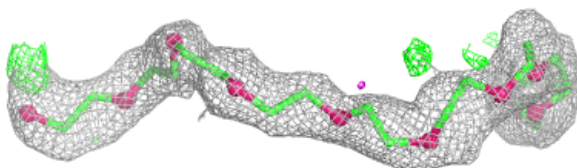
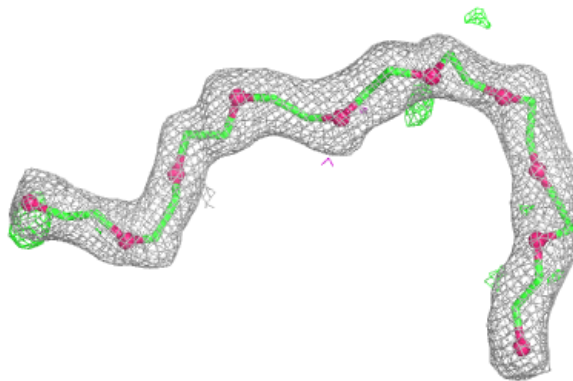
Electron density around 2PE C 201:

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 2PE D 203:

$2mF_o-DF_c$ (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.