



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 09:09 pm BST

PDB ID : 5FIP  
Title : Discovery and characterization of a novel thermostable and highly halotolerant GH5 cellulase from an Icelandic hot spring isolate  
Authors : Zarafeta, D.; Kissas, D.; Sayer, C.; Gudbergdottir, S.R.; Ladoukakis, E.; Isupov, M.N.; Chatziioannou, A.; Peng, X.; Littlechild, J.A.; Skretas, G.; Kolisis, F.N.  
Deposited on : 2015-10-01  
Resolution : 1.88 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

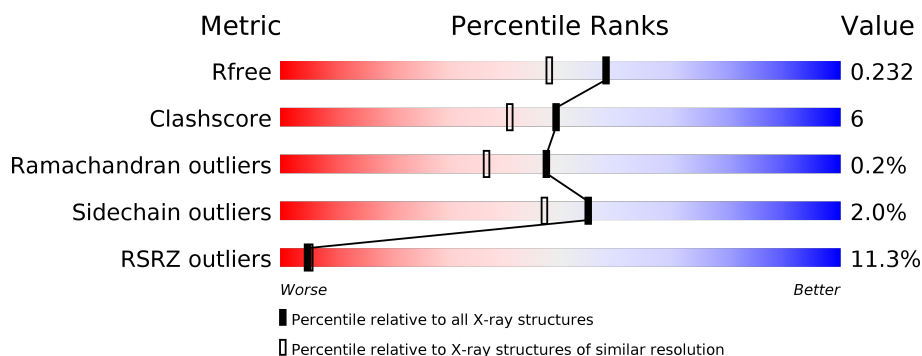
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.88 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	334	<div> <div>5%</div> <div>86%</div> <div>13%</div> <div>..</div> </div>
1	B	334	<div> <div>6%</div> <div>93%</div> <div>6%</div> <div>..</div> </div>
1	C	334	<div> <div>15%</div> <div>90%</div> <div>8%</div> <div>..</div> </div>
1	D	334	<div> <div>19%</div> <div>86%</div> <div>12%</div> <div>..</div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PEG	A	1386	-	-	X	-
5	IPA	A	1395	-	-	X	-
5	IPA	B	1394	-	-	X	-
5	IPA	B	1395	-	-	X	-
5	IPA	C	1384	-	-	X	-
5	IPA	D	1391	-	-	X	-

## 2 Entry composition [i](#)

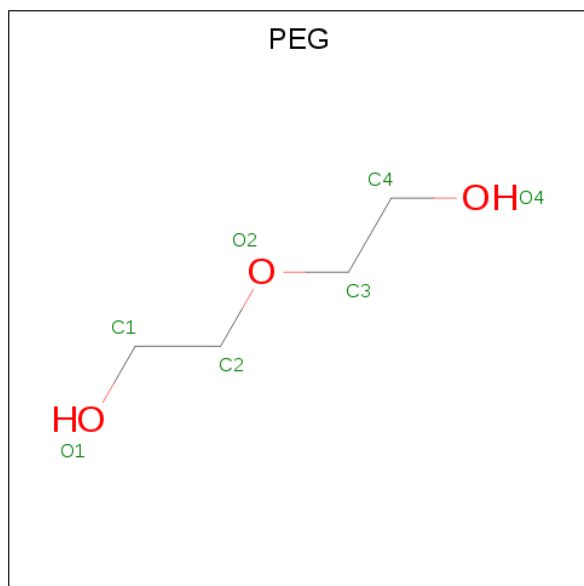
There are 9 unique types of molecules in this entry. The entry contains 11615 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GH5 CELLULASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	20	0
			2715	1736	454	516	9			
1	B	332	Total	C	N	O	S	0	19	0
			2711	1737	454	511	9			
1	C	331	Total	C	N	O	S	0	14	0
			2677	1710	449	510	8			
1	D	328	Total	C	N	O	S	0	10	0
			2648	1690	450	499	9			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



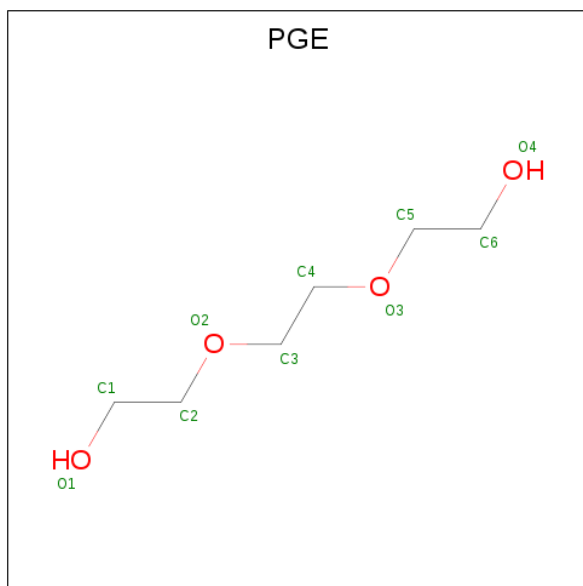
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		

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

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



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

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



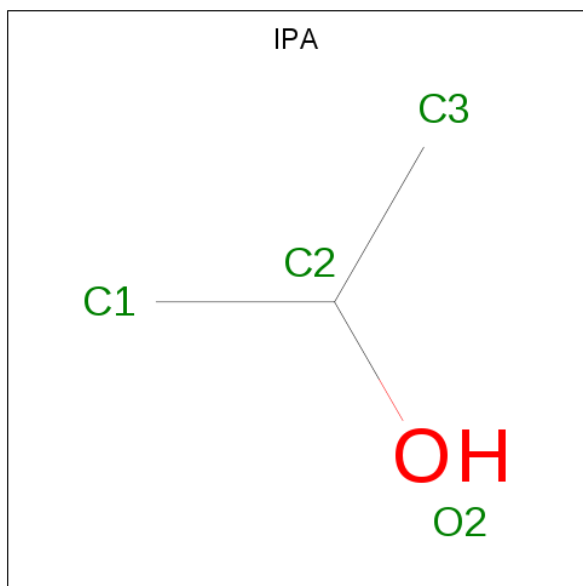
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 5 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C<sub>3</sub>H<sub>8</sub>O).



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

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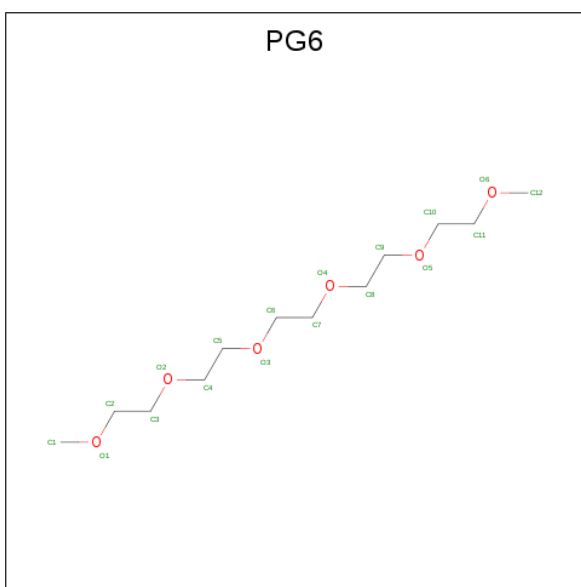
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	3	1		
5	B	1	Total	C	O	0	0
			4	3	1		
5	B	1	Total	C	O	0	0
			4	3	1		
5	B	1	Total	C	O	0	0
			4	3	1		
5	B	1	Total	C	O	0	0
			4	3	1		
5	B	1	Total	C	O	0	0
			4	3	1		
5	C	1	Total	C	O	0	0
			4	3	1		
5	D	1	Total	C	O	0	0
			4	3	1		
5	D	1	Total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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Cl	0	0
			2	2		
6	A	3	Total	Cl	0	0
			3	3		
6	D	1	Total	Cl	0	0
			1	1		
6	C	1	Total	Cl	0	0
			1	1		

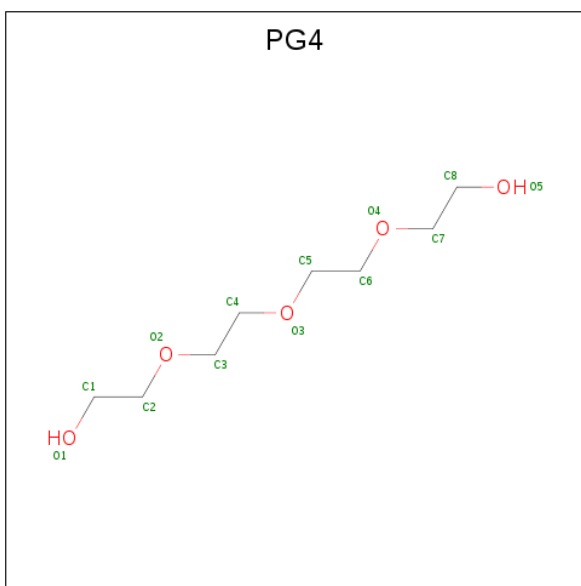
- Molecule 7 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHANE (three-letter code: PG6) (formula: C<sub>12</sub>H<sub>26</sub>O<sub>6</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			18	12	6		

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



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

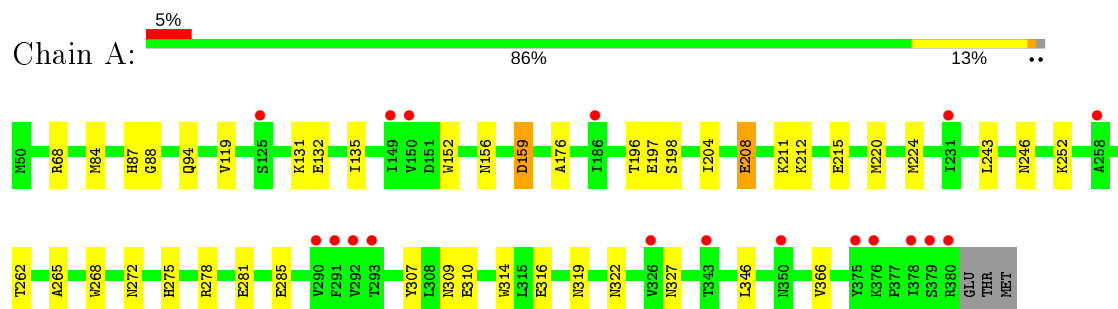
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	206	Total 206	O 206	0	0
9	B	196	Total 196	O 196	0	0
9	C	94	Total 94	O 94	0	0
9	D	89	Total 89	O 89	0	0

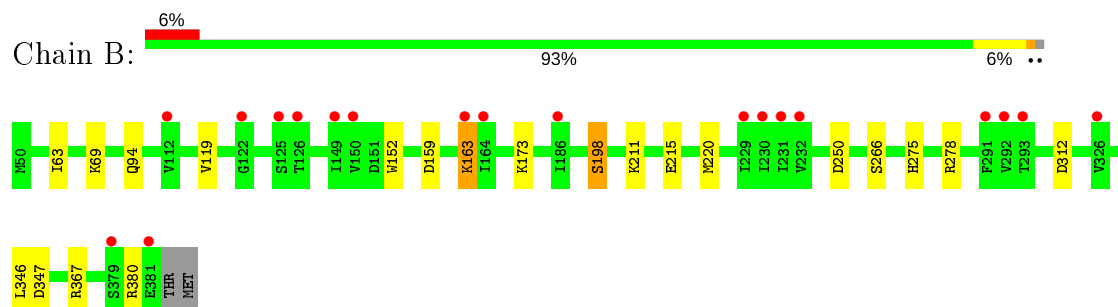
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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.

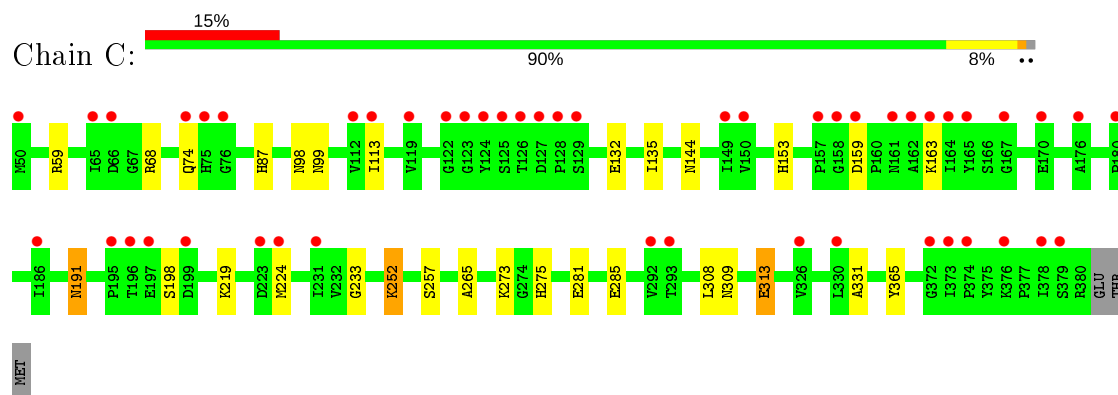
#### • Molecule 1: GH5 CELLULASE



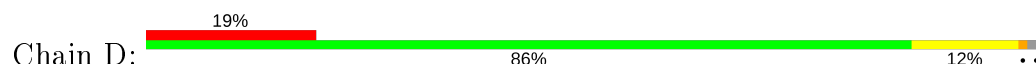
#### • Molecule 1: GH5 CELLULASE

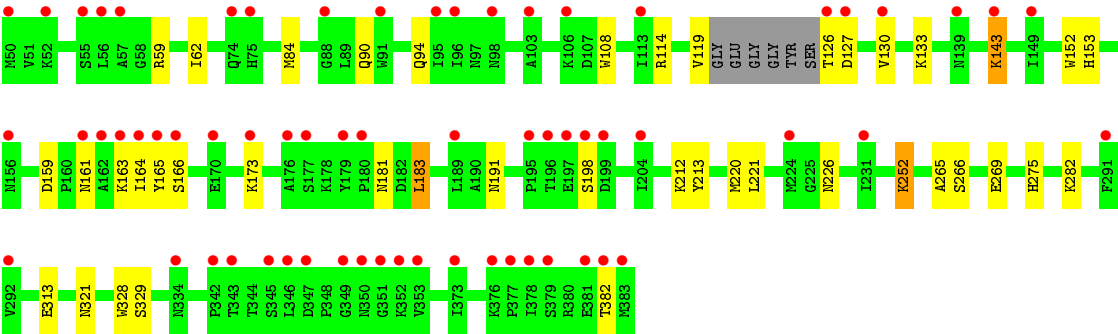


#### • Molecule 1: GH5 CELLULASE



#### • Molecule 1: GH5 CELLULASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.34Å 137.45Å 121.34Å 90.00° 114.44° 90.00°	Depositor
Resolution (Å)	36.38 – 1.88 36.38 – 1.88	Depositor EDS
% Data completeness (in resolution range)	97.4 (36.38-1.88) 97.4 (36.38-1.88)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, $R_{free}$	0.193 , 0.234 0.192 , 0.232	Depositor DCC
$R_{free}$ test set	6406 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.3	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 62.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11615	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, CL, EDO, PG6, PG4, IPA, PEG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.68	1/2841 (0.0%)	0.73	1/3855 (0.0%)
1	B	0.69	0/2833	0.74	5/3843 (0.1%)
1	C	0.55	0/2784	0.71	0/3781
1	D	0.57	0/2742	0.69	1/3720 (0.0%)
All	All	0.62	1/11200 (0.0%)	0.72	7/15199 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	GLU	CD-OE2	-5.18	1.20	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	312	ASP	CB-CG-OD1	6.58	124.22	118.30
1	B	278	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	B	278	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	B	347	ASP	CB-CG-OD1	5.86	123.57	118.30
1	A	159	ASP	CB-CG-OD1	5.70	123.43	118.30
1	B	380	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	D	183	LEU	CA-CB-CG	5.15	127.14	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2715	0	2706	50	0
1	B	2711	0	2722	16	0
1	C	2677	0	2656	22	0
1	D	2648	0	2630	33	0
2	A	49	0	70	14	0
2	B	14	0	20	1	0
2	C	7	0	10	0	0
2	D	7	0	10	0	0
3	A	20	0	28	4	0
3	B	10	0	14	0	0
3	C	10	0	14	1	0
4	A	16	0	24	0	0
4	B	32	0	48	0	0
4	C	4	0	6	0	0
4	D	20	0	30	0	0
5	A	8	0	16	6	0
5	B	24	0	48	10	0
5	C	4	0	8	5	0
5	D	16	0	32	13	0
6	A	3	0	0	1	0
6	B	2	0	0	1	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	B	18	0	26	3	0
8	D	13	0	18	0	0
9	A	206	0	0	14	0
9	B	196	0	0	4	0
9	C	94	0	0	2	0
9	D	89	0	0	3	0
All	All	11615	0	11136	130	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 6.

All (130) 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:132[A]:GLU:OE1	9:A:2075:HOH:O	1.59	1.18
9:A:2023:HOH:O	1:C:313[B]:GLU:OE1	1.62	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309[B]:ASN:OD1	9:C:2074:HOH:O	1.62	1.16
1:A:132[A]:GLU:CD	9:A:2075:HOH:O	1.80	1.15
1:A:197[B]:GLU:OE2	6:A:1397:CL:CL	2.13	1.04
1:D:159:ASP:HB2	1:D:198:SER:HB2	1.45	0.97
1:A:132[A]:GLU:OE2	9:A:2075:HOH:O	1.81	0.91
1:A:268:TRP:HE1	2:A:1387:PEG:H31	1.35	0.90
1:D:59[B]:ARG:HE	1:D:183:LEU:HA	1.38	0.86
1:D:282[B]:LYS:NZ	9:D:2043:HOH:O	1.95	0.86
1:C:265:ALA:HA	5:C:1384:IPA:H11	1.59	0.85
1:A:84[B]:MET:CE	1:A:366:VAL:HG11	2.07	0.84
1:A:319:ASN:HD22	2:A:1384:PEG:H11	1.45	0.81
1:A:252:LYS:HE3	2:A:1381:PEG:H11	1.63	0.81
1:A:275:HIS:H	5:A:1395:IPA:H12	1.47	0.78
2:A:1382:PEG:C2	9:A:2120:HOH:O	2.33	0.76
1:B:159:ASP:HB2	1:B:198:SER:HB2	1.65	0.76
1:B:211:LYS:NZ	5:B:1395:IPA:H31	2.00	0.75
1:A:159:ASP:HB2	1:A:198:SER:HB2	1.69	0.74
1:A:252:LYS:H	2:A:1381:PEG:H42	1.51	0.74
1:A:68:ARG:HD3	3:A:1389:PGE:H42	1.70	0.74
1:D:275[A]:HIS:H	5:D:1391:IPA:H33	1.54	0.72
1:C:159:ASP:HB2	1:C:198:SER:HB2	1.72	0.72
1:A:84[B]:MET:HE1	1:A:366:VAL:HG11	1.72	0.71
1:D:275[B]:HIS:H	5:D:1391:IPA:H33	1.55	0.71
1:D:275[B]:HIS:H	5:D:1391:IPA:C3	2.05	0.69
1:D:275[A]:HIS:H	5:D:1391:IPA:C3	2.05	0.69
1:A:84[B]:MET:CE	1:A:366:VAL:CG1	2.72	0.67
1:B:250:ASP:HB2	5:B:1395:IPA:H11	1.79	0.65
1:B:367:ARG:HH12	5:B:1397:IPA:H12	1.61	0.65
1:D:282[B]:LYS:CE	9:D:2043:HOH:O	2.38	0.64
1:D:321:ASN:HD21	5:D:1393:IPA:H33	1.62	0.63
1:D:265:ALA:HA	5:D:1391:IPA:H11	1.79	0.63
1:D:161:ASN:OD1	1:D:213:TYR:HB2	1.99	0.61
1:A:94[A]:GLN:HG2	1:A:346:LEU:HD12	1.81	0.60
1:A:275:HIS:H	5:A:1395:IPA:C1	2.14	0.60
1:A:309[B]:ASN:HB3	2:A:1386:PEG:H41	1.82	0.60
1:B:211:LYS:HZ1	5:B:1395:IPA:H31	1.64	0.60
1:A:84[B]:MET:HE2	1:A:327:ASN:HB3	1.84	0.60
1:A:87:HIS:CD2	1:A:88:GLY:H	2.20	0.60
1:A:307:TYR:HB3	2:A:1386:PEG:H42	1.84	0.60
2:A:1382:PEG:H22	9:A:2120:HOH:O	2.01	0.59
7:B:1393:PG6:H81	1:D:313:GLU:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59[B]:ARG:NH1	1:D:181:ASN:OD1	2.36	0.59
1:C:275:HIS:H	5:C:1384:IPA:H33	1.68	0.58
2:A:1382:PEG:H21	9:A:2120:HOH:O	1.99	0.57
5:B:1394:IPA:H33	9:B:2139:HOH:O	2.05	0.56
1:A:68:ARG:HB3	3:A:1389:PGE:H22	1.86	0.56
1:A:156[B]:ASN:ND2	9:A:2088:HOH:O	1.58	0.56
1:D:119:VAL:HB	1:D:165:TYR:HE1	1.72	0.55
1:A:322:ASN:HB2	3:A:1389:PGE:H62	1.88	0.54
1:B:275:HIS:H	5:B:1394:IPA:H12	1.73	0.54
1:D:119:VAL:HB	1:D:165:TYR:CE1	2.43	0.54
1:A:272:ASN:HB3	1:A:278[B]:ARG:NH2	2.23	0.54
5:A:1395:IPA:H33	9:A:2150:HOH:O	2.07	0.54
1:A:272:ASN:HB3	1:A:278[B]:ARG:HH22	1.72	0.54
1:B:94[B]:GLN:HG2	1:B:346:LEU:HD12	1.90	0.53
1:D:275[A]:HIS:HB2	5:D:1391:IPA:H31	1.90	0.53
1:D:59[B]:ARG:NE	1:D:183:LEU:HA	2.17	0.53
1:A:310[B]:GLU:H	2:A:1386:PEG:H41	1.74	0.52
1:C:275:HIS:HD2	5:C:1384:IPA:H31	1.74	0.52
1:C:233:GLY:HA2	1:C:257[B]:SER:OG	2.10	0.52
1:A:310[A]:GLU:H	2:A:1386:PEG:H41	1.75	0.51
1:B:211:LYS:O	1:B:215:GLU:HG3	2.10	0.51
1:A:131[A]:LYS:HE2	1:A:135:ILE:HD11	1.92	0.51
1:A:84[B]:MET:HE2	1:A:366:VAL:HG11	1.90	0.51
1:D:143:LYS:HE3	1:D:143:LYS:HA	1.92	0.50
1:A:204[B]:ILE:HD13	1:A:243:LEU:HD22	1.93	0.50
7:B:1393:PG6:H42	9:B:2024:HOH:O	2.11	0.50
1:B:275:HIS:H	5:B:1394:IPA:C1	2.25	0.50
9:A:2023:HOH:O	1:C:313[B]:GLU:CD	2.31	0.50
1:A:220:MET:SD	1:A:224:MET:HE2	2.52	0.49
1:A:204[B]:ILE:HD11	1:A:246:ASN:OD1	2.12	0.49
1:B:250:ASP:CB	5:B:1395:IPA:H11	2.42	0.49
1:B:211:LYS:HZ3	5:B:1395:IPA:H31	1.74	0.49
1:D:321:ASN:HD21	5:D:1393:IPA:C3	2.23	0.49
1:D:282[B]:LYS:HE3	5:D:1392:IPA:H11	1.95	0.49
3:A:1388:PGE:H3	9:A:2165:HOH:O	2.13	0.49
1:C:275:HIS:H	5:C:1384:IPA:C3	2.25	0.49
1:D:127:ASP:O	1:D:130:VAL:HG22	2.13	0.48
1:D:269:GLU:OE2	5:D:1391:IPA:H32	2.13	0.48
1:D:282[A]:LYS:NZ	5:D:1394:IPA:H11	2.29	0.48
2:B:1382:PEG:H42	2:B:1383:PEG:H21	1.95	0.48
1:C:275:HIS:CD2	5:C:1384:IPA:H31	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ALA:HB3	1:A:224:MET:HE3	1.96	0.47
1:A:156[B]:ASN:HD22	1:A:196:THR:HG21	1.79	0.47
1:A:211:LYS:O	1:A:215:GLU:HG3	2.16	0.46
1:A:281:GLU:HG2	1:C:285:GLU:OE2	2.15	0.46
7:B:1393:PG6:H92	9:B:2024:HOH:O	2.14	0.46
1:A:285:GLU:OE2	1:C:281:GLU:HG2	2.16	0.46
1:A:87:HIS:HD2	1:A:88:GLY:H	1.61	0.46
1:C:99:ASN:ND2	9:C:2027:HOH:O	2.41	0.46
1:C:308:LEU:HD22	1:C:365:TYR:CG	2.52	0.45
1:D:266:SER:H	5:D:1391:IPA:H11	1.82	0.45
1:A:275:HIS:N	5:A:1395:IPA:H12	2.25	0.45
1:A:119:VAL:HG21	1:A:152:TRP:CE2	2.52	0.44
1:A:281:GLU:O	1:A:285:GLU:HG3	2.18	0.44
1:D:62:ILE:O	1:D:252[A]:LYS:HE3	2.17	0.44
1:C:98:ASN:ND2	1:C:144:ASN:HD21	2.15	0.44
1:D:84[B]:MET:CE	1:D:108:TRP:HZ3	2.30	0.44
1:C:132:GLU:HA	1:C:135:ILE:HD12	1.99	0.44
1:D:221:LEU:O	1:D:226:ASN:HB2	2.17	0.44
1:B:163[A]:LYS:HE3	1:B:163[A]:LYS:HA	1.99	0.44
1:A:316[A]:GLU:HG3	2:A:1384:PEG:H31	1.99	0.44
1:C:68:ARG:HB3	3:C:1382:PGE:H42	1.98	0.43
1:A:275:HIS:CD2	5:A:1395:IPA:H13	2.53	0.43
1:C:153:HIS:HA	1:C:191:ASN:HB2	1.99	0.43
1:C:252:LYS:HG3	1:C:252:LYS:H	1.50	0.43
1:B:275:HIS:CD2	5:B:1394:IPA:H13	2.54	0.42
1:C:87:HIS:HB2	1:C:331:ALA:HB2	2.00	0.42
1:C:59:ARG:HB2	1:C:74:GLN:HG3	2.01	0.42
1:B:119:VAL:HG21	1:B:152:TRP:CE2	2.54	0.42
2:A:1387:PEG:H21	9:A:2200:HOH:O	2.19	0.42
1:A:265:ALA:HB1	5:A:1395:IPA:H31	2.00	0.42
1:A:262:THR:HG22	1:A:314:TRP:CD1	2.54	0.41
1:A:212[A]:LYS:HD3	1:A:212[A]:LYS:HA	1.93	0.41
1:C:59:ARG:HG3	1:C:74:GLN:OE1	2.19	0.41
1:A:132[B]:GLU:HG2	9:A:2076:HOH:O	2.20	0.41
1:A:309[A]:ASN:HB2	2:A:1386:PEG:H41	2.00	0.41
1:D:282[A]:LYS:HZ3	5:D:1394:IPA:H11	1.85	0.41
1:B:63:ILE:O	1:B:69:LYS:HA	2.20	0.41
1:D:328:TRP:HA	1:D:329:SER:HA	1.92	0.41
1:B:173[B]:LYS:HE3	1:B:220[B]:MET:SD	2.61	0.41
1:D:114:ARG:NH2	1:D:191:ASN:OD1	2.53	0.41
1:D:153:HIS:HA	1:D:191:ASN:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282[B]:LYS:HE2	9:D:2043:HOH:O	2.15	0.40
1:D:328:TRP:CG	1:D:329:SER:HB3	2.56	0.40
1:A:94[A]:GLN:NE2	9:A:2047:HOH:O	2.54	0.40
1:A:208:GLU:O	1:A:212[A]:LYS:HG2	2.22	0.40
6:B:1401:CL:CL	9:B:2163:HOH:O	2.59	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	349/334 (104%)	340 (97%)	9 (3%)	0	100	100
1	B	349/334 (104%)	336 (96%)	13 (4%)	0	100	100
1	C	343/334 (103%)	331 (96%)	11 (3%)	1 (0%)	41	30
1	D	334/334 (100%)	321 (96%)	11 (3%)	2 (1%)	25	14
All	All	1375/1336 (103%)	1328 (97%)	44 (3%)	3 (0%)	47	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	163	LYS
1	C	191	ASN
1	D	152	TRP

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	299/282 (106%)	299 (100%)	0	100	100
1	B	299/282 (106%)	294 (98%)	5 (2%)	60	54
1	C	293/282 (104%)	284 (97%)	9 (3%)	40	29
1	D	289/282 (102%)	275 (95%)	14 (5%)	25	14
All	All	1180/1128 (105%)	1152 (98%)	28 (2%)	55	39

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	163[A]	LYS
1	B	163[B]	LYS
1	B	198	SER
1	B	266[A]	SER
1	B	266[B]	SER
1	C	113[A]	ILE
1	C	113[B]	ILE
1	C	163	LYS
1	C	219	LYS
1	C	224	MET
1	C	252	LYS
1	C	273	LYS
1	C	313[A]	GLU
1	C	313[B]	GLU
1	D	90	GLN
1	D	94	GLN
1	D	126	THR
1	D	133	LYS
1	D	143	LYS
1	D	164	ILE
1	D	166	SER
1	D	173	LYS
1	D	212[A]	LYS
1	D	212[B]	LYS
1	D	220	MET
1	D	252[A]	LYS
1	D	252[B]	LYS
1	D	382	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	HIS
1	A	139	ASN
1	A	275	HIS
1	B	275	HIS
1	C	98	ASN
1	C	99	ASN
1	C	275	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 55 ligands modelled in this entry, 7 are monoatomic - leaving 48 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	EDO	A	1392	-	3,3,3	0.42	0	2,2,2	0.41	0
4	EDO	D	1387	-	3,3,3	0.46	0	2,2,2	0.50	0
5	IPA	B	1395	-	3,3,3	0.48	0	3,3,3	0.79	0
5	IPA	B	1394	-	3,3,3	0.45	0	3,3,3	0.63	0
2	PEG	A	1387	-	6,6,6	0.76	0	5,5,5	0.70	0
2	PEG	A	1383	-	6,6,6	0.35	0	5,5,5	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	PG4	D	1390	-	12,12,12	0.45	0	11,11,11	0.26	0
4	EDO	A	1391	-	3,3,3	0.47	0	2,2,2	0.13	0
7	PG6	B	1393	-	17,17,17	0.57	0	16,16,16	0.40	0
4	EDO	B	1387	-	3,3,3	0.39	0	2,2,2	0.50	0
5	IPA	B	1397	-	3,3,3	0.47	0	3,3,3	0.19	0
2	PEG	A	1381	-	6,6,6	0.45	0	5,5,5	0.31	0
4	EDO	B	1390	-	3,3,3	0.56	0	2,2,2	0.14	0
2	PEG	C	1381	-	6,6,6	0.43	0	5,5,5	0.28	0
4	EDO	D	1389	-	3,3,3	0.39	0	2,2,2	0.48	0
5	IPA	A	1394	-	3,3,3	0.55	0	3,3,3	0.52	0
5	IPA	A	1395	-	3,3,3	0.28	0	3,3,3	0.64	0
4	EDO	B	1385	-	3,3,3	0.46	0	2,2,2	0.24	0
4	EDO	D	1386	-	3,3,3	0.41	0	2,2,2	0.45	0
5	IPA	B	1396	-	3,3,3	0.50	0	3,3,3	0.47	0
2	PEG	B	1382	-	6,6,6	0.48	0	5,5,5	0.25	0
5	IPA	B	1399	-	3,3,3	0.38	0	3,3,3	0.72	0
5	IPA	D	1394	-	3,3,3	0.41	0	3,3,3	0.75	0
4	EDO	B	1389	-	3,3,3	0.53	0	2,2,2	0.32	0
2	PEG	D	1384	-	6,6,6	0.48	0	5,5,5	0.39	0
4	EDO	D	1385	-	3,3,3	0.44	0	2,2,2	0.25	0
2	PEG	A	1384	-	6,6,6	0.39	0	5,5,5	0.40	0
5	IPA	D	1393	-	3,3,3	0.48	0	3,3,3	0.37	0
4	EDO	B	1392	-	3,3,3	0.41	0	2,2,2	0.56	0
3	PGE	A	1389	-	9,9,9	0.58	0	8,8,8	0.89	0
5	IPA	B	1398	-	3,3,3	0.56	0	3,3,3	0.17	0
4	EDO	B	1391	-	3,3,3	0.44	0	2,2,2	0.48	0
2	PEG	B	1383	-	6,6,6	0.47	0	5,5,5	0.32	0
4	EDO	B	1386	-	3,3,3	0.51	0	2,2,2	0.34	0
4	EDO	B	1388	-	3,3,3	0.37	0	2,2,2	0.59	0
5	IPA	C	1384	-	3,3,3	0.43	0	3,3,3	0.86	0
5	IPA	D	1391	-	3,3,3	0.89	0	3,3,3	0.65	0
3	PGE	A	1388	-	9,9,9	0.61	0	8,8,8	0.55	0
4	EDO	A	1393	-	3,3,3	0.57	0	2,2,2	0.37	0
2	PEG	A	1382	-	6,6,6	0.43	0	5,5,5	0.45	0
4	EDO	A	1390	-	3,3,3	0.47	0	2,2,2	0.37	0
5	IPA	D	1392	-	3,3,3	0.54	0	3,3,3	0.20	0
3	PGE	B	1384	-	9,9,9	0.53	0	8,8,8	0.35	0
4	EDO	D	1388	-	3,3,3	0.49	0	2,2,2	0.39	0
2	PEG	A	1386	-	6,6,6	0.28	0	5,5,5	0.81	0
3	PGE	C	1382	-	9,9,9	0.56	0	8,8,8	0.52	0
4	EDO	C	1383	-	3,3,3	0.44	0	2,2,2	0.51	0
2	PEG	A	1385	-	6,6,6	0.39	0	5,5,5	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	1392	-	-	1/1/1/1	-
4	EDO	D	1387	-	-	0/1/1/1	-
2	PEG	A	1387	-	-	3/4/4/4	-
2	PEG	A	1383	-	-	3/4/4/4	-
8	PG4	D	1390	-	-	2/10/10/10	-
4	EDO	A	1391	-	-	1/1/1/1	-
7	PG6	B	1393	-	-	9/15/15/15	-
4	EDO	B	1387	-	-	1/1/1/1	-
4	EDO	C	1383	-	-	1/1/1/1	-
2	PEG	A	1381	-	-	1/4/4/4	-
4	EDO	B	1390	-	-	1/1/1/1	-
2	PEG	C	1381	-	-	2/4/4/4	-
4	EDO	D	1389	-	-	1/1/1/1	-
4	EDO	B	1385	-	-	1/1/1/1	-
4	EDO	D	1386	-	-	0/1/1/1	-
2	PEG	B	1382	-	-	1/4/4/4	-
4	EDO	B	1389	-	-	0/1/1/1	-
2	PEG	D	1384	-	-	2/4/4/4	-
4	EDO	D	1385	-	-	1/1/1/1	-
2	PEG	A	1384	-	-	2/4/4/4	-
4	EDO	B	1392	-	-	0/1/1/1	-
3	PGE	A	1389	-	-	5/7/7/7	-
4	EDO	B	1391	-	-	1/1/1/1	-
2	PEG	B	1383	-	-	2/4/4/4	-
4	EDO	B	1386	-	-	1/1/1/1	-
4	EDO	B	1388	-	-	1/1/1/1	-
3	PGE	A	1388	-	-	6/7/7/7	-
4	EDO	A	1393	-	-	1/1/1/1	-
2	PEG	A	1382	-	-	3/4/4/4	-
4	EDO	A	1390	-	-	1/1/1/1	-
4	EDO	D	1388	-	-	1/1/1/1	-
3	PGE	B	1384	-	-	6/7/7/7	-
2	PEG	A	1386	-	-	4/4/4/4	-
3	PGE	C	1382	-	-	4/7/7/7	-
2	PEG	A	1385	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1382	PGE	C1-C2-O2-C3
7	B	1393	PG6	O1-C2-C3-O2
7	B	1393	PG6	O4-C8-C9-O5
3	B	1384	PGE	O2-C3-C4-O3
3	A	1388	PGE	O2-C3-C4-O3
2	C	1381	PEG	O2-C3-C4-O4
3	A	1389	PGE	O1-C1-C2-O2
2	B	1383	PEG	O1-C1-C2-O2
2	B	1383	PEG	O2-C3-C4-O4
3	B	1384	PGE	O3-C5-C6-O4
4	D	1389	EDO	O1-C1-C2-O2
3	A	1389	PGE	O2-C3-C4-O3
3	C	1382	PGE	O2-C3-C4-O3
2	D	1384	PEG	O2-C3-C4-O4
2	A	1386	PEG	O2-C3-C4-O4
7	B	1393	PG6	O2-C4-C5-O3
2	A	1383	PEG	O1-C1-C2-O2
3	B	1384	PGE	O1-C1-C2-O2
2	A	1386	PEG	O1-C1-C2-O2
2	A	1383	PEG	O2-C3-C4-O4
4	B	1387	EDO	O1-C1-C2-O2
4	C	1383	EDO	O1-C1-C2-O2
4	B	1385	EDO	O1-C1-C2-O2
4	B	1391	EDO	O1-C1-C2-O2
4	A	1393	EDO	O1-C1-C2-O2
4	A	1390	EDO	O1-C1-C2-O2
2	A	1387	PEG	O2-C3-C4-O4
2	A	1381	PEG	O1-C1-C2-O2
3	A	1388	PGE	O3-C5-C6-O4
4	B	1388	EDO	O1-C1-C2-O2
3	C	1382	PGE	O3-C5-C6-O4
3	A	1389	PGE	C4-C3-O2-C2
2	C	1381	PEG	O1-C1-C2-O2
7	B	1393	PG6	C3-C2-O1-C1
7	B	1393	PG6	O5-C10-C11-O6
4	A	1392	EDO	O1-C1-C2-O2
4	D	1385	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	A	1384	PEG	C4-C3-O2-C2
3	B	1384	PGE	C3-C4-O3-C5
3	B	1384	PGE	C6-C5-O3-C4
2	A	1382	PEG	C4-C3-O2-C2
7	B	1393	PG6	C11-C10-O5-C9
3	A	1388	PGE	C4-C3-O2-C2
2	B	1382	PEG	C1-C2-O2-C3
2	A	1386	PEG	C4-C3-O2-C2
3	A	1389	PGE	C6-C5-O3-C4
2	A	1382	PEG	O1-C1-C2-O2
7	B	1393	PG6	C4-C5-O3-C6
2	A	1387	PEG	C4-C3-O2-C2
8	D	1390	PG4	O1-C1-C2-O2
4	B	1390	EDO	O1-C1-C2-O2
4	B	1386	EDO	O1-C1-C2-O2
7	B	1393	PG6	C6-C7-O4-C8
3	C	1382	PGE	C3-C4-O3-C5
3	A	1389	PGE	O3-C5-C6-O4
3	A	1388	PGE	O1-C1-C2-O2
2	A	1383	PEG	C4-C3-O2-C2
2	A	1386	PEG	C1-C2-O2-C3
2	D	1384	PEG	C1-C2-O2-C3
2	A	1382	PEG	C1-C2-O2-C3
8	D	1390	PG4	C5-C6-O4-C7
2	A	1387	PEG	C1-C2-O2-C3
4	A	1391	EDO	O1-C1-C2-O2
3	A	1388	PGE	C1-C2-O2-C3
3	A	1388	PGE	C6-C5-O3-C4
3	B	1384	PGE	C4-C3-O2-C2
2	A	1384	PEG	O2-C3-C4-O4
7	B	1393	PG6	C9-C8-O4-C7
4	D	1388	EDO	O1-C1-C2-O2

There are no ring outliers.

20 monomers are involved in 57 short contacts:

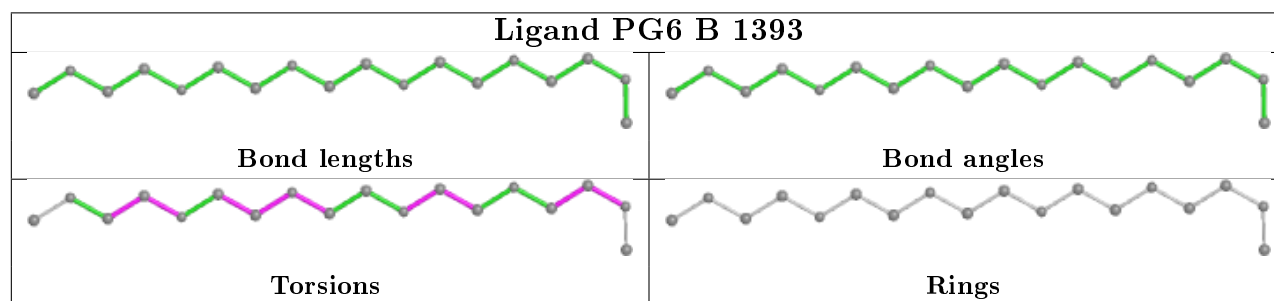
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1395	IPA	5	0
5	B	1394	IPA	4	0
2	A	1387	PEG	2	0
7	B	1393	PG6	3	0
5	B	1397	IPA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1381	PEG	2	0
5	A	1395	IPA	6	0
2	B	1382	PEG	1	0
5	D	1394	IPA	2	0
2	A	1384	PEG	2	0
5	D	1393	IPA	2	0
3	A	1389	PGE	3	0
2	B	1383	PEG	1	0
5	C	1384	IPA	5	0
5	D	1391	IPA	8	0
3	A	1388	PGE	1	0
2	A	1382	PEG	3	0
5	D	1392	IPA	1	0
2	A	1386	PEG	5	0
3	C	1382	PGE	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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	331/334 (99%)	0.10	18 (5%) 25 27	19, 33, 53, 72	0
1	B	332/334 (99%)	0.04	19 (5%) 23 25	20, 30, 53, 93	0
1	C	331/334 (99%)	0.56	49 (14%) 2 2	29, 45, 80, 110	0
1	D	328/334 (98%)	0.84	64 (19%) 1 1	23, 51, 93, 132	0
All	All	1322/1336 (98%)	0.38	150 (11%) 5 5	19, 39, 74, 132	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	126	THR	6.5
1	D	383	MET	6.1
1	C	50	MET	5.7
1	D	349	GLY	5.7
1	D	197	GLU	5.3
1	D	91	TRP	5.1
1	D	382	THR	5.0
1	D	179	TYR	4.8
1	D	180	PRO	4.8
1	D	224	MET	4.7
1	D	161	ASN	4.5
1	C	197	GLU	4.5
1	C	163	LYS	4.4
1	C	164	ILE	4.4
1	D	177	SER	4.3
1	C	149	ILE	4.3
1	D	75	HIS	4.3
1	D	55	SER	4.2
1	A	380	ARG	4.2
1	C	65	ILE	4.2
1	C	326	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	350	ASN	4.0
1	C	128	PRO	4.0
1	C	224	MET	4.0
1	A	379	SER	4.0
1	B	149	ILE	4.0
1	C	126	THR	4.0
1	B	231	ILE	3.9
1	B	122	GLY	3.8
1	C	122	GLY	3.8
1	D	127	ASP	3.8
1	C	162	ALA	3.7
1	D	156	ASN	3.7
1	A	231	ILE	3.6
1	C	165	TYR	3.6
1	C	199	ASP	3.6
1	A	291	PHE	3.5
1	C	231	ILE	3.5
1	D	373	ILE	3.5
1	B	126	THR	3.5
1	B	292	VAL	3.5
1	C	161	ASN	3.5
1	C	119	VAL	3.5
1	C	186	ILE	3.4
1	C	180	PRO	3.4
1	C	373	ILE	3.4
1	D	149	ILE	3.4
1	C	293	THR	3.4
1	A	149	ILE	3.4
1	B	326	VAL	3.3
1	C	125	SER	3.3
1	D	379	SER	3.3
1	D	352	LYS	3.3
1	D	162	ALA	3.3
1	A	326	VAL	3.2
1	B	379	SER	3.2
1	A	292	VAL	3.2
1	D	292	VAL	3.2
1	D	381	GLU	3.1
1	B	125	SER	3.1
1	B	291	PHE	3.1
1	C	124	TYR	3.1
1	C	150	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	378	ILE	3.0
1	D	170	GLU	3.0
1	D	163	LYS	3.0
1	D	343	THR	3.0
1	C	158	GLY	3.0
1	B	230	ILE	3.0
1	C	75	HIS	2.9
1	C	378	ILE	2.9
1	C	74	GLN	2.8
1	C	379	SER	2.8
1	D	353	VAL	2.8
1	D	164	ILE	2.8
1	C	376	LYS	2.8
1	A	375	TYR	2.8
1	D	199	ASP	2.8
1	D	88	GLY	2.7
1	C	195	PRO	2.7
1	A	186	ILE	2.7
1	D	98	ASN	2.7
1	C	170	GLU	2.7
1	B	150	VAL	2.7
1	D	377	PRO	2.7
1	D	95	ILE	2.6
1	D	334	ASN	2.6
1	D	57	ALA	2.6
1	D	196	THR	2.6
1	C	330	LEU	2.6
1	D	106	LYS	2.6
1	B	186	ILE	2.6
1	C	76	GLY	2.6
1	D	378	ILE	2.6
1	D	165	TYR	2.5
1	D	56	LEU	2.5
1	C	127	ASP	2.5
1	C	112	VAL	2.5
1	C	129	SER	2.5
1	D	346	LEU	2.5
1	A	343	THR	2.5
1	A	350[A]	ASN	2.5
1	B	164	ILE	2.5
1	B	293	THR	2.5
1	D	195	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	342	PRO	2.4
1	D	143	LYS	2.4
1	D	176	ALA	2.4
1	B	229	ILE	2.4
1	D	231	ILE	2.4
1	A	293	THR	2.4
1	D	130	VAL	2.4
1	B	112	VAL	2.4
1	C	374	PRO	2.4
1	C	176	ALA	2.4
1	D	351	GLY	2.4
1	C	113[A]	ILE	2.4
1	D	74	GLN	2.3
1	C	123	GLY	2.3
1	A	258	ALA	2.3
1	C	372	GLY	2.3
1	D	345	SER	2.3
1	C	167	GLY	2.3
1	D	50	MET	2.3
1	D	291	PHE	2.3
1	D	173	LYS	2.3
1	D	347	ASP	2.3
1	A	376	LYS	2.2
1	C	196	THR	2.2
1	C	292	VAL	2.2
1	A	125	SER	2.2
1	D	166	SER	2.2
1	D	103	ALA	2.2
1	C	157	PRO	2.2
1	C	223	ASP	2.2
1	D	113	ILE	2.2
1	D	52	LYS	2.2
1	B	232	VAL	2.2
1	C	66	ASP	2.1
1	A	150	VAL	2.1
1	D	139	ASN	2.1
1	D	198	SER	2.1
1	A	290	VAL	2.1
1	C	159	ASP	2.1
1	D	204	ILE	2.1
1	D	189	LEU	2.1
1	B	163[A]	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	376	LYS	2.0
1	D	96	ILE	2.0
1	B	381	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	A	1390	4/4	0.66	0.19	75,77,80,82	0
4	EDO	D	1388	4/4	0.66	0.23	71,79,79,81	0
4	EDO	B	1389	4/4	0.68	0.22	63,72,72,78	0
3	PGE	B	1384	10/10	0.70	0.21	68,77,85,85	0
2	PEG	A	1387	7/7	0.71	0.17	36,47,57,61	0
4	EDO	A	1391	4/4	0.72	0.25	59,59,66,81	0
2	PEG	B	1382	7/7	0.73	0.18	63,66,77,78	0
4	EDO	D	1387	4/4	0.74	0.18	45,58,65,72	0
4	EDO	B	1386	4/4	0.75	0.14	60,67,69,70	0
4	EDO	A	1392	4/4	0.76	0.17	72,80,82,91	0
2	PEG	A	1386	7/7	0.78	0.23	40,49,72,80	0
2	PEG	C	1381	7/7	0.81	0.12	59,61,64,68	0
5	IPA	D	1391	4/4	0.81	0.15	29,29,37,51	0
5	IPA	A	1394	4/4	0.82	0.30	37,47,51,53	4
4	EDO	A	1393	4/4	0.83	0.15	49,51,68,74	0
4	EDO	C	1383	4/4	0.84	0.13	50,53,59,63	0
3	PGE	C	1382	10/10	0.84	0.16	43,51,64,71	0
2	PEG	D	1384	7/7	0.85	0.17	52,70,76,79	0
4	EDO	D	1385	4/4	0.85	0.20	49,56,62,63	0
5	IPA	D	1393	4/4	0.86	0.18	37,45,53,62	0

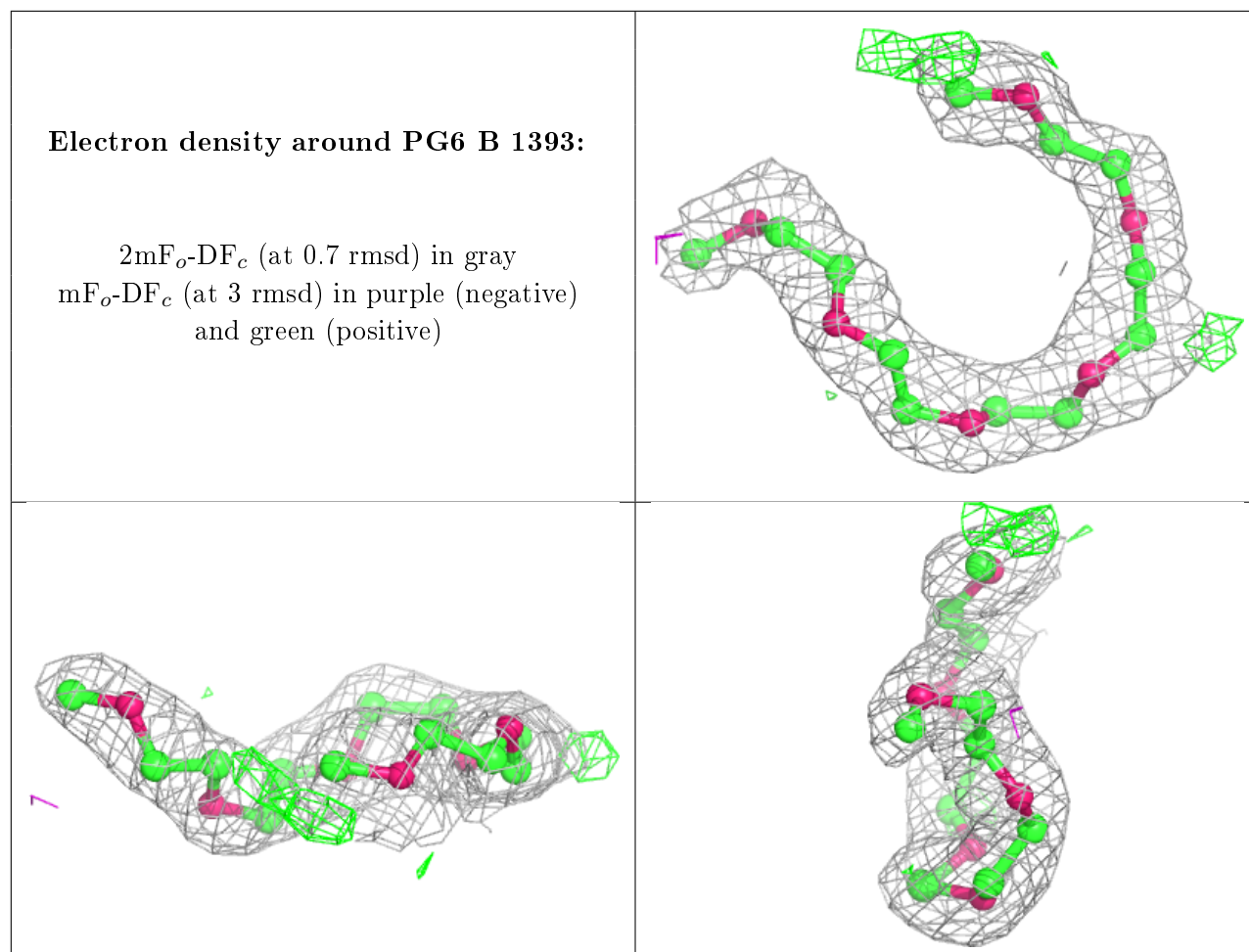
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PEG	B	1383	7/7	0.86	0.25	58,62,69,83	0
4	EDO	B	1391	4/4	0.87	0.38	70,71,73,78	0
4	EDO	B	1392	4/4	0.87	0.12	55,61,62,75	0
3	PGE	A	1388	10/10	0.87	0.10	50,60,69,70	0
3	PGE	A	1389	10/10	0.88	0.14	34,50,59,62	0
4	EDO	B	1390	4/4	0.88	0.17	42,62,62,74	0
4	EDO	B	1385	4/4	0.88	0.20	43,60,64,73	0
4	EDO	D	1386	4/4	0.89	0.11	53,59,64,64	0
2	PEG	A	1385	7/7	0.89	0.12	57,72,77,84	0
2	PEG	A	1384	7/7	0.90	0.14	49,59,67,78	0
2	PEG	A	1381	7/7	0.90	0.15	31,49,53,57	0
5	IPA	D	1392	4/4	0.90	0.11	49,55,57,59	0
6	CL	A	1400	1/1	0.91	0.13	59,59,59,59	1
7	PG6	B	1393	18/18	0.91	0.09	44,52,78,78	0
4	EDO	B	1387	4/4	0.92	0.08	46,52,57,65	0
6	CL	C	1385	1/1	0.92	0.06	56,56,56,56	1
4	EDO	D	1389	4/4	0.92	0.12	58,62,64,75	0
4	EDO	B	1388	4/4	0.92	0.14	37,47,50,61	0
2	PEG	A	1383	7/7	0.92	0.17	45,49,58,72	0
5	IPA	B	1396	4/4	0.92	0.14	48,49,50,67	0
5	IPA	B	1398	4/4	0.92	0.13	50,57,74,78	0
6	CL	A	1396	1/1	0.93	0.06	53,53,53,53	0
6	CL	A	1397	1/1	0.93	0.07	30,30,30,30	1
5	IPA	B	1394	4/4	0.93	0.10	19,29,29,42	0
5	IPA	B	1395	4/4	0.94	0.11	26,35,41,41	0
8	PG4	D	1390	13/13	0.94	0.14	43,51,61,63	0
5	IPA	A	1395	4/4	0.94	0.16	22,23,27,42	0
5	IPA	D	1394	4/4	0.94	0.11	38,41,44,46	0
5	IPA	B	1397	4/4	0.95	0.09	42,46,54,61	0
5	IPA	C	1384	4/4	0.95	0.13	31,33,36,37	0
6	CL	D	1395	1/1	0.96	0.09	52,52,52,52	1
5	IPA	B	1399	4/4	0.97	0.26	33,36,40,45	0
2	PEG	A	1382	7/7	0.98	0.08	26,31,45,48	7
6	CL	B	1400	1/1	0.98	0.03	47,47,47,47	0
6	CL	B	1401	1/1	0.98	0.13	39,39,39,39	1

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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.