



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 11:19 PM UTC

PDB ID : 5AII / pdb_00005aai
Title : Discovery and characterization of thermophilic limonene-1,2-epoxide hydrolases from hot spring metagenomic libraries. CH55-sample-PEG complex
Authors : Ferrandi, E.; Sayer, C.; Isupov, M.N.; Annovazzi, C.; Marchesi, C.; Iacobone, G.; Peng, X.; Bonch-Osmolovskaya, E.; Wohlgemuth, R.; Littlechild, J.A.; Montia, D.
Deposited on : 2015-02-13
Resolution : 1.47 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](#) ①) were used in the production of this report:

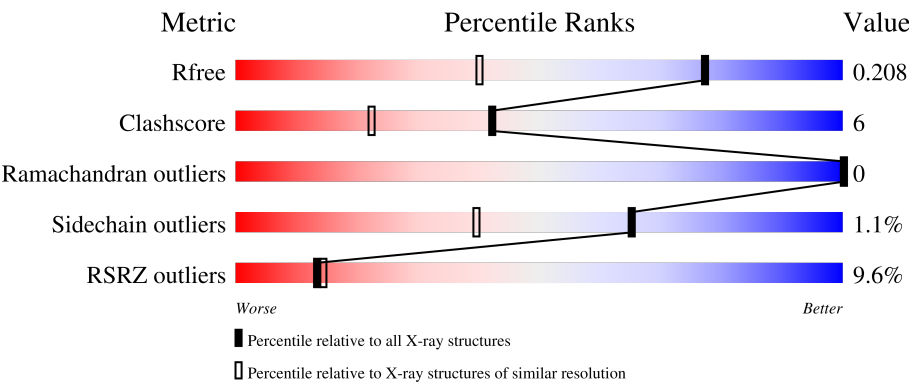
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.47 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	6779 (1.50-1.46)
Clashscore	190562	7025 (1.50-1.46)
Ramachandran outliers	187476	6917 (1.50-1.46)
Sidechain outliers	187428	6914 (1.50-1.46)
RSRZ outliers	180081	6781 (1.50-1.46)

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	135	15% 87% 5% 7%
1	B	135	7% 84% 10% 6%
1	C	135	7% 84% 10% 7%
1	D	135	6% 88% • 7%
1	E	135	26% 86% 6% • 7%

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Mol	Chain	Length	Quality of chain
1	F	135	
1	G	135	
1	H	135	
1	I	135	
1	J	135	
1	K	135	
1	L	135	
1	M	135	
1	N	135	
1	O	135	
1	P	135	

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
4	ACT	M	1128	-	-	X	-
4	ACT	P	1128	-	-	X	-

2 Entry composition

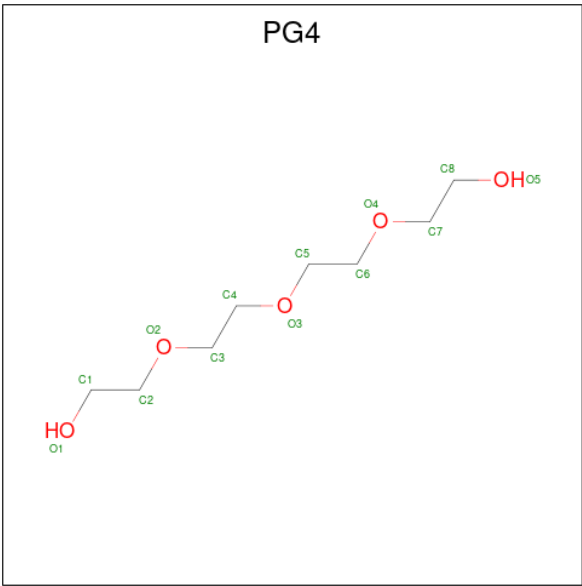
There are 10 unique types of molecules in this entry. The entry contains 18828 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 LIMONENE-1,2-EPOXIDE HYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	125	Total	C	N	O	S	0	15	0
			1031	664	177	181	9			
1	B	127	Total	C	N	O	S	0	16	0
			1046	675	176	186	9			
1	C	126	Total	C	N	O	S	0	10	0
			1006	641	172	185	8			
1	D	125	Total	C	N	O	S	0	12	0
			1013	647	175	183	8			
1	E	125	Total	C	N	O	S	0	10	0
			1005	641	174	182	8			
1	F	124	Total	C	N	O	S	0	14	0
			1018	653	176	180	9			
1	G	125	Total	C	N	O	S	0	7	0
			983	623	171	182	7			
1	H	130	Total	C	N	O	S	0	13	1
			1062	679	188	187	8			
1	I	125	Total	C	N	O	S	0	13	0
			1017	651	174	184	8			
1	J	125	Total	C	N	O	S	0	14	0
			1025	654	176	187	8			
1	K	125	Total	C	N	O	S	0	7	0
			980	626	167	180	7			
1	L	125	Total	C	N	O	S	0	12	0
			1015	649	176	182	8			
1	M	125	Total	C	N	O	S	0	11	0
			1009	645	174	182	8			
1	N	130	Total	C	N	O	S	0	17	1
			1078	693	187	190	8			
1	O	125	Total	C	N	O	S	0	12	0
			1018	653	173	183	9			
1	P	126	Total	C	N	O	S	0	14	0
			1029	663	172	185	9			

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



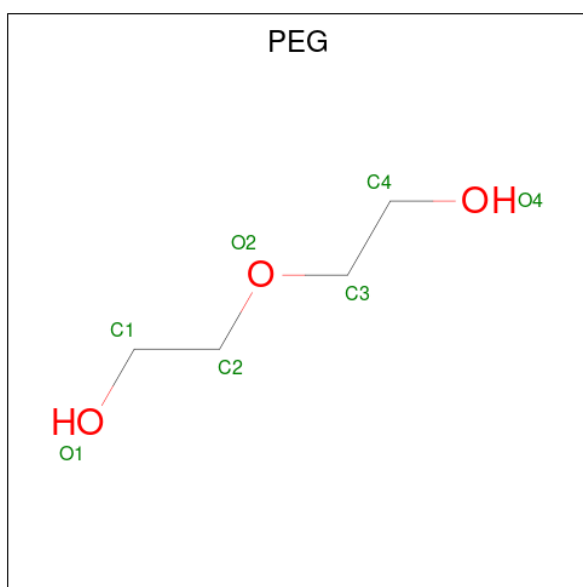
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		
2	B	1	Total	C	O	0	0
			13	8	5		
2	B	1	Total	C	O	0	0
			13	8	5		
2	C	1	Total	C	O	0	0
			13	8	5		
2	D	1	Total	C	O	0	0
			13	8	5		
2	D	1	Total	C	O	0	0
			13	8	5		
2	D	1	Total	C	O	0	0
			13	8	5		
2	E	1	Total	C	O	0	0
			13	8	5		
2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

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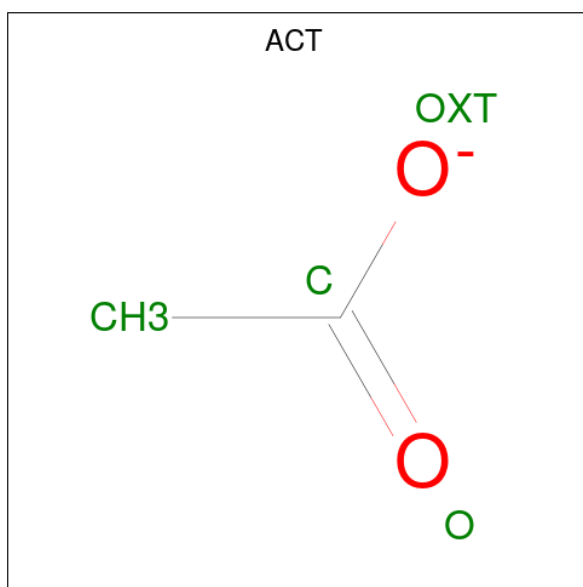
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	C	O	0	0
			13	8	5		
2	I	1	Total	C	O	0	0
			13	8	5		
2	I	1	Total	C	O	0	0
			13	8	5		
2	J	1	Total	C	O	0	0
			13	8	5		
2	K	1	Total	C	O	0	0
			13	8	5		
2	L	1	Total	C	O	0	0
			13	8	5		
2	M	1	Total	C	O	0	0
			13	8	5		
2	N	1	Total	C	O	0	0
			13	8	5		
2	O	1	Total	C	O	0	0
			13	8	5		
2	O	1	Total	C	O	0	0
			13	8	5		
2	P	1	Total	C	O	0	0
			13	8	5		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	D	1	Total C O 7 4 3	0	0
3	F	1	Total C O 7 4 3	0	0
3	F	1	Total C O 7 4 3	0	0
3	H	1	Total C O 7 4 3	0	0
3	I	1	Total C O 7 4 3	0	0
3	I	1	Total C O 7 4 3	0	0
3	K	1	Total C O 7 4 3	0	0
3	K	1	Total C O 7 4 3	0	0
3	L	1	Total C O 7 4 3	0	0
3	L	1	Total C O 7 4 3	0	0
3	M	1	Total C O 7 4 3	0	0
3	O	1	Total C O 7 4 3	0	0
3	O	1	Total C O 7 4 3	0	0

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	J	1	Total	C	O	0	0
			4	2	2		
4	K	1	Total	C	O	0	0
			4	2	2		
4	L	1	Total	C	O	0	0
			4	2	2		
4	M	1	Total	C	O	0	0
			4	2	2		
4	P	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



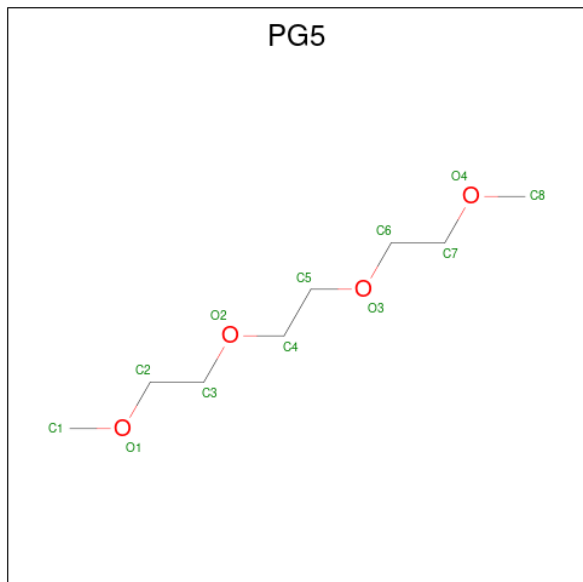
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	L	1	Total	C	O	0	0
			4	2	2		
5	M	1	Total	C	O	0	0
			4	2	2		
5	M	1	Total	C	O	0	0
			4	2	2		
5	N	1	Total	C	O	0	0
			4	2	2		

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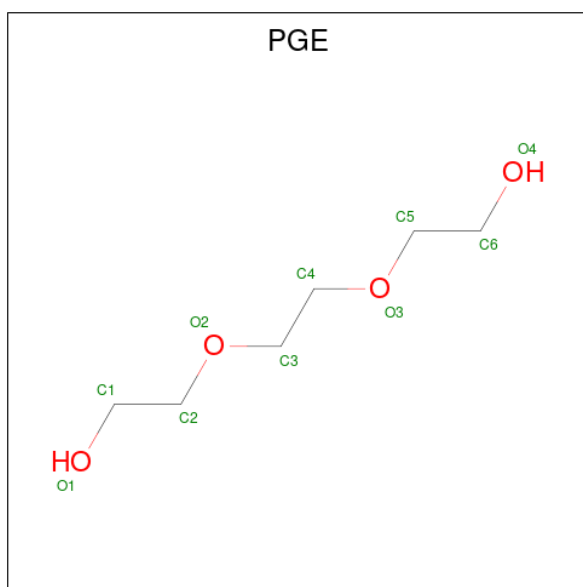
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	P	1	Total	C	O	0	0
			4	2	2		
5	P	1	Total	C	O	0	0
			4	2	2		
5	P	1	Total	C	O	0	0
			4	2	2		
5	P	1	Total	C	O	0	0
			4	2	2		
5	P	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is 1-METHOXY-2-[2-(2-METHOXY-ETHOXY)]-ETHANE (CCD ID: PG5) (formula: C₈H₁₈O₄).



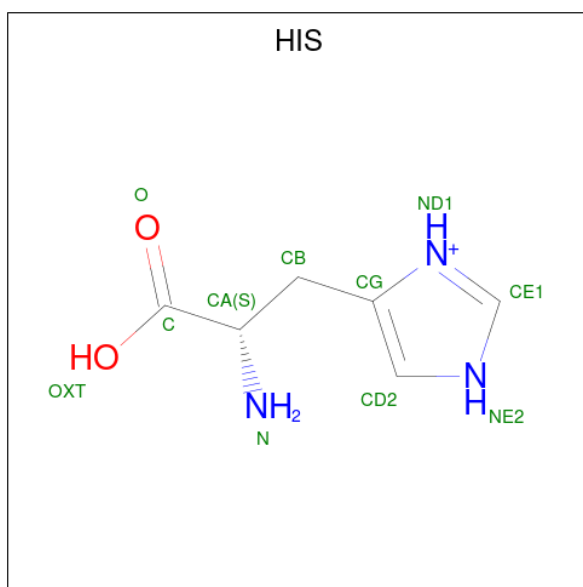
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			12	8	4		

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



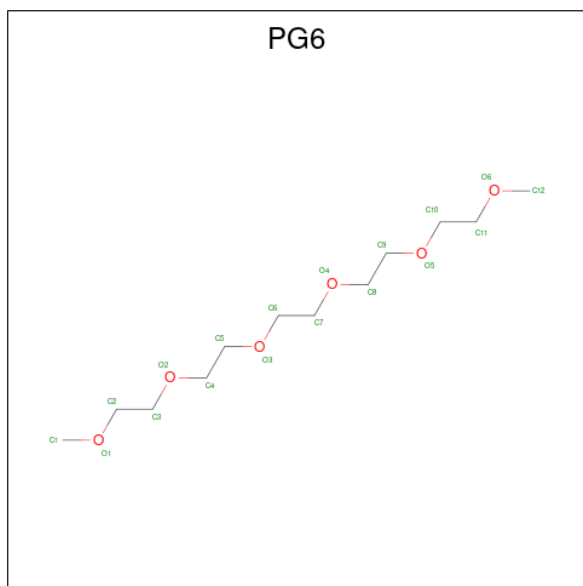
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			10	6	4		
7	D	1	Total	C	O	0	0
			10	6	4		
7	K	1	Total	C	O	0	0
			10	6	4		
7	M	1	Total	C	O	0	0
			10	6	4		
7	N	1	Total	C	O	0	0
			10	6	4		
7	N	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is HISTIDINE (CCD ID: HIS) (formula: C₆H₁₀N₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	F	1	Total	C	N	O	0	0
			11	6	3	2		

- Molecule 9 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANE (CCD ID: PG6) (formula: $C_{12}H_{26}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	I	1	Total	C	O	0	0
			18	12	6		
9	N	1	Total	C	O	0	0
			18	12	6		

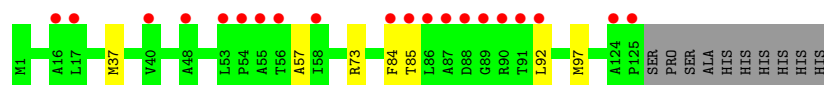
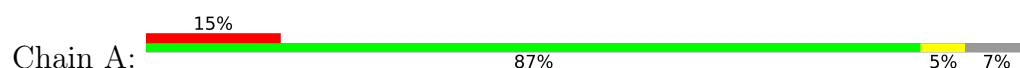
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	124	Total 124	O 124	0	0
10	B	114	Total 114	O 114	0	0
10	C	146	Total 146	O 146	0	0
10	D	140	Total 140	O 140	0	0
10	E	84	Total 84	O 84	0	0
10	F	94	Total 94	O 94	0	0
10	G	126	Total 126	O 126	0	0
10	H	97	Total 97	O 97	0	0
10	I	137	Total 137	O 137	0	0
10	J	95	Total 95	O 95	0	0
10	K	109	Total 109	O 109	0	0
10	L	80	Total 80	O 80	0	0
10	M	126	Total 126	O 126	0	0
10	N	137	Total 137	O 137	0	0
10	O	114	Total 114	O 114	0	0
10	P	107	Total 107	O 107	0	0

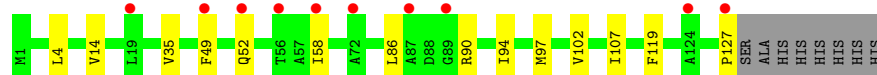
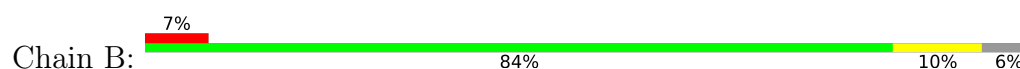
3 Residue-property plots [i](#)

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.

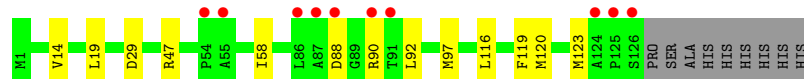
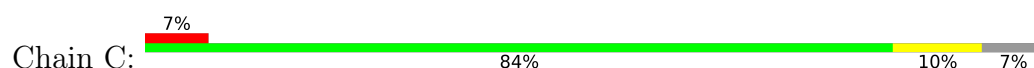
- Molecule 1: LIMONENE-1,2-EPOXIDE HYDROLASE



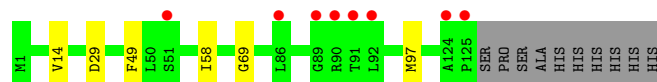
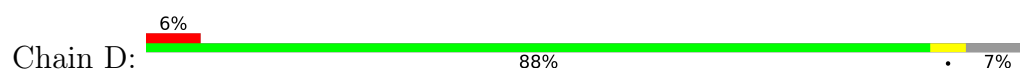
- Molecule 1: LIMONENE-1,2-EPOXIDE HYDROLASE



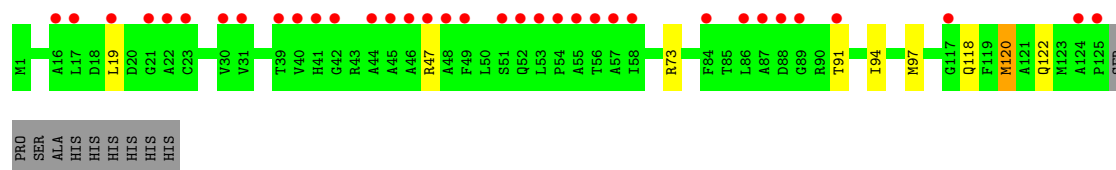
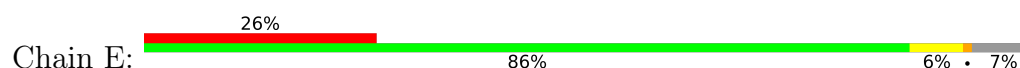
- Molecule 1: LIMONENE-1,2-EPOXIDE HYDROLASE



- Molecule 1: LIMONENE-1,2-EPOXIDE HYDROLASE



- Molecule 1: LIMONENE-1,2-EPOXIDE HYDROLASE



Chain F:

[illegible]

Chain H:

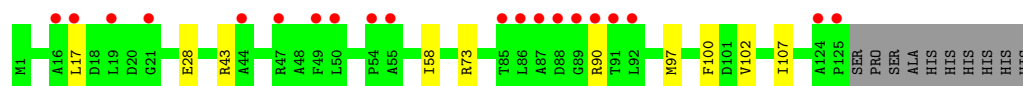
Chain I:

[illegible]

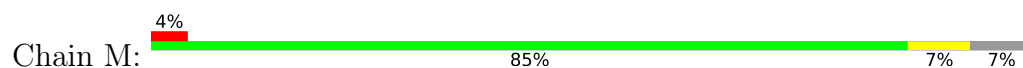
Chain K:

Amino Acid	Percentage
Ala	86%
Arg	86%
Asn	86%
Asp	86%
Glu	86%
Gly	86%
Ile	86%
Leu	86%
Met	86%
Phe	86%
Pro	86%
Ser	86%
Thr	86%
Val	86%
Lys	8%
Gln	7%
His	7%

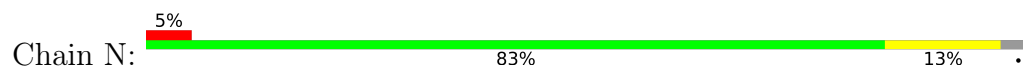
Chain L: 15% 85% 7% 7%



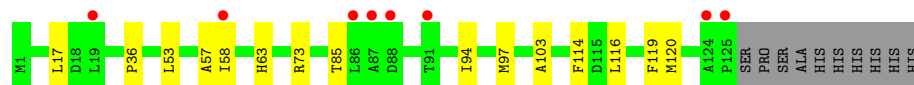
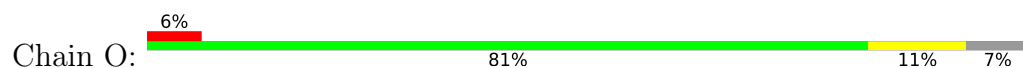
• Molecule 1: LIMONENE-1,2-EPOXIDE HYDROLASE



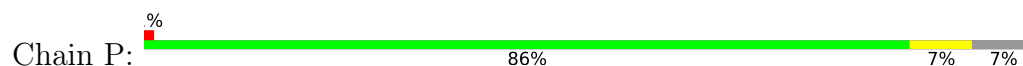
• Molecule 1: LIMONENE-1,2-EPOXIDE HYDROLASE



• Molecule 1: LIMONENE-1,2-EPOXIDE HYDROLASE



• Molecule 1: LIMONENE-1,2-EPOXIDE HYDROLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.97Å 104.23Å 148.00Å 90.00° 102.41° 90.00°	Depositor
Resolution (Å)	104.23 – 1.47 104.23 – 1.47	Depositor EDS
% Data completeness (in resolution range)	97.4 (104.23-1.47) 97.3 (104.23-1.47)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 1.47Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.175 , 0.208 0.175 , 0.208	Depositor DCC
R_{free} test set	16691 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18828	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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 53.72 % 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 4.0485e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, ACT, EDO, PG6, PGE, PG4, PG5

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	0.82	0/1094	0.95	4/1489 (0.3%)
1	B	0.80	0/1113	0.88	1/1517 (0.1%)
1	C	0.93	0/1054	0.95	0/1435
1	D	0.93	0/1068	0.94	0/1453
1	E	0.81	0/1053	0.95	0/1433
1	F	0.86	0/1077	0.86	0/1464
1	G	0.95	0/1022	0.92	0/1392
1	H	0.87	1/1124 (0.1%)	0.93	0/1529
1	I	0.81	0/1074	0.86	0/1463
1	J	0.78	0/1085	0.87	0/1475
1	K	0.84	0/1019	0.93	1/1390 (0.1%)
1	L	0.75	0/1069	0.89	0/1453
1	M	0.86	0/1060	0.87	0/1442
1	N	0.95	1/1152 (0.1%)	0.94	0/1568
1	O	0.97	0/1067	0.97	0/1452
1	P	0.91	0/1090	0.97	0/1484
All	All	0.87	2/17221 (0.0%)	0.92	6/23439 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	133	HIS	C-N	-7.05	1.23	1.33
1	N	133	HIS	C-N	-6.77	1.23	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37[A]	MET	CA-C-N	-5.35	114.45	119.85
1	A	37[A]	MET	C-N-CA	-5.35	114.45	119.85
1	A	37[B]	MET	CA-C-N	-5.35	114.45	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37[B]	MET	C-N-CA	-5.35	114.45	119.85
1	B	35	VAL	O-C-N	5.31	123.82	120.42
1	K	35	VAL	O-C-N	5.22	123.76	120.42

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	1031	0	1087	6	0
1	B	1046	0	1103	11	0
1	C	1006	0	1028	16	0
1	D	1013	0	1044	7	0
1	E	1005	0	1031	15	0
1	F	1018	0	1069	14	0
1	G	983	0	995	9	0
1	H	1062	0	1080	14	0
1	I	1017	0	1056	9	0
1	J	1025	0	1060	18	0
1	K	980	0	998	10	0
1	L	1015	0	1052	10	0
1	M	1009	0	1038	10	0
1	N	1078	0	1105	35	0
1	O	1018	0	1046	19	0
1	P	1029	0	1068	20	0
2	A	13	0	18	0	0
2	B	26	0	36	3	0
2	C	13	0	18	0	0
2	D	39	0	54	7	0
2	E	13	0	18	0	0
2	F	26	0	36	1	0
2	G	26	0	36	1	0
2	H	26	0	36	3	0
2	I	26	0	36	5	0
2	J	13	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	13	0	18	3	0
2	L	13	0	18	0	0
2	M	13	0	18	1	0
2	N	13	0	18	2	0
2	O	26	0	36	2	0
2	P	13	0	18	5	0
3	A	7	0	10	0	0
3	B	14	0	20	0	0
3	D	7	0	10	1	0
3	F	14	0	20	1	0
3	H	7	0	10	0	0
3	I	14	0	20	0	0
3	K	14	0	20	3	0
3	L	14	0	20	1	0
3	M	7	0	10	2	0
3	O	14	0	20	1	0
4	A	4	0	3	0	0
4	C	8	0	6	1	0
4	G	4	0	3	0	0
4	H	8	0	6	0	0
4	J	4	0	3	0	0
4	K	4	0	3	0	0
4	L	4	0	3	0	0
4	M	4	0	3	2	0
4	P	4	0	3	10	0
5	A	4	0	6	0	0
5	C	4	0	6	3	0
5	D	16	0	24	0	0
5	F	4	0	6	0	0
5	G	8	0	12	0	0
5	H	4	0	6	1	0
5	L	4	0	6	0	0
5	M	8	0	12	0	0
5	N	4	0	6	0	0
5	P	20	0	30	5	0
6	A	12	0	18	0	0
7	C	10	0	14	0	0
7	D	10	0	14	1	0
7	K	10	0	14	0	0
7	M	10	0	14	0	0
7	N	20	0	28	4	0
8	F	11	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	18	0	26	2	0
9	N	18	0	26	4	0
10	A	124	0	0	0	0
10	B	114	0	0	0	0
10	C	146	0	0	2	0
10	D	140	0	0	2	0
10	E	84	0	0	1	0
10	F	94	0	0	1	0
10	G	126	0	0	1	0
10	H	97	0	0	0	0
10	I	137	0	0	2	0
10	J	95	0	0	0	0
10	K	109	0	0	0	0
10	L	80	0	0	1	0
10	M	126	0	0	1	0
10	N	137	0	0	3	0
10	O	114	0	0	1	0
10	P	107	0	0	1	0
All	All	18828	0	17759	220	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 (220) 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:N:92[B]:LEU:HD11	1:N:123[B]:MET:CE	1.36	1.53
1:N:92[B]:LEU:CD1	1:N:123[B]:MET:CE	2.19	1.20
1:J:61[B]:GLU:OE2	1:J:83[B]:ARG:NE	1.74	1.19
1:N:120[A]:MET:CE	10:N:2119:HOH:O	1.85	1.19
1:E:73[B]:ARG:HG3	1:E:73[B]:ARG:HH11	1.10	1.13
1:J:88[A]:ASP:CG	1:J:90[A]:ARG:NH1	2.07	1.12
1:J:88[A]:ASP:CG	1:J:90[A]:ARG:HH11	1.59	1.10
1:N:92[B]:LEU:HD11	1:N:123[B]:MET:HE1	1.23	1.06
1:N:120[A]:MET:HE1	10:N:2119:HOH:O	1.47	1.05
1:N:92[B]:LEU:CD1	1:N:123[B]:MET:HE2	1.84	1.05
1:P:49[B]:PHE:CE2	2:P:1127:PG4:H42	1.90	1.04
1:E:19[B]:LEU:CD2	1:E:47[B]:ARG:HD3	1.89	1.01
1:J:88[A]:ASP:OD1	1:J:90[A]:ARG:NH1	1.94	1.01
1:N:92[B]:LEU:CD2	1:N:123[B]:MET:HE2	1.95	0.97
1:E:73[B]:ARG:HH11	1:E:73[B]:ARG:CG	1.78	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:49[B]:PHE:CE2	2:H:1134:PG4:H42	2.03	0.94
1:N:92[B]:LEU:HD11	1:N:123[B]:MET:HE3	1.50	0.91
1:H:49[B]:PHE:HE2	2:H:1134:PG4:H42	1.35	0.90
1:J:88[A]:ASP:HB2	1:J:90[A]:ARG:HD3	1.51	0.90
1:M:121:ALA:HB2	5:P:1131:EDO:H12	1.50	0.89
1:O:17[B]:LEU:HD13	1:O:58[B]:ILE:HD12	1.55	0.89
1:P:49[B]:PHE:HE2	2:P:1127:PG4:H42	1.37	0.88
1:D:49:PHE:CE2	2:D:1126:PG4:H42	2.09	0.87
1:E:19[B]:LEU:HD21	1:E:47[B]:ARG:HD3	1.58	0.85
1:O:17[B]:LEU:CD1	1:O:58[B]:ILE:HD12	2.06	0.85
1:A:73[B]:ARG:NH1	1:F:73[B]:ARG:HD2	1.92	0.84
1:L:102:VAL:HG22	1:L:107[B]:ILE:HD13	1.59	0.82
1:N:92[B]:LEU:HD21	1:N:123[B]:MET:HE2	1.60	0.82
1:G:93:ALA:H	1:G:122:GLN:HE22	1.28	0.81
1:C:123[B]:MET:HE2	1:C:123[B]:MET:HA	1.62	0.80
1:E:73[B]:ARG:HG3	1:E:73[B]:ARG:NH1	1.87	0.79
1:H:111:ARG:HD3	1:N:73[B]:ARG:CZ	2.14	0.78
1:N:92[B]:LEU:HD21	1:N:123[B]:MET:CE	2.17	0.75
1:F:120[A]:MET:HE2	1:F:120[A]:MET:HA	1.70	0.74
1:F:86:LEU:HD12	1:F:90[B]:ARG:HE	1.53	0.73
1:P:115:ASP:CB	4:P:1128:ACT:H1	2.21	0.71
5:C:1131:EDO:H11	10:C:2073:HOH:O	1.90	0.70
1:E:118[B]:GLN:HG3	10:E:2079:HOH:O	1.92	0.70
1:I:49:PHE:CE2	2:I:1126:PG4:H42	2.27	0.70
1:C:123[B]:MET:HA	1:C:123[B]:MET:CE	2.21	0.69
1:E:19[B]:LEU:HD21	1:E:47[B]:ARG:CD	2.22	0.69
1:B:102:VAL:HG22	1:B:107[B]:ILE:HD13	1.72	0.69
1:J:61[B]:GLU:CD	1:J:83[B]:ARG:HH21	1.98	0.69
1:M:94[B]:ILE:HG21	2:M:1126:PG4:H72	1.75	0.69
1:P:115:ASP:CB	4:P:1128:ACT:CH3	2.71	0.69
1:D:69:GLY:HA2	3:D:1127:PEG:H21	1.76	0.68
1:C:19[B]:LEU:HD21	1:C:47[B]:ARG:HG2	1.74	0.68
1:P:115:ASP:HB3	4:P:1128:ACT:CH3	2.23	0.68
1:P:115:ASP:HB3	4:P:1128:ACT:H1	1.75	0.68
5:C:1131:EDO:H22	10:C:2146:HOH:O	1.94	0.67
1:N:92[B]:LEU:CG	1:N:123[B]:MET:HE2	2.25	0.66
1:P:49[B]:PHE:CE2	2:P:1127:PG4:C4	2.76	0.66
1:D:49:PHE:HE2	2:D:1126:PG4:H42	1.56	0.66
1:J:88[A]:ASP:CB	1:J:90[A]:ARG:HD3	2.24	0.66
1:N:123[A]:MET:HG3	7:N:1137:PGE:H5	1.78	0.65
1:J:61[B]:GLU:OE1	1:J:83[B]:ARG:NH2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:120[A]:MET:HB2	5:P:1130:EDO:H21	1.80	0.64
1:F:94[A]:ILE:HD12	1:F:119:PHE:HB2	1.78	0.64
1:J:61[B]:GLU:OE2	1:J:83[B]:ARG:CZ	2.43	0.63
1:I:1[A]:MET:H3	2:I:1130:PG4:H41	1.63	0.63
1:B:49:PHE:CE2	2:B:1128:PG4:H42	2.35	0.62
1:C:116:LEU:HD11	1:C:120[A]:MET:HE2	1.82	0.62
1:A:73[B]:ARG:CZ	1:F:73[B]:ARG:HD2	2.29	0.62
1:I:1[B]:MET:HE1	1:I:9:LEU:HD22	1.80	0.62
1:F:94[A]:ILE:HD11	1:F:114:PHE:CD2	2.35	0.61
1:O:116:LEU:O	1:O:120[B]:MET:HG2	2.01	0.61
1:L:102:VAL:HG22	1:L:107[B]:ILE:CD1	2.28	0.61
1:E:19[B]:LEU:HD23	1:E:47[B]:ARG:HD3	1.82	0.60
1:I:1[B]:MET:H2	2:I:1130:PG4:H41	1.65	0.60
1:N:119[B]:PHE:CE2	2:N:1134:PG4:H52	2.36	0.60
1:H:111:ARG:HD3	1:N:73[B]:ARG:NE	2.16	0.60
1:J:88[A]:ASP:CB	1:J:90[A]:ARG:HH11	2.15	0.59
1:G:47[A]:ARG:NH1	1:G:51[A]:SER:OG	2.36	0.59
9:I:1129:PG6:H92	10:I:2134:HOH:O	2.01	0.59
1:E:73[B]:ARG:CG	1:E:73[B]:ARG:NH1	2.50	0.58
1:N:86:LEU:HD11	1:N:123[B]:MET:HE1	1.87	0.57
1:N:119[B]:PHE:HE2	2:N:1134:PG4:H52	1.68	0.57
1:N:134:HIS:N	1:O:73[A]:ARG:HH22	2.02	0.57
1:E:94[B]:ILE:CD1	1:E:118[B]:GLN:HE21	2.17	0.57
1:O:57:ALA:HB3	1:O:85:THR:HB	1.85	0.57
1:P:115:ASP:HB2	4:P:1128:ACT:H1	1.86	0.57
1:N:92[B]:LEU:CD1	1:N:123[B]:MET:HE1	2.11	0.56
4:C:1129:ACT:H3	1:G:123:MET:HB2	1.88	0.56
1:O:36:PRO:HA	4:P:1128:ACT:H3	1.87	0.56
1:C:92:LEU:HD21	1:C:123[B]:MET:HE3	1.88	0.55
1:N:1:MET:H1	9:N:1135:PG6:H22	1.70	0.55
1:N:73[B]:ARG:HG2	1:N:103:ALA:HA	1.87	0.55
1:H:49[B]:PHE:CE2	2:H:1134:PG4:C4	2.85	0.55
1:O:94[B]:ILE:CD1	1:O:119[B]:PHE:HD2	2.20	0.55
1:P:120[B]:MET:HB2	5:P:1130:EDO:H21	1.89	0.55
1:C:119:PHE:O	1:C:123[B]:MET:HG2	2.07	0.54
1:N:120[A]:MET:HE3	10:N:2119:HOH:O	1.81	0.54
7:D:1130:PGE:H52	10:D:2109:HOH:O	2.07	0.54
1:H:73[A]:ARG:HG2	1:H:103:ALA:HA	1.88	0.54
1:L:17:LEU:HG	1:L:58[B]:ILE:HG22	1.90	0.54
1:E:94[B]:ILE:HD12	1:E:118[B]:GLN:HE21	1.72	0.54
1:B:14:VAL:O	1:B:58[B]:ILE:HG21	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:93:ALA:H	1:G:122:GLN:NE2	2.00	0.54
1:K:53[B]:LEU:HD11	1:K:123[B]:MET:SD	2.49	0.53
1:H:111:ARG:HH11	1:N:73[B]:ARG:NH2	2.07	0.52
1:P:115:ASP:CB	4:P:1128:ACT:H2	2.38	0.52
1:A:97:MET:HE2	1:B:97:MET:HE2	1.92	0.52
1:P:53[A]:LEU:HD12	2:P:1127:PG4:H31	1.90	0.52
1:P:4[A]:LEU:HD23	5:P:1131:EDO:H22	1.92	0.52
1:I:49:PHE:HE2	2:I:1126:PG4:H42	1.72	0.52
4:M:1128:ACT:H1	10:M:2045:HOH:O	2.09	0.52
5:P:1131:EDO:H11	10:P:2003:HOH:O	2.09	0.52
1:K:1:MET:H2	3:K:1128:PEG:H12	1.74	0.52
1:D:29:ASP:HB3	2:D:1129:PG4:H31	1.92	0.51
1:O:94[B]:ILE:HD11	1:O:114:PHE:CD2	2.45	0.51
1:K:1:MET:N	3:K:1128:PEG:H12	2.26	0.51
1:L:28[B]:GLU:HG2	1:L:43:ARG:HH12	1.76	0.51
1:C:19[B]:LEU:HD21	1:C:47[B]:ARG:NE	2.25	0.51
1:I:19[B]:LEU:HD21	1:I:50:LEU:HB3	1.92	0.51
1:A:84:PHE:CD1	1:A:92[A]:LEU:HD23	2.46	0.51
1:C:19[B]:LEU:CD2	1:C:47[B]:ARG:NE	2.75	0.50
1:B:94[B]:ILE:HG21	2:B:1128:PG4:H72	1.93	0.50
1:L:28[B]:GLU:HG3	10:L:2024:HOH:O	2.12	0.50
1:O:73[B]:ARG:HG3	1:O:103:ALA:HA	1.93	0.50
1:O:36:PRO:CA	4:P:1128:ACT:H3	2.41	0.50
1:N:116:LEU:O	1:N:120[B]:MET:HG2	2.11	0.50
1:P:86:LEU:HD11	1:P:92[B]:LEU:HD11	1.94	0.50
3:F:1126:PEG:H22	10:F:2091:HOH:O	2.12	0.49
1:P:115:ASP:HB2	4:P:1128:ACT:CH3	2.41	0.49
1:N:123[B]:MET:HG3	7:N:1137:PGE:H5	1.93	0.49
1:J:61[B]:GLU:CD	1:J:83[B]:ARG:NH2	2.69	0.49
1:M:103:ALA:HB2	3:M:1127:PEG:H12	1.95	0.49
1:N:92[B]:LEU:CD2	1:N:123[B]:MET:CE	2.74	0.49
1:B:127:PRO:HG3	1:H:47[B]:ARG:HD2	1.95	0.49
1:E:73[B]:ARG:HH11	1:E:73[B]:ARG:CB	2.27	0.48
1:P:49[B]:PHE:CZ	2:P:1127:PG4:H42	2.44	0.48
7:N:1137:PGE:H2	1:P:13:ARG:HG2	1.95	0.48
1:G:37:MET:HE1	2:G:1126:PG4:H12	1.96	0.48
1:K:94[B]:ILE:HG21	2:K:1126:PG4:H72	1.94	0.48
1:E:97:MET:HE2	1:F:97:MET:HE2	1.96	0.47
1:K:72:ALA:HA	3:K:1128:PEG:H32	1.96	0.47
1:G:91[B]:THR:HG22	10:G:2099:HOH:O	2.14	0.47
1:H:103:ALA:HB2	5:H:1139:EDO:H11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:61[B]:GLU:OE2	1:J:83[B]:ARG:NH2	2.48	0.47
1:H:130:HIS:HB2	1:H:132:HIS:O	2.14	0.47
1:I:83[B]:ARG:HA	1:I:92:LEU:O	2.15	0.47
1:F:104:ASP:HA	2:F:1128:PG4:H62	1.97	0.46
1:C:123[B]:MET:CE	1:C:123[B]:MET:CA	2.90	0.46
1:G:97:MET:HE2	1:H:97:MET:HE2	1.96	0.46
1:I:83[A]:ARG:HA	1:I:92:LEU:O	2.15	0.46
1:B:49:PHE:HE2	2:B:1128:PG4:H42	1.80	0.46
1:L:28[B]:GLU:HG2	1:L:43:ARG:NH1	2.31	0.46
1:J:88[A]:ASP:CG	1:J:90[A]:ARG:HH12	2.13	0.46
1:L:73[A]:ARG:HH21	3:L:1127:PEG:H22	1.80	0.46
1:A:57:ALA:HB3	1:A:85[B]:THR:HG22	1.98	0.45
1:F:47[A]:ARG:NH1	1:F:51[A]:SER:OG	2.48	0.45
1:F:79:GLU:HA	1:F:97:MET:HG2	1.98	0.45
1:M:94[B]:ILE:HD11	1:M:114:PHE:CD2	2.51	0.45
1:C:19[B]:LEU:HD21	1:C:47[B]:ARG:CG	2.43	0.45
1:P:53[A]:LEU:HA	1:P:53[A]:LEU:HD23	1.83	0.45
1:C:14:VAL:O	1:C:58[B]:ILE:HG21	2.17	0.45
1:C:123[B]:MET:HE2	1:C:123[B]:MET:CA	2.33	0.45
2:D:1129:PG4:H11	1:O:63:HIS:HB3	1.99	0.45
1:E:118[A]:GLN:HG3	1:E:122:GLN:HE21	1.81	0.45
1:H:131[B]:HIS:CE1	1:H:132:HIS:HD2	2.34	0.45
1:N:92[B]:LEU:CG	1:N:123[B]:MET:CE	2.85	0.45
1:B:52[B]:GLN:NE2	1:B:52[B]:GLN:HA	2.31	0.44
1:F:94[A]:ILE:HD11	1:F:114:PHE:HD2	1.82	0.44
1:J:90[B]:ARG:NH1	1:J:124:ALA:O	2.41	0.44
2:D:1129:PG4:H31	2:D:1129:PG4:H12	1.65	0.44
1:K:94[B]:ILE:HG23	2:K:1126:PG4:H82	2.00	0.44
1:F:37[B]:MET:HE3	1:F:114:PHE:HZ	1.83	0.44
1:J:79:GLU:HA	1:J:97:MET:HG2	2.00	0.44
1:J:90[B]:ARG:HH22	1:J:125:PRO:HA	1.83	0.44
1:P:84:PHE:CD1	1:P:92[A]:LEU:HD23	2.53	0.43
1:M:118:GLN:NE2	4:M:1128:ACT:H3	2.33	0.43
1:M:97:MET:HE2	1:N:97:MET:HE2	2.00	0.43
1:B:86:LEU:HD12	1:B:90:ARG:HD2	2.00	0.43
2:D:1129:PG4:H32	10:D:2128:HOH:O	2.18	0.43
1:J:53:LEU:HA	1:J:54:PRO:HD3	1.88	0.42
1:O:53:LEU:HB2	2:O:1126:PG4:H31	2.01	0.42
1:H:53[A]:LEU:HG	1:H:86:LEU:HD21	2.01	0.42
1:M:79:GLU:HA	1:M:97:MET:HG2	2.01	0.42
1:M:94[B]:ILE:HD12	1:M:119:PHE:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:94[B]:ILE:HG23	2:O:1126:PG4:H82	2.01	0.42
1:D:14:VAL:O	1:D:58[B]:ILE:HG21	2.19	0.42
1:F:59:ASP:CG	8:F:1130:HIS:HE2	2.28	0.42
1:H:79:GLU:HA	1:H:97:MET:HG2	2.02	0.42
1:B:52[B]:GLN:NE2	1:B:52[B]:GLN:CA	2.82	0.42
1:J:19[B]:LEU:HD11	1:J:50:LEU:HD13	2.01	0.42
1:N:14:VAL:O	1:N:58[B]:ILE:HG21	2.19	0.42
1:D:29:ASP:HB3	2:D:1129:PG4:C3	2.49	0.42
1:M:123[B]:MET:HE2	1:M:123[B]:MET:HB3	1.69	0.42
3:O:1128:PEG:H21	10:O:2078:HOH:O	2.19	0.42
1:N:79:GLU:HA	1:N:97:MET:HG2	2.01	0.42
1:B:94[A]:ILE:HD11	1:B:119:PHE:HA	2.02	0.41
1:K:53[B]:LEU:HD12	1:K:53[B]:LEU:HA	1.92	0.41
1:N:72:ALA:C	1:N:73[A]:ARG:HG3	2.44	0.41
1:O:17[B]:LEU:CD1	1:O:58[B]:ILE:CD1	2.89	0.41
1:L:100:PHE:HB3	1:L:107[B]:ILE:HD12	2.02	0.41
1:M:101:ASP:HB3	3:M:1127:PEG:H22	2.02	0.41
1:O:94[B]:ILE:HD13	1:O:119[B]:PHE:HD2	1.83	0.41
1:C:19[B]:LEU:CD2	1:C:47[B]:ARG:HG2	2.46	0.41
1:K:97:MET:HE2	1:L:97:MET:HE2	2.02	0.41
1:N:1:MET:HG3	9:N:1135:PG6:H22	2.03	0.41
1:N:123[A]:MET:HE2	7:N:1137:PGE:H42	2.01	0.41
1:N:1:MET:N	9:N:1135:PG6:H42	2.35	0.41
1:N:1:MET:H1	9:N:1135:PG6:H42	1.85	0.41
1:K:79:GLU:HA	1:K:97:MET:HG2	2.01	0.41
9:I:1129:PG6:H22	10:I:2133:HOH:O	2.21	0.41
1:O:97:MET:HE2	1:P:97:MET:HE2	2.03	0.41
1:C:88:ASP:OD1	1:C:90:ARG:HG2	2.21	0.41
1:C:29:ASP:HB2	5:C:1131:EDO:H11	2.03	0.41
1:G:1[A]:MET:HG3	1:G:5:GLU:HB2	2.02	0.41
1:O:94[B]:ILE:HD12	1:O:119[B]:PHE:CD2	2.56	0.41
1:E:120[A]:MET:HA	1:E:120[A]:MET:HE2	2.02	0.41
1:I:19[B]:LEU:HD12	1:I:19[B]:LEU:HA	1.74	0.41
1:O:36:PRO:HA	4:P:1128:ACT:CH3	2.50	0.40
1:L:107[B]:ILE:HD12	1:L:107[B]:ILE:HG23	1.87	0.40
1:A:73[B]:ARG:HH11	1:F:73[B]:ARG:HD2	1.78	0.40
1:G:53:LEU:HD12	1:G:53:LEU:HA	2.00	0.40
1:K:94[B]:ILE:CG2	2:K:1126:PG4:H82	2.51	0.40
1:C:97:MET:HE2	1:D:97:MET:HE2	2.03	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	138/135 (102%)	135 (98%)	3 (2%)	0	100	100
1	B	140/135 (104%)	138 (99%)	2 (1%)	0	100	100
1	C	134/135 (99%)	133 (99%)	1 (1%)	0	100	100
1	D	134/135 (99%)	133 (99%)	1 (1%)	0	100	100
1	E	133/135 (98%)	129 (97%)	4 (3%)	0	100	100
1	F	135/135 (100%)	134 (99%)	1 (1%)	0	100	100
1	G	129/135 (96%)	127 (98%)	2 (2%)	0	100	100
1	H	138/135 (102%)	133 (96%)	5 (4%)	0	100	100
1	I	135/135 (100%)	133 (98%)	2 (2%)	0	100	100
1	J	136/135 (101%)	132 (97%)	4 (3%)	0	100	100
1	K	130/135 (96%)	129 (99%)	1 (1%)	0	100	100
1	L	135/135 (100%)	132 (98%)	3 (2%)	0	100	100
1	M	134/135 (99%)	131 (98%)	3 (2%)	0	100	100
1	N	142/135 (105%)	141 (99%)	1 (1%)	0	100	100
1	O	134/135 (99%)	133 (99%)	1 (1%)	0	100	100
1	P	138/135 (102%)	136 (99%)	2 (1%)	0	100	100
All	All	2165/2160 (100%)	2129 (98%)	36 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	109/103 (106%)	109 (100%)	0	100	100
1	B	112/103 (109%)	111 (99%)	1 (1%)	70	48
1	C	105/103 (102%)	105 (100%)	0	100	100
1	D	106/103 (103%)	106 (100%)	0	100	100
1	E	104/103 (101%)	101 (97%)	3 (3%)	37	9
1	F	107/103 (104%)	105 (98%)	2 (2%)	50	20
1	G	101/103 (98%)	101 (100%)	0	100	100
1	H	111/103 (108%)	109 (98%)	2 (2%)	51	22
1	I	107/103 (104%)	105 (98%)	2 (2%)	50	20
1	J	108/103 (105%)	99 (92%)	9 (8%)	10	1
1	K	101/103 (98%)	100 (99%)	1 (1%)	68	43
1	L	106/103 (103%)	104 (98%)	2 (2%)	50	20
1	M	105/103 (102%)	105 (100%)	0	100	100
1	N	115/103 (112%)	112 (97%)	3 (3%)	40	12
1	O	106/103 (103%)	106 (100%)	0	100	100
1	P	109/103 (106%)	109 (100%)	0	100	100
All	All	1712/1648 (104%)	1687 (98%)	25 (2%)	65	28

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4	LEU
1	E	91	THR
1	E	120[A]	MET
1	E	120[B]	MET
1	F	73[A]	ARG
1	F	73[B]	ARG
1	H	90	ARG
1	H	130	HIS
1	I	91[A]	THR
1	I	91[B]	THR
1	J	1[A]	MET
1	J	1[B]	MET
1	J	51[A]	SER
1	J	51[B]	SER
1	J	53	LEU
1	J	88[A]	ASP

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Mol	Chain	Res	Type
1	J	88[B]	ASP
1	J	90[A]	ARG
1	J	90[B]	ARG
1	K	90	ARG
1	L	90[A]	ARG
1	L	90[B]	ARG
1	N	17[A]	LEU
1	N	17[B]	LEU
1	N	131	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	34	ASN
1	G	122	GLN
1	H	132	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

80 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
2	PG4	O	1129	-	12,12,12	0.66	0	11,11,11	0.73	0
3	PEG	O	1128	-	6,6,6	0.48	0	5,5,5	0.33	0
5	EDO	P	1132	-	3,3,3	0.45	0	2,2,2	0.16	0
2	PG4	L	1126	-	12,12,12	0.43	0	11,11,11	0.50	0
2	PG4	A	1126	-	12,12,12	0.49	0	11,11,11	0.42	0
3	PEG	M	1127	-	6,6,6	0.43	0	5,5,5	0.71	0
3	PEG	F	1127	-	6,6,6	0.53	0	5,5,5	0.31	0
6	PG5	A	1130	-	11,11,11	0.58	0	10,10,10	0.40	0
4	ACT	J	1127	-	3,3,3	0.87	0	3,3,3	0.76	0
4	ACT	P	1128	-	3,3,3	0.84	0	3,3,3	0.79	0
4	ACT	A	1128	-	3,3,3	0.88	0	3,3,3	1.05	0
5	EDO	D	1131	-	3,3,3	0.38	0	2,2,2	0.34	0
2	PG4	G	1128	-	12,12,12	0.49	0	11,11,11	0.67	0
2	PG4	H	1134	-	12,12,12	0.49	0	11,11,11	0.44	0
5	EDO	L	1130	-	3,3,3	0.42	0	2,2,2	0.37	0
3	PEG	B	1131	-	6,6,6	0.52	0	5,5,5	0.47	0
2	PG4	B	1128	-	12,12,12	0.54	0	11,11,11	0.33	0
2	PG4	J	1126	-	12,12,12	0.50	0	11,11,11	0.53	0
5	EDO	G	1130	-	3,3,3	0.42	0	2,2,2	0.18	0
5	EDO	D	1134	-	3,3,3	0.46	0	2,2,2	0.32	0
3	PEG	L	1128	-	6,6,6	0.48	0	5,5,5	0.39	0
7	PGE	M	1129	-	9,9,9	0.41	0	8,8,8	0.71	0
2	PG4	D	1126	-	12,12,12	0.60	0	11,11,11	0.53	0
5	EDO	H	1139	-	3,3,3	0.26	0	2,2,2	0.77	0
5	EDO	G	1129	-	3,3,3	0.44	0	2,2,2	0.31	0
2	PG4	E	1126	-	12,12,12	0.56	0	11,11,11	0.45	0
2	PG4	D	1128	-	12,12,12	0.54	0	11,11,11	0.36	0
3	PEG	L	1127	-	6,6,6	0.45	0	5,5,5	0.38	0
2	PG4	M	1126	-	12,12,12	0.57	0	11,11,11	0.63	0
5	EDO	A	1129	-	3,3,3	0.43	0	2,2,2	0.43	0
5	EDO	D	1133	-	3,3,3	0.44	0	2,2,2	0.39	0
2	PG4	K	1126	-	12,12,12	0.50	0	11,11,11	0.49	0
2	PG4	D	1129	-	12,12,12	0.50	0	11,11,11	0.50	0
3	PEG	I	1127	-	6,6,6	0.53	0	5,5,5	0.28	0
7	PGE	C	1130	-	9,9,9	0.56	0	8,8,8	0.46	0
9	PG6	N	1135	-	17,17,17	0.55	0	16,16,16	0.50	0
2	PG4	H	1138	-	12,12,12	0.52	0	11,11,11	0.25	0
7	PGE	K	1130	-	9,9,9	0.43	0	8,8,8	0.47	0
2	PG4	C	1127	-	12,12,12	0.58	0	11,11,11	0.51	0
4	ACT	L	1129	-	3,3,3	0.62	0	3,3,3	1.10	0
5	EDO	D	1132	-	3,3,3	0.40	0	2,2,2	0.48	0
5	EDO	P	1131	-	3,3,3	0.67	0	2,2,2	0.37	0
2	PG4	B	1129	-	12,12,12	0.55	0	11,11,11	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ACT	K	1129	-	3,3,3	0.81	0	3,3,3	0.65	0
2	PG4	P	1127	-	12,12,12	0.46	0	11,11,11	0.76	0
4	ACT	C	1128	-	3,3,3	0.71	0	3,3,3	1.18	0
7	PGE	N	1137	-	9,9,9	0.45	0	8,8,8	0.34	0
5	EDO	F	1129	-	3,3,3	0.45	0	2,2,2	0.37	0
2	PG4	F	1125	-	12,12,12	0.55	0	11,11,11	0.38	0
5	EDO	M	1130	-	3,3,3	0.44	0	2,2,2	0.37	0
4	ACT	G	1127	-	3,3,3	0.80	0	3,3,3	0.71	0
3	PEG	K	1128	-	6,6,6	0.47	0	5,5,5	0.22	0
3	PEG	H	1135	-	6,6,6	0.44	0	5,5,5	0.31	0
2	PG4	F	1128	-	12,12,12	0.56	0	11,11,11	0.39	0
2	PG4	O	1126	-	12,12,12	0.58	0	11,11,11	0.41	0
3	PEG	K	1127	-	6,6,6	0.45	0	5,5,5	0.52	0
8	HIS	F	1130	-	10,11,11	0.75	1 (10%)	10,14,14	1.26	1 (10%)
4	ACT	M	1128	-	3,3,3	1.04	0	3,3,3	1.62	1 (33%)
4	ACT	H	1136	-	3,3,3	0.70	0	3,3,3	1.07	0
2	PG4	I	1126	-	12,12,12	0.49	0	11,11,11	0.43	0
5	EDO	P	1130	-	3,3,3	0.49	0	2,2,2	0.10	0
5	EDO	C	1131	-	3,3,3	0.32	0	2,2,2	0.87	0
9	PG6	I	1129	-	17,17,17	0.66	0	16,16,16	0.51	0
3	PEG	B	1130	-	6,6,6	0.47	0	5,5,5	0.24	0
3	PEG	D	1127	-	6,6,6	0.46	0	5,5,5	0.57	0
5	EDO	P	1129	-	3,3,3	0.33	0	2,2,2	0.41	0
3	PEG	O	1127	-	6,6,6	0.40	0	5,5,5	0.35	0
7	PGE	N	1136	-	9,9,9	0.48	0	8,8,8	0.55	0
7	PGE	D	1130	-	9,9,9	0.73	0	8,8,8	1.10	0
4	ACT	H	1137	-	3,3,3	0.82	0	3,3,3	0.75	0
3	PEG	F	1126	-	6,6,6	0.36	0	5,5,5	0.52	0
2	PG4	G	1126	-	12,12,12	0.62	0	11,11,11	0.51	0
2	PG4	I	1130	-	12,12,12	0.54	0	11,11,11	0.19	0
3	PEG	I	1128	-	6,6,6	0.49	0	5,5,5	0.22	0
3	PEG	A	1127	-	6,6,6	0.32	0	5,5,5	0.79	0
5	EDO	P	1133	-	3,3,3	0.45	0	2,2,2	0.36	0
4	ACT	C	1129	-	3,3,3	0.83	0	3,3,3	0.82	0
5	EDO	N	1138	-	3,3,3	0.48	0	2,2,2	0.38	0
2	PG4	N	1134	-	12,12,12	0.49	0	11,11,11	0.39	0
5	EDO	M	1131	-	3,3,3	0.37	0	2,2,2	0.46	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
2	PG4	O	1129	-	-	1/10/10/10	-
5	EDO	H	1139	-	-	1/1/1/1	-
3	PEG	O	1128	-	-	3/4/4/4	-
2	PG4	N	1134	-	-	2/10/10/10	-
5	EDO	G	1129	-	-	1/1/1/1	-
5	EDO	P	1132	-	-	0/1/1/1	-
2	PG4	L	1126	-	-	2/10/10/10	-
2	PG4	A	1126	-	-	1/10/10/10	-
2	PG4	I	1126	-	-	5/10/10/10	-
3	PEG	M	1127	-	-	3/4/4/4	-
5	EDO	P	1130	-	-	1/1/1/1	-
5	EDO	C	1131	-	-	1/1/1/1	-
5	EDO	D	1132	-	-	1/1/1/1	-
9	PG6	I	1129	-	-	4/15/15/15	-
5	EDO	P	1131	-	-	1/1/1/1	-
3	PEG	F	1127	-	-	3/4/4/4	-
2	PG4	B	1129	-	-	1/10/10/10	-
2	PG4	E	1126	-	-	2/10/10/10	-
2	PG4	D	1128	-	-	2/10/10/10	-
2	PG4	P	1127	-	-	2/10/10/10	-
3	PEG	B	1130	-	-	2/4/4/4	-
6	PG5	A	1130	-	-	4/9/9/9	-
3	PEG	D	1127	-	-	1/4/4/4	-
3	PEG	L	1127	-	-	2/4/4/4	-
7	PGE	N	1137	-	-	6/7/7/7	-
5	EDO	P	1129	-	-	0/1/1/1	-
2	PG4	M	1126	-	-	1/10/10/10	-
5	EDO	F	1129	-	-	0/1/1/1	-
5	EDO	A	1129	-	-	1/1/1/1	-
3	PEG	O	1127	-	-	4/4/4/4	-
2	PG4	K	1126	-	-	4/10/10/10	-
2	PG4	F	1125	-	-	3/10/10/10	-
5	EDO	D	1133	-	-	1/1/1/1	-
7	PGE	D	1130	-	-	4/7/7/7	-
7	PGE	N	1136	-	-	1/7/7/7	-
5	EDO	D	1131	-	-	0/1/1/1	-
5	EDO	M	1130	-	-	1/1/1/1	-
3	PEG	F	1126	-	-	4/4/4/4	-
2	PG4	G	1128	-	-	5/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PG4	H	1134	-	-	2/10/10/10	-
5	EDO	L	1130	-	-	1/1/1/1	-
3	PEG	B	1131	-	-	3/4/4/4	-
2	PG4	G	1126	-	-	2/10/10/10	-
2	PG4	D	1129	-	-	6/10/10/10	-
3	PEG	I	1127	-	-	3/4/4/4	-
2	PG4	B	1128	-	-	3/10/10/10	-
3	PEG	H	1135	-	-	3/4/4/4	-
3	PEG	K	1128	-	-	3/4/4/4	-
2	PG4	F	1128	-	-	3/10/10/10	-
2	PG4	O	1126	-	-	3/10/10/10	-
5	EDO	N	1138	-	-	1/1/1/1	-
2	PG4	J	1126	-	-	0/10/10/10	-
5	EDO	G	1130	-	-	1/1/1/1	-
7	PGE	C	1130	-	-	4/7/7/7	-
3	PEG	K	1127	-	-	2/4/4/4	-
9	PG6	N	1135	-	-	9/15/15/15	-
8	HIS	F	1130	-	-	1/8/8/8	0/1/1/1
2	PG4	I	1130	-	-	5/10/10/10	-
3	PEG	I	1128	-	-	4/4/4/4	-
3	PEG	A	1127	-	-	3/4/4/4	-
3	PEG	L	1128	-	-	1/4/4/4	-
5	EDO	D	1134	-	-	1/1/1/1	-
7	PGE	M	1129	-	-	1/7/7/7	-
5	EDO	P	1133	-	-	1/1/1/1	-
7	PGE	K	1130	-	-	1/7/7/7	-
2	PG4	H	1138	-	-	2/10/10/10	-
2	PG4	D	1126	-	-	3/10/10/10	-
2	PG4	C	1127	-	-	1/10/10/10	-
5	EDO	M	1131	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	1130	HIS	OXT-C	-2.19	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	1130	HIS	OXT-C-O	-2.75	117.85	124.08
4	M	1128	ACT	O-C-CH3	-2.01	114.30	122.53

There are no chirality outliers.

All (155) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	1130	PG4	O3-C5-C6-O4
9	N	1135	PG6	O2-C4-C5-O3
9	I	1129	PG6	O3-C6-C7-O4
2	F	1125	PG4	O2-C3-C4-O3
3	I	1127	PEG	O1-C1-C2-O2
3	I	1128	PEG	O2-C3-C4-O4
9	N	1135	PG6	O5-C10-C11-O6
2	D	1129	PG4	O2-C3-C4-O3
7	K	1130	PGE	O2-C3-C4-O3
6	A	1130	PG5	O3-C6-C7-O4
7	C	1130	PGE	O2-C3-C4-O3
2	D	1129	PG4	O4-C7-C8-O5
3	K	1127	PEG	O2-C3-C4-O4
3	M	1127	PEG	O1-C1-C2-O2
3	O	1127	PEG	O1-C1-C2-O2
7	M	1129	PGE	O1-C1-C2-O2
7	N	1137	PGE	O2-C3-C4-O3
2	E	1126	PG4	O2-C3-C4-O3
9	N	1135	PG6	O4-C8-C9-O5
2	B	1128	PG4	O1-C1-C2-O2
2	G	1126	PG4	O1-C1-C2-O2
2	I	1130	PG4	O1-C1-C2-O2
3	D	1127	PEG	O2-C3-C4-O4
3	F	1126	PEG	O1-C1-C2-O2
3	F	1127	PEG	O1-C1-C2-O2
3	K	1127	PEG	O1-C1-C2-O2
3	O	1128	PEG	O1-C1-C2-O2
7	N	1137	PGE	O1-C1-C2-O2
9	I	1129	PG6	O5-C10-C11-O6
2	D	1129	PG4	C1-C2-O2-C3
2	F	1125	PG4	O1-C1-C2-O2
2	I	1126	PG4	O1-C1-C2-O2
3	B	1130	PEG	O2-C3-C4-O4
3	I	1128	PEG	O1-C1-C2-O2
3	K	1128	PEG	O2-C3-C4-O4
3	O	1128	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
7	C	1130	PGE	O1-C1-C2-O2
2	O	1126	PG4	O4-C7-C8-O5
7	D	1130	PGE	O1-C1-C2-O2
7	N	1136	PGE	O1-C1-C2-O2
5	G	1130	EDO	O1-C1-C2-O2
5	H	1139	EDO	O1-C1-C2-O2
5	N	1138	EDO	O1-C1-C2-O2
2	E	1126	PG4	O1-C1-C2-O2
2	K	1126	PG4	O3-C5-C6-O4
2	G	1128	PG4	O3-C5-C6-O4
2	G	1128	PG4	O1-C1-C2-O2
3	A	1127	PEG	O1-C1-C2-O2
3	F	1126	PEG	O2-C3-C4-O4
3	L	1127	PEG	O1-C1-C2-O2
3	O	1127	PEG	O2-C3-C4-O4
2	I	1130	PG4	O2-C3-C4-O3
2	G	1128	PG4	O2-C3-C4-O3
5	A	1129	EDO	O1-C1-C2-O2
5	D	1134	EDO	O1-C1-C2-O2
5	L	1130	EDO	O1-C1-C2-O2
5	P	1131	EDO	O1-C1-C2-O2
5	P	1133	EDO	O1-C1-C2-O2
2	D	1129	PG4	O3-C5-C6-O4
3	B	1131	PEG	O2-C3-C4-O4
8	F	1130	HIS	OXT-C-CA-N
6	A	1130	PG5	O1-C2-C3-O2
2	D	1129	PG4	C5-C6-O4-C7
2	H	1134	PG4	O1-C1-C2-O2
7	C	1130	PGE	O3-C5-C6-O4
2	G	1126	PG4	C4-C3-O2-C2
2	G	1128	PG4	C3-C4-O3-C5
3	K	1128	PEG	C4-C3-O2-C2
3	M	1127	PEG	C4-C3-O2-C2
2	D	1128	PG4	C8-C7-O4-C6
2	F	1128	PG4	C1-C2-O2-C3
3	F	1126	PEG	C1-C2-O2-C3
3	A	1127	PEG	C1-C2-O2-C3
3	I	1128	PEG	C4-C3-O2-C2
3	B	1131	PEG	C4-C3-O2-C2
3	O	1127	PEG	C1-C2-O2-C3
2	B	1128	PG4	C4-C3-O2-C2
2	F	1125	PG4	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
3	O	1128	PEG	C1-C2-O2-C3
2	K	1126	PG4	O1-C1-C2-O2
2	K	1126	PG4	O4-C7-C8-O5
3	H	1135	PEG	O1-C1-C2-O2
3	F	1127	PEG	C4-C3-O2-C2
2	I	1130	PG4	C6-C5-O3-C4
5	M	1131	EDO	O1-C1-C2-O2
2	H	1138	PG4	O2-C3-C4-O3
3	H	1135	PEG	C4-C3-O2-C2
2	B	1128	PG4	C3-C4-O3-C5
2	D	1129	PG4	C3-C4-O3-C5
2	H	1138	PG4	O4-C7-C8-O5
2	I	1130	PG4	C4-C3-O2-C2
3	I	1127	PEG	C1-C2-O2-C3
2	I	1126	PG4	C4-C3-O2-C2
2	I	1126	PG4	C6-C5-O3-C4
9	N	1135	PG6	C6-C7-O4-C8
2	D	1126	PG4	O1-C1-C2-O2
2	F	1128	PG4	O1-C1-C2-O2
2	F	1128	PG4	O4-C7-C8-O5
2	O	1129	PG4	O1-C1-C2-O2
3	F	1127	PEG	C1-C2-O2-C3
2	O	1126	PG4	C6-C5-O3-C4
2	P	1127	PG4	C4-C3-O2-C2
2	O	1126	PG4	O1-C1-C2-O2
2	A	1126	PG4	O3-C5-C6-O4
5	D	1132	EDO	O1-C1-C2-O2
3	B	1130	PEG	O1-C1-C2-O2
7	D	1130	PGE	O3-C5-C6-O4
7	N	1137	PGE	O3-C5-C6-O4
9	N	1135	PG6	C9-C8-O4-C7
2	I	1126	PG4	O4-C7-C8-O5
3	A	1127	PEG	C4-C3-O2-C2
2	N	1134	PG4	C6-C5-O3-C4
7	N	1137	PGE	C1-C2-O2-C3
9	N	1135	PG6	O3-C6-C7-O4
2	K	1126	PG4	C6-C5-O3-C4
2	L	1126	PG4	C3-C4-O3-C5
3	F	1126	PEG	C4-C3-O2-C2
7	D	1130	PGE	O2-C3-C4-O3
2	D	1126	PG4	O3-C5-C6-O4
2	M	1126	PG4	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
9	I	1129	PG6	C5-C4-O2-C3
7	D	1130	PGE	C3-C4-O3-C5
3	H	1135	PEG	C1-C2-O2-C3
7	N	1137	PGE	C4-C3-O2-C2
2	L	1126	PG4	C4-C3-O2-C2
2	H	1134	PG4	C4-C3-O2-C2
7	C	1130	PGE	C1-C2-O2-C3
7	N	1137	PGE	C3-C4-O3-C5
2	D	1126	PG4	C3-C4-O3-C5
5	C	1131	EDO	O1-C1-C2-O2
5	D	1133	EDO	O1-C1-C2-O2
5	G	1129	EDO	O1-C1-C2-O2
5	P	1130	EDO	O1-C1-C2-O2
3	L	1127	PEG	O2-C3-C4-O4
2	G	1128	PG4	C8-C7-O4-C6
9	N	1135	PG6	C3-C2-O1-C1
3	I	1128	PEG	C1-C2-O2-C3
2	C	1127	PG4	C4-C3-O2-C2
6	A	1130	PG5	C6-C7-O4-C8
5	M	1130	EDO	O1-C1-C2-O2
2	N	1134	PG4	O1-C1-C2-O2
3	M	1127	PEG	O2-C3-C4-O4
9	N	1135	PG6	C8-C9-O5-C10
3	I	1127	PEG	O2-C3-C4-O4
9	I	1129	PG6	O4-C8-C9-O5
3	O	1127	PEG	C4-C3-O2-C2
3	K	1128	PEG	C1-C2-O2-C3
2	P	1127	PG4	O1-C1-C2-O2
3	L	1128	PEG	O1-C1-C2-O2
9	N	1135	PG6	O1-C2-C3-O2
2	B	1129	PG4	O1-C1-C2-O2
3	B	1131	PEG	O1-C1-C2-O2
6	A	1130	PG5	O2-C4-C5-O3
2	I	1126	PG4	C3-C4-O3-C5
2	D	1128	PG4	C1-C2-O2-C3

There are no ring outliers.

31 monomers are involved in 76 short contacts:

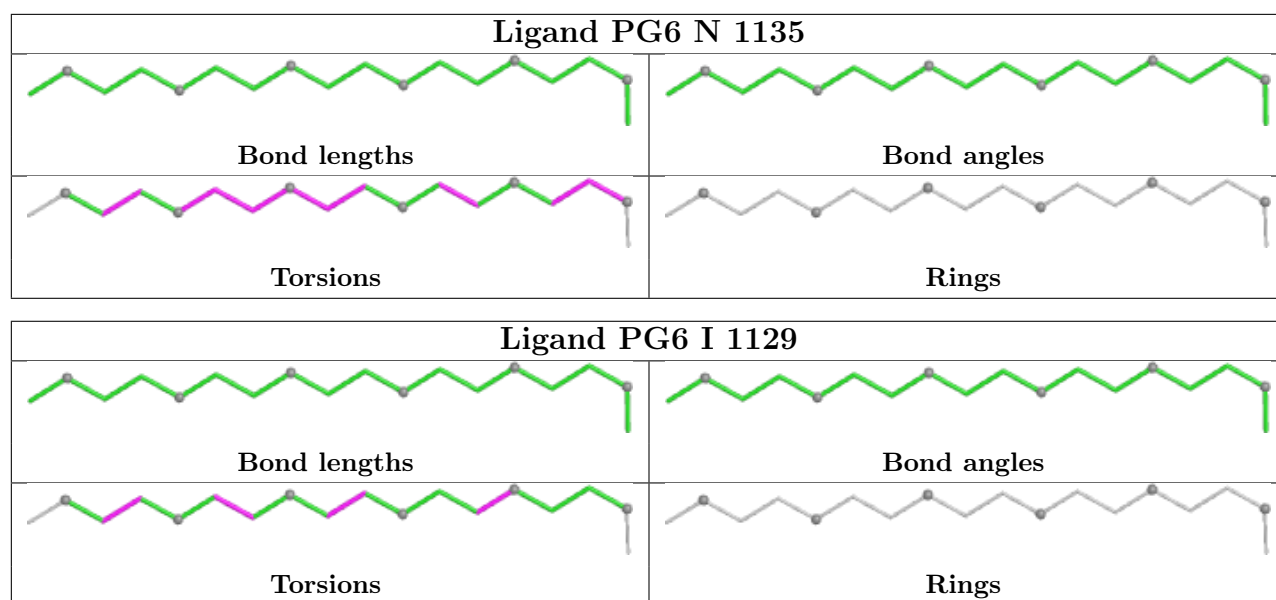
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	1128	PEG	1	0
3	M	1127	PEG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	P	1128	ACT	10	0
2	H	1134	PG4	3	0
2	B	1128	PG4	3	0
2	D	1126	PG4	2	0
5	H	1139	EDO	1	0
3	L	1127	PEG	1	0
2	M	1126	PG4	1	0
2	K	1126	PG4	3	0
2	D	1129	PG4	5	0
9	N	1135	PG6	4	0
5	P	1131	EDO	3	0
2	P	1127	PG4	5	0
7	N	1137	PGE	4	0
3	K	1128	PEG	3	0
2	F	1128	PG4	1	0
2	O	1126	PG4	2	0
8	F	1130	HIS	1	0
4	M	1128	ACT	2	0
2	I	1126	PG4	2	0
5	P	1130	EDO	2	0
5	C	1131	EDO	3	0
9	I	1129	PG6	2	0
3	D	1127	PEG	1	0
7	D	1130	PGE	1	0
3	F	1126	PEG	1	0
2	G	1126	PG4	1	0
2	I	1130	PG4	3	0
4	C	1129	ACT	1	0
2	N	1134	PG4	2	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	125/135 (92%)	0.73	20 (16%) 5 5	11, 24, 48, 94	15 (12%)
1	B	127/135 (94%)	0.58	10 (7%) 18 20	12, 24, 44, 71	16 (12%)
1	C	126/135 (93%)	0.06	10 (7%) 18 20	10, 17, 45, 86	10 (7%)
1	D	125/135 (92%)	0.05	8 (6%) 25 27	10, 17, 41, 85	12 (9%)
1	E	125/135 (92%)	1.38	35 (28%) 1 1	14, 30, 56, 76	10 (8%)
1	F	124/135 (91%)	0.59	11 (8%) 15 16	15, 23, 52, 72	14 (11%)
1	G	125/135 (92%)	0.12	9 (7%) 21 23	13, 18, 41, 82	7 (5%)
1	H	130/135 (96%)	0.60	15 (11%) 9 10	13, 22, 45, 67	13 (10%)
1	I	125/135 (92%)	0.23	8 (6%) 25 27	14, 21, 39, 96	13 (10%)
1	J	125/135 (92%)	0.38	13 (10%) 11 12	10, 22, 53, 76	14 (11%)
1	K	125/135 (92%)	0.42	11 (8%) 15 17	11, 23, 47, 79	7 (5%)
1	L	125/135 (92%)	0.81	20 (16%) 5 5	12, 24, 62, 90	12 (9%)
1	M	125/135 (92%)	0.23	6 (4%) 35 39	9, 20, 37, 55	11 (8%)
1	N	130/135 (96%)	0.14	7 (5%) 31 34	10, 17, 35, 81	17 (13%)
1	O	125/135 (92%)	0.05	8 (6%) 25 27	10, 15, 46, 70	12 (9%)
1	P	126/135 (93%)	-0.18	2 (1%) 70 74	8, 15, 29, 61	14 (11%)
All	All	2013/2160 (93%)	0.39	193 (9%) 13 14	8, 21, 47, 96	197 (9%)

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	86	LEU	5.9
1	E	45	ALA	5.3
1	A	87	ALA	5.2
1	E	86	LEU	4.9
1	F	87	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	124	ALA	4.7
1	J	91[A]	THR	4.7
1	F	124	ALA	4.6
1	L	87	ALA	4.5
1	L	125	PRO	4.3
1	N	125	PRO	4.2
1	H	124	ALA	4.2
1	H	130	HIS	4.1
1	J	89	GLY	4.1
1	E	49	PHE	4.0
1	D	125	PRO	4.0
1	E	125	PRO	4.0
1	E	51	SER	3.9
1	C	124	ALA	3.9
1	D	124	ALA	3.9
1	J	86	LEU	3.9
1	L	86	LEU	3.9
1	L	54	PRO	3.8
1	H	125	PRO	3.8
1	L	124	ALA	3.8
1	I	125	PRO	3.7
1	A	55	ALA	3.7
1	E	48	ALA	3.7
1	F	121	ALA	3.7
1	J	87	ALA	3.7
1	A	54	PRO	3.7
1	G	125	PRO	3.6
1	E	19[A]	LEU	3.6
1	C	86	LEU	3.6
1	E	16	ALA	3.6
1	J	125	PRO	3.6
1	L	91	THR	3.6
1	M	89	GLY	3.6
1	O	125	PRO	3.5
1	M	91	THR	3.5
1	M	125	PRO	3.5
1	E	52	GLN	3.4
1	L	19[A]	LEU	3.4
1	L	90[A]	ARG	3.4
1	L	17	LEU	3.3
1	C	91	THR	3.3
1	C	87	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	89	GLY	3.3
1	E	40	VAL	3.3
1	C	54	PRO	3.3
1	A	84	PHE	3.3
1	E	53	LEU	3.2
1	A	125	PRO	3.2
1	K	125	PRO	3.2
1	E	84	PHE	3.1
1	F	91	THR	3.1
1	E	54	PRO	3.1
1	E	46	ALA	3.1
1	J	90[A]	ARG	3.1
1	G	124	ALA	3.1
1	I	124	ALA	3.1
1	A	53[A]	LEU	3.1
1	L	49	PHE	3.1
1	E	58[A]	ILE	3.0
1	H	87	ALA	3.0
1	J	55	ALA	3.0
1	M	87	ALA	3.0
1	N	134	HIS	3.0
1	D	91[A]	THR	3.0
1	K	48	ALA	3.0
1	L	89	GLY	2.9
1	E	17	LEU	2.9
1	L	92[A]	LEU	2.9
1	O	86	LEU	2.9
1	A	85[A]	THR	2.9
1	O	91	THR	2.9
1	B	72	ALA	2.9
1	E	44	ALA	2.9
1	J	124	ALA	2.9
1	C	126	SER	2.9
1	J	54	PRO	2.9
1	J	53	LEU	2.9
1	N	131	HIS	2.8
1	I	91[A]	THR	2.8
1	A	92[A]	LEU	2.8
1	N	130[A]	HIS	2.8
1	K	87	ALA	2.8
1	N	91[A]	THR	2.8
1	E	87	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	132	HIS	2.7
1	E	56	THR	2.7
1	A	58	ILE	2.7
1	A	17[A]	LEU	2.6
1	J	50	LEU	2.6
1	L	50	LEU	2.6
1	A	91	THR	2.6
1	K	90	ARG	2.6
1	M	54	PRO	2.6
1	B	127	PRO	2.6
1	E	124	ALA	2.6
1	G	123	MET	2.6
1	O	87	ALA	2.6
1	A	40	VAL	2.6
1	K	88	ASP	2.6
1	A	90[A]	ARG	2.6
1	C	55	ALA	2.5
1	E	55	ALA	2.5
1	L	44	ALA	2.5
1	M	55	ALA	2.5
1	D	89	GLY	2.5
1	E	30	VAL	2.5
1	H	131[A]	HIS	2.5
1	F	92	LEU	2.5
1	E	89	GLY	2.5
1	E	31	VAL	2.5
1	B	52[A]	GLN	2.5
1	L	55	ALA	2.5
1	E	88	ASP	2.5
1	O	58[A]	ILE	2.5
1	L	16	ALA	2.4
1	D	90[A]	ARG	2.4
1	E	57	ALA	2.4
1	P	58[A]	ILE	2.4
1	B	56	THR	2.4
1	B	49	PHE	2.4
1	A	89	GLY	2.4
1	L	88	ASP	2.4
1	H	17[A]	LEU	2.4
1	H	91[A]	THR	2.4
1	A	48	ALA	2.3
1	H	103	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	O	124	ALA	2.3
1	F	54	PRO	2.3
1	K	123[A]	MET	2.3
1	K	91	THR	2.3
1	K	58	ILE	2.3
1	G	90	ARG	2.3
1	K	53[A]	LEU	2.3
1	E	39	THR	2.3
1	E	47[A]	ARG	2.3
1	H	133	HIS	2.3
1	D	86	LEU	2.3
1	F	86	LEU	2.3
1	N	58[A]	ILE	2.3
1	D	51[A]	SER	2.3
1	A	16	ALA	2.2
1	B	124	ALA	2.2
1	E	23	CYS	2.2
1	H	54	PRO	2.2
1	A	88	ASP	2.2
1	L	85	THR	2.2
1	D	92	LEU	2.2
1	O	19[A]	LEU	2.2
1	B	58[A]	ILE	2.2
1	B	87	ALA	2.2
1	C	88	ASP	2.2
1	C	90	ARG	2.2
1	E	91	THR	2.2
1	K	89	GLY	2.2
1	G	86	LEU	2.2
1	J	19[A]	LEU	2.2
1	H	16	ALA	2.2
1	I	54	PRO	2.2
1	E	42	GLY	2.2
1	E	117	GLY	2.2
1	J	49	PHE	2.2
1	E	22	ALA	2.1
1	I	87	ALA	2.1
1	E	21	GLY	2.1
1	G	89	GLY	2.1
1	I	92	LEU	2.1
1	K	19[A]	LEU	2.1
1	F	56	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	88	ASP	2.1
1	I	58[A]	ILE	2.1
1	I	123	MET	2.1
1	E	41	HIS	2.1
1	F	51[A]	SER	2.1
1	L	21	GLY	2.1
1	P	126	SER	2.1
1	B	89	GLY	2.1
1	H	105	GLY	2.1
1	C	125	PRO	2.1
1	A	56	THR	2.0
1	G	87	ALA	2.0
1	H	72	ALA	2.0
1	B	19[A]	LEU	2.0
1	G	53	LEU	2.0
1	F	117	GLY	2.0
1	L	47[A]	ARG	2.0
1	N	132	HIS	2.0
1	H	53[A]	LEU	2.0
1	O	88	ASP	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 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	H	1139	4/4	0.73	0.20	39,43,49,50	0
4	ACT	H	1137	4/4	0.77	0.16	43,46,54,62	0
4	ACT	K	1129	4/4	0.80	0.13	47,50,50,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PG4	F	1128	13/13	0.81	0.16	31,42,51,57	13
3	PEG	B	1131	7/7	0.81	0.18	41,54,63,72	0
3	PEG	L	1128	7/7	0.81	0.18	31,37,40,49	7
5	EDO	F	1129	4/4	0.82	0.17	46,50,52,59	0
3	PEG	K	1127	7/7	0.82	0.12	45,54,59,61	0
3	PEG	K	1128	7/7	0.83	0.15	44,52,56,58	0
5	EDO	M	1130	4/4	0.83	0.15	52,58,62,67	0
5	EDO	M	1131	4/4	0.83	0.17	49,50,54,62	0
8	HIS	F	1130	11/11	0.83	0.11	36,42,64,70	0
2	PG4	D	1128	13/13	0.84	0.14	33,41,53,55	0
5	EDO	L	1130	4/4	0.85	0.15	37,52,55,62	0
2	PG4	I	1130	13/13	0.85	0.13	43,51,57,60	0
4	ACT	G	1127	4/4	0.85	0.13	48,53,55,61	0
3	PEG	F	1126	7/7	0.85	0.12	38,50,56,65	0
2	PG4	G	1128	13/13	0.86	0.18	27,31,43,45	13
3	PEG	O	1128	7/7	0.86	0.13	44,47,55,58	0
5	EDO	A	1129	4/4	0.86	0.12	57,60,64,67	0
3	PEG	A	1127	7/7	0.86	0.14	33,51,65,70	0
5	EDO	P	1133	4/4	0.86	0.11	44,48,56,62	0
7	PGE	D	1130	10/10	0.86	0.11	22,34,45,47	0
5	EDO	G	1130	4/4	0.86	0.13	38,39,45,46	0
5	EDO	N	1138	4/4	0.87	0.12	42,45,46,51	0
2	PG4	A	1126	13/13	0.87	0.14	26,48,81,81	0
6	PG5	A	1130	12/12	0.87	0.12	33,40,49,55	0
2	PG4	D	1129	13/13	0.87	0.12	27,42,54,56	0
7	PGE	N	1137	10/10	0.87	0.15	28,35,42,52	10
5	EDO	D	1132	4/4	0.87	0.15	45,48,50,54	0
9	PG6	N	1135	18/18	0.87	0.14	28,46,60,64	0
3	PEG	D	1127	7/7	0.88	0.13	35,48,54,60	0
2	PG4	H	1138	13/13	0.88	0.13	30,41,57,66	0
3	PEG	M	1127	7/7	0.88	0.13	34,40,52,53	0
3	PEG	F	1127	7/7	0.88	0.09	39,46,53,56	0
5	EDO	D	1134	4/4	0.88	0.09	48,51,57,59	0
9	PG6	I	1129	18/18	0.88	0.12	26,35,45,62	0
2	PG4	O	1129	13/13	0.88	0.11	30,37,42,45	0
4	ACT	C	1129	4/4	0.89	0.11	23,34,38,56	0
3	PEG	I	1128	7/7	0.89	0.09	43,54,58,64	0
5	EDO	G	1129	4/4	0.89	0.09	44,44,47,54	0
3	PEG	H	1135	7/7	0.89	0.11	49,54,62,67	0
3	PEG	O	1127	7/7	0.89	0.12	32,47,55,59	0
4	ACT	L	1129	4/4	0.89	0.11	30,30,32,34	0
3	PEG	I	1127	7/7	0.89	0.11	31,43,50,50	0

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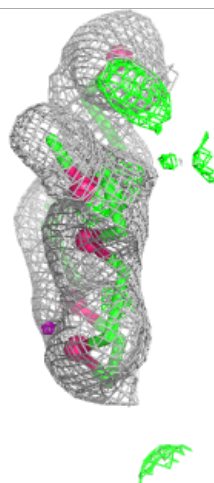
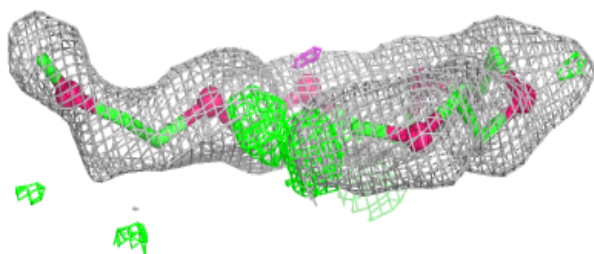
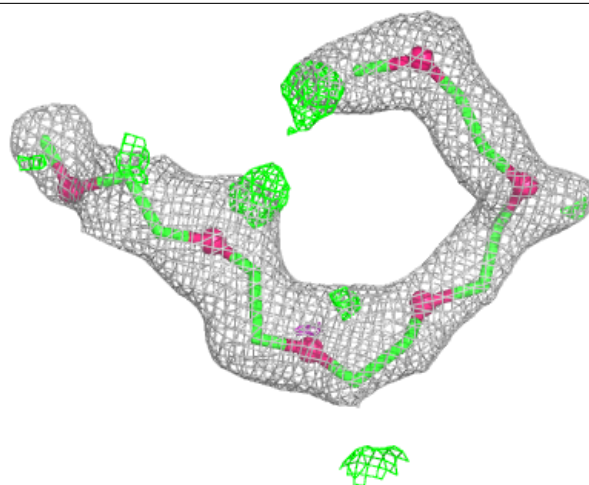
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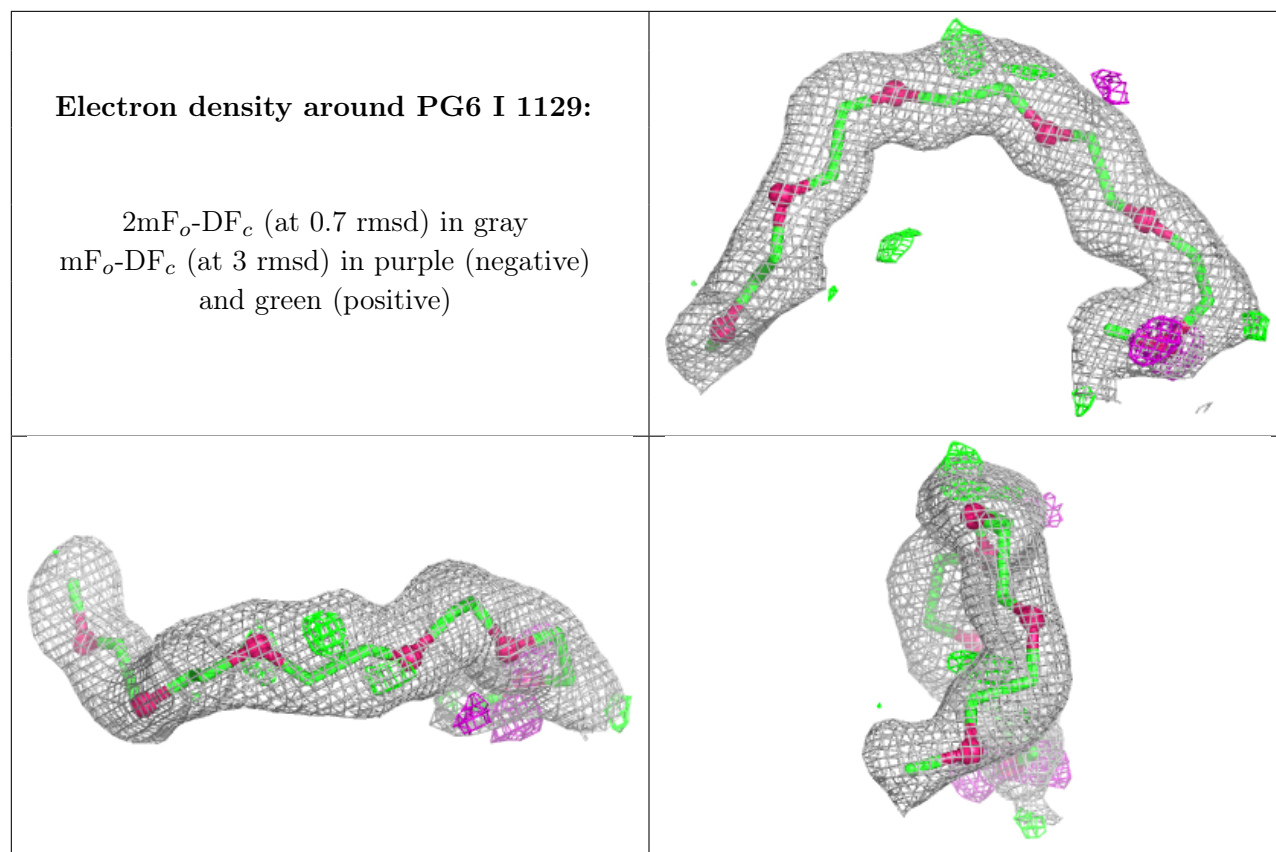
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACT	A	1128	4/4	0.89	0.12	37,37,41,42	0
5	EDO	P	1129	4/4	0.90	0.11	28,29,37,41	0
7	PGE	K	1130	10/10	0.90	0.10	32,42,44,57	0
5	EDO	P	1131	4/4	0.90	0.12	18,32,33,37	0
2	PG4	B	1129	13/13	0.90	0.11	32,45,53,57	0
2	PG4	F	1125	13/13	0.90	0.15	29,44,99,106	0
7	PGE	C	1130	10/10	0.90	0.11	25,35,49,54	0
7	PGE	M	1129	10/10	0.91	0.11	27,30,49,50	0
7	PGE	N	1136	10/10	0.91	0.11	29,37,50,51	0
2	PG4	B	1128	13/13	0.91	0.13	26,38,76,79	0
4	ACT	C	1128	4/4	0.91	0.10	26,27,28,29	0
3	PEG	L	1127	7/7	0.91	0.11	36,40,49,56	0
5	EDO	D	1133	4/4	0.91	0.12	35,46,53,57	0
5	EDO	P	1132	4/4	0.92	0.10	35,42,43,46	0
4	ACT	M	1128	4/4	0.92	0.12	18,20,22,25	0
3	PEG	B	1130	7/7	0.92	0.08	41,48,56,59	0
2	PG4	E	1126	13/13	0.92	0.11	27,51,68,72	0
2	PG4	L	1126	13/13	0.93	0.12	27,37,61,64	0
2	PG4	N	1134	13/13	0.93	0.11	18,34,46,61	0
5	EDO	P	1130	4/4	0.93	0.11	21,21,22,60	0
2	PG4	G	1126	13/13	0.93	0.13	18,31,57,63	0
5	EDO	D	1131	4/4	0.93	0.10	39,43,49,54	0
2	PG4	I	1126	13/13	0.93	0.13	22,41,62,70	0
4	ACT	J	1127	4/4	0.93	0.09	30,32,33,33	0
2	PG4	D	1126	13/13	0.93	0.11	18,34,52,53	0
5	EDO	C	1131	4/4	0.94	0.09	21,22,33,35	0
2	PG4	P	1127	13/13	0.94	0.10	17,29,53,55	0
2	PG4	K	1126	13/13	0.94	0.11	22,41,72,76	0
2	PG4	C	1127	13/13	0.94	0.10	19,29,48,49	0
4	ACT	P	1128	4/4	0.95	0.11	24,28,36,42	0
2	PG4	O	1126	13/13	0.95	0.10	21,36,51,52	0
2	PG4	M	1126	13/13	0.95	0.09	18,26,39,44	0
4	ACT	H	1136	4/4	0.95	0.09	20,25,25,25	0
2	PG4	H	1134	13/13	0.95	0.09	21,28,48,57	0
2	PG4	J	1126	13/13	0.96	0.09	22,32,56,61	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 PG6 N 1135:

$2mF_o-DF_c$ (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.