Full wwPDB X-ray Structure Validation Report (i)

Apr 2, 2025 – 02:12 PM JST

PDB ID	:	9J61 / pdb_00009j61
Title	:	Crystal structure of a cyclodipeptide synthase from Streptomyces sapporonensis
Authors	:	Li, P.; Ren, Y.; He, J.; Wu, S.; Wang, J.; Tang, G.; Fang, P.
Deposited on	:	2024-08-14
Resolution	:	2.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

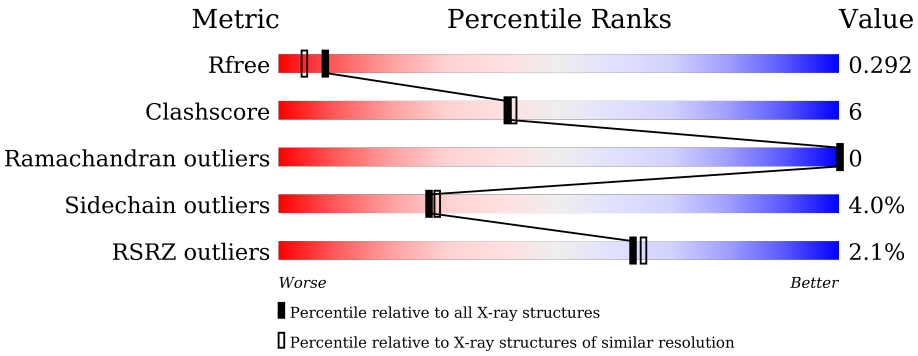
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	249	73% 14% • 12%
1	B	249	78% 12% 9%
1	C	249	4% 73% 11% 15%
1	D	249	2% 76% 8% • 15%
1	E	249	% 68% 16% • 14%
1	F	249	4% 71% 13% 15%

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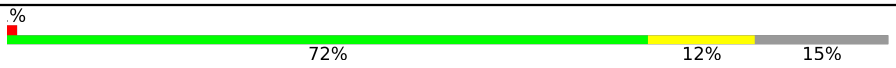
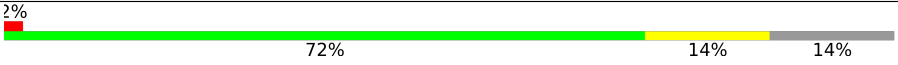
Mol	Chain	Length	Quality of chain
1	G	249	
1	H	249	

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
2	EDO	B	301	-	-	X	-
2	EDO	B	302	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14511 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 Cyclodipeptide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1762	1107	314	334	7			
1	B	226	Total	C	N	O	S	0	0	0
			1803	1130	325	341	7			
1	C	212	Total	C	N	O	S	0	0	0
			1690	1061	305	317	7			
1	D	211	Total	C	N	O	S	0	0	0
			1683	1059	299	318	7			
1	E	213	Total	C	N	O	S	0	0	0
			1704	1072	303	322	7			
1	F	212	Total	C	N	O	S	0	0	0
			1699	1070	305	317	7			
1	G	211	Total	C	N	O	S	0	0	0
			1694	1065	304	318	7			
1	H	214	Total	C	N	O	S	0	0	0
			1722	1084	307	324	7			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP A0A2G1XAZ9
A	-6	GLY	-	expression tag	UNP A0A2G1XAZ9
A	-5	HIS	-	expression tag	UNP A0A2G1XAZ9
A	-4	HIS	-	expression tag	UNP A0A2G1XAZ9
A	-3	HIS	-	expression tag	UNP A0A2G1XAZ9
A	-2	HIS	-	expression tag	UNP A0A2G1XAZ9
A	-1	HIS	-	expression tag	UNP A0A2G1XAZ9
A	0	HIS	-	expression tag	UNP A0A2G1XAZ9
A	1	GLY	-	expression tag	UNP A0A2G1XAZ9
B	-7	MET	-	initiating methionine	UNP A0A2G1XAZ9
B	-6	GLY	-	expression tag	UNP A0A2G1XAZ9
B	-5	HIS	-	expression tag	UNP A0A2G1XAZ9
B	-4	HIS	-	expression tag	UNP A0A2G1XAZ9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	HIS	-	expression tag	UNP A0A2G1XAZ9
B	-2	HIS	-	expression tag	UNP A0A2G1XAZ9
B	-1	HIS	-	expression tag	UNP A0A2G1XAZ9
B	0	HIS	-	expression tag	UNP A0A2G1XAZ9
B	1	GLY	-	expression tag	UNP A0A2G1XAZ9
C	-7	MET	-	initiating methionine	UNP A0A2G1XAZ9
C	-6	GLY	-	expression tag	UNP A0A2G1XAZ9
C	-5	HIS	-	expression tag	UNP A0A2G1XAZ9
C	-4	HIS	-	expression tag	UNP A0A2G1XAZ9
C	-3	HIS	-	expression tag	UNP A0A2G1XAZ9
C	-2	HIS	-	expression tag	UNP A0A2G1XAZ9
C	-1	HIS	-	expression tag	UNP A0A2G1XAZ9
C	0	HIS	-	expression tag	UNP A0A2G1XAZ9
C	1	GLY	-	expression tag	UNP A0A2G1XAZ9
D	-7	MET	-	initiating methionine	UNP A0A2G1XAZ9
D	-6	GLY	-	expression tag	UNP A0A2G1XAZ9
D	-5	HIS	-	expression tag	UNP A0A2G1XAZ9
D	-4	HIS	-	expression tag	UNP A0A2G1XAZ9
D	-3	HIS	-	expression tag	UNP A0A2G1XAZ9
D	-2	HIS	-	expression tag	UNP A0A2G1XAZ9
D	-1	HIS	-	expression tag	UNP A0A2G1XAZ9
D	0	HIS	-	expression tag	UNP A0A2G1XAZ9
D	1	GLY	-	expression tag	UNP A0A2G1XAZ9
E	-7	MET	-	initiating methionine	UNP A0A2G1XAZ9
E	-6	GLY	-	expression tag	UNP A0A2G1XAZ9
E	-5	HIS	-	expression tag	UNP A0A2G1XAZ9
E	-4	HIS	-	expression tag	UNP A0A2G1XAZ9
E	-3	HIS	-	expression tag	UNP A0A2G1XAZ9
E	-2	HIS	-	expression tag	UNP A0A2G1XAZ9
E	-1	HIS	-	expression tag	UNP A0A2G1XAZ9
E	0	HIS	-	expression tag	UNP A0A2G1XAZ9
E	1	GLY	-	expression tag	UNP A0A2G1XAZ9
F	-7	MET	-	initiating methionine	UNP A0A2G1XAZ9
F	-6	GLY	-	expression tag	UNP A0A2G1XAZ9
F	-5	HIS	-	expression tag	UNP A0A2G1XAZ9
F	-4	HIS	-	expression tag	UNP A0A2G1XAZ9
F	-3	HIS	-	expression tag	UNP A0A2G1XAZ9
F	-2	HIS	-	expression tag	UNP A0A2G1XAZ9
F	-1	HIS	-	expression tag	UNP A0A2G1XAZ9
F	0	HIS	-	expression tag	UNP A0A2G1XAZ9
F	1	GLY	-	expression tag	UNP A0A2G1XAZ9
G	-7	MET	-	initiating methionine	UNP A0A2G1XAZ9

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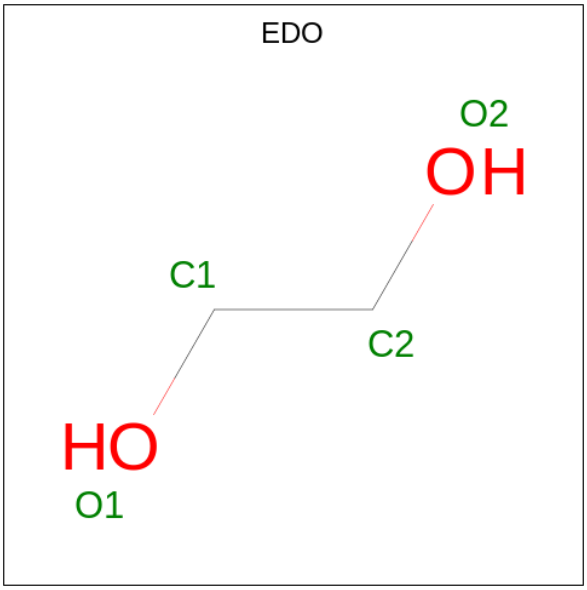
Chain	Residue	Modelled	Actual	Comment	Reference
G	-6	GLY	-	expression tag	UNP A0A2G1XAZ9
G	-5	HIS	-	expression tag	UNP A0A2G1XAZ9
G	-4	HIS	-	expression tag	UNP A0A2G1XAZ9
G	-3	HIS	-	expression tag	UNP A0A2G1XAZ9
G	-2	HIS	-	expression tag	UNP A0A2G1XAZ9
G	-1	HIS	-	expression tag	UNP A0A2G1XAZ9
G	0	HIS	-	expression tag	UNP A0A2G1XAZ9
G	1	GLY	-	expression tag	UNP A0A2G1XAZ9
H	-7	MET	-	initiating methionine	UNP A0A2G1XAZ9
H	-6	GLY	-	expression tag	UNP A0A2G1XAZ9
H	-5	HIS	-	expression tag	UNP A0A2G1XAZ9
H	-4	HIS	-	expression tag	UNP A0A2G1XAZ9
H	-3	HIS	-	expression tag	UNP A0A2G1XAZ9
H	-2	HIS	-	expression tag	UNP A0A2G1XAZ9
H	-1	HIS	-	expression tag	UNP A0A2G1XAZ9
H	0	HIS	-	expression tag	UNP A0A2G1XAZ9
H	1	GLY	-	expression tag	UNP A0A2G1XAZ9

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



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

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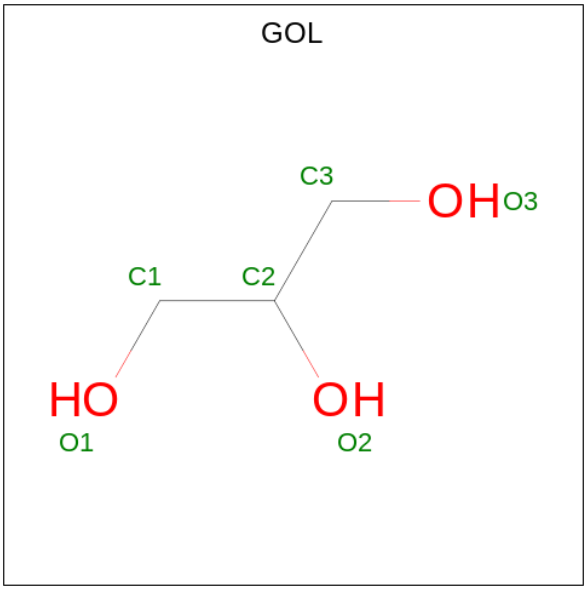
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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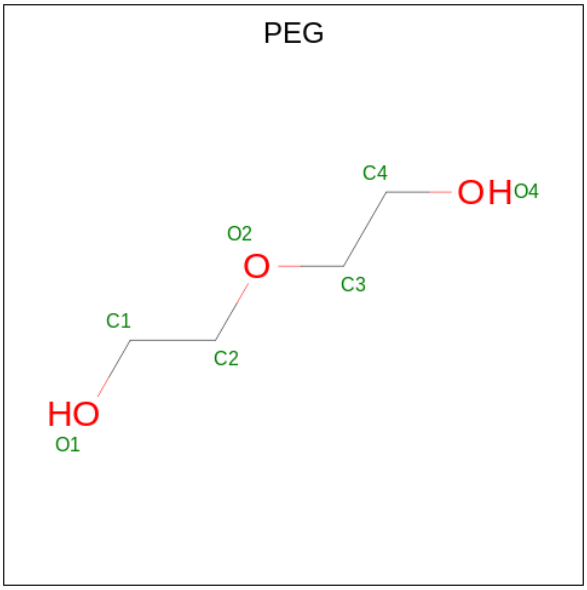
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	102	Total O 102 102	0	0
5	B	90	Total O 90 90	0	0
5	C	66	Total O 66 66	0	0
5	D	99	Total O 99 99	0	0
5	E	81	Total O 81 81	0	0
5	F	87	Total O 87 87	0	0
5	G	78	Total O 78 78	0	0

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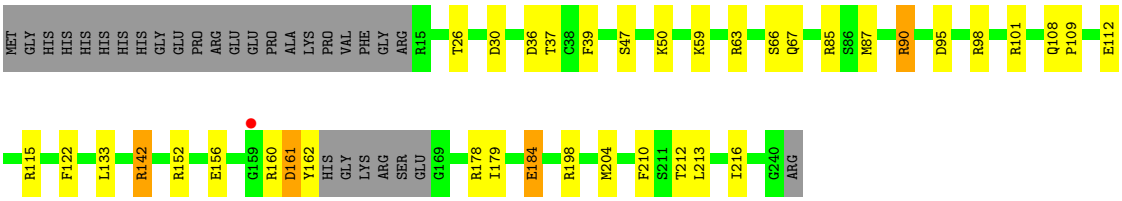
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	80	Total	O	0	0
			80	80		

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.

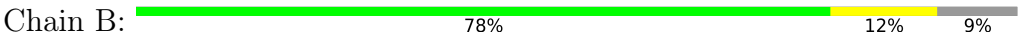
• Molecule 1: Cyclodipeptide synthase

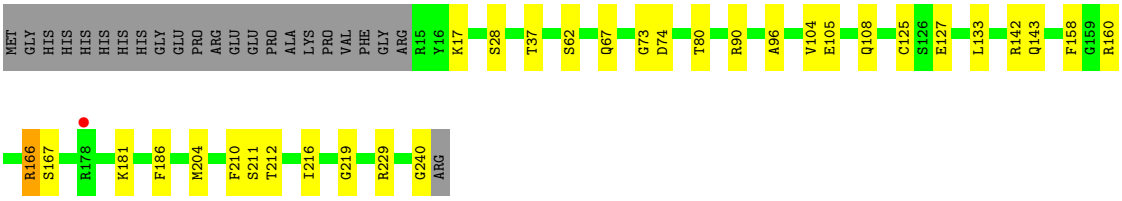
Chain A:



• Molecule 1: Cyclodipeptide synthase

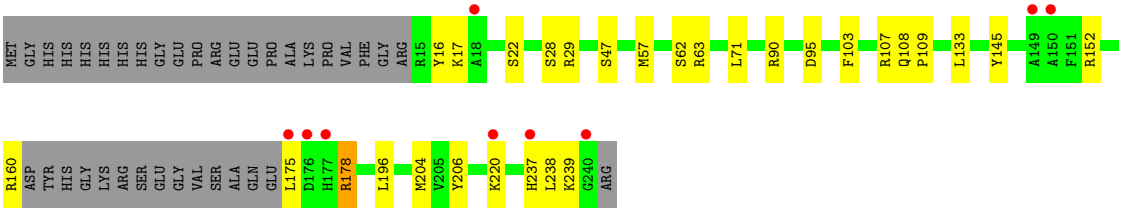
Chain B:





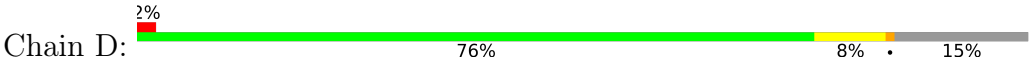
• Molecule 1: Cyclodipeptide synthase

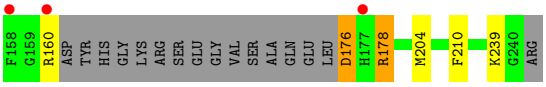
Chain C:



• Molecule 1: Cyclodipeptide synthase

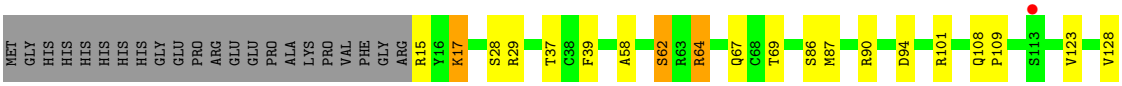
Chain D:

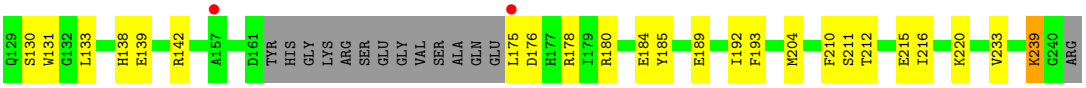




• Molecule 1: Cyclodipeptide synthase

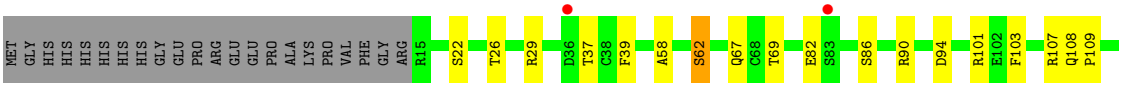
Chain E:

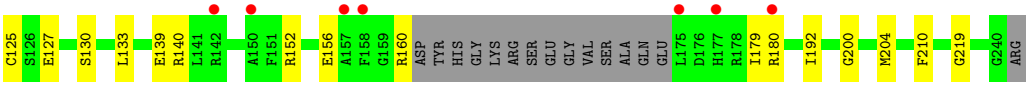




• Molecule 1: Cyclodipeptide synthase

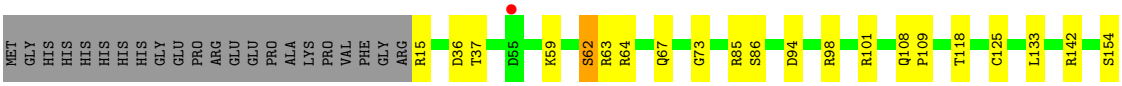
Chain F:

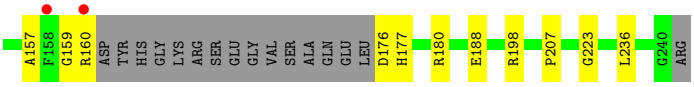




• Molecule 1: Cyclodipeptide synthase

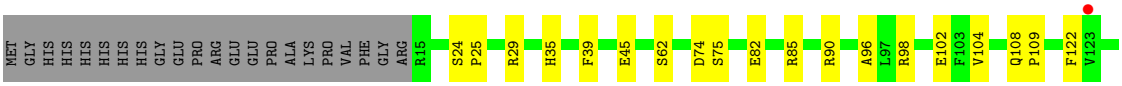
Chain G:

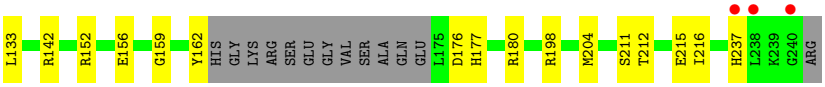




• Molecule 1: Cyclodipeptide synthase

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	85.59Å 89.44Å 93.35Å 70.85° 67.04° 61.54°	Depositor
Resolution (Å)	28.62 – 2.10 28.62 – 2.10	Depositor EDS
% Data completeness (in resolution range)	91.1 (28.62-2.10) 91.1 (28.62-2.10)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.234 , 0.292 0.234 , 0.292	Depositor DCC
R_{free} test set	6616 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å^2)	38.7	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 32.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14511	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, GOL, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.46	0/1802	0.74	0/2430
1	B	0.46	0/1845	0.76	0/2489
1	C	0.44	0/1728	0.74	0/2330
1	D	0.47	0/1721	0.74	0/2321
1	E	0.49	0/1743	0.76	0/2351
1	F	0.45	0/1738	0.76	0/2343
1	G	0.46	0/1733	0.77	0/2336
1	H	0.43	0/1762	0.74	0/2376
All	All	0.46	0/14072	0.75	0/18976

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	1
1	D	0	3
1	E	0	2
1	F	0	2
1	G	0	1
1	H	0	1
All	All	0	13

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	ARG	Sidechain
1	A	90	ARG	Sidechain
1	B	166	ARG	Sidechain
1	C	160	ARG	Sidechain
1	D	101	ARG	Sidechain
1	D	160	ARG	Sidechain
1	D	178	ARG	Sidechain
1	E	101	ARG	Sidechain
1	E	64	ARG	Sidechain
1	F	101	ARG	Sidechain
1	F	140	ARG	Sidechain
1	G	198	ARG	Sidechain
1	H	98	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1762	0	1701	27	0
1	B	1803	0	1734	24	0
1	C	1690	0	1634	18	0
1	D	1683	0	1625	15	0
1	E	1704	0	1645	27	0
1	F	1699	0	1650	19	0
1	G	1694	0	1641	22	0
1	H	1722	0	1665	21	0
2	A	4	0	6	0	0
2	B	12	0	18	14	0
2	C	4	0	6	0	0
2	D	4	0	6	0	0
2	E	4	0	6	1	0
2	F	8	0	12	0	0
2	G	16	0	24	3	0
3	B	6	0	8	0	0
3	D	6	0	8	2	0
4	D	7	0	10	1	0
5	A	102	0	0	3	0
5	B	90	0	0	9	0
5	C	66	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	99	0	0	4	0
5	E	81	0	0	9	0
5	F	87	0	0	6	0
5	G	78	0	0	6	0
5	H	80	0	0	6	0
All	All	14511	0	13399	174	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 (174) 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:E:128:VAL:HB	5:E:456:HOH:O	1.53	1.05
1:B:80:THR:OG1	2:B:302:EDO:H21	1.59	1.01
1:D:37:THR:HB	5:D:489:HOH:O	1.66	0.95
1:B:211:SER:HB2	5:B:410:HOH:O	1.68	0.93
1:E:192:ILE:HG12	5:E:456:HOH:O	1.68	0.93
1:F:26:THR:HB	5:F:465:HOH:O	1.68	0.92
1:C:145:TYR:HA	5:C:452:HOH:O	1.73	0.88
1:B:143:GLN:HB3	5:B:411:HOH:O	1.76	0.85
1:H:180:ARG:HD2	5:H:359:HOH:O	1.78	0.83
1:H:142:ARG:HG3	1:H:142:ARG:HH11	1.45	0.82
1:C:145:TYR:CD2	5:C:452:HOH:O	2.35	0.80
1:F:82:GLU:HB3	5:F:401:HOH:O	1.84	0.78
1:A:142:ARG:HH11	1:A:142:ARG:HG3	1.51	0.75
1:A:26:THR:HG23	1:B:219:GLY:HA3	1.68	0.74
1:A:122:PHE:CE2	5:A:447:HOH:O	2.41	0.73
1:F:180:ARG:HD2	5:F:445:HOH:O	1.88	0.73
1:A:162:TYR:CE2	1:A:178:ARG:HB3	2.26	0.70
1:D:176:ASP:N	5:D:402:HOH:O	2.27	0.68
1:G:37:THR:HG22	1:G:67:GLN:HB2	1.75	0.68
1:E:130:SER:HB3	5:E:467:HOH:O	1.94	0.67
1:B:80:THR:HG1	2:B:302:EDO:H21	1.59	0.66
1:F:37:THR:HG22	1:F:67:GLN:HB2	1.79	0.65
1:D:17:LYS:HE3	1:D:239:LYS:HD2	1.77	0.65
2:B:301:EDO:O1	2:B:302:EDO:H22	1.98	0.64
1:B:127:GLU:HB3	5:B:446:HOH:O	1.98	0.63
2:B:301:EDO:C2	2:B:302:EDO:O2	2.47	0.63
1:C:29:ARG:NH1	5:C:402:HOH:O	2.31	0.61
1:G:188:GLU:OE2	2:G:302:EDO:H22	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:154:SER:HA	5:G:428:HOH:O	2.01	0.60
1:A:112:GLU:O	1:A:115:ARG:NH1	2.34	0.60
1:C:145:TYR:CG	5:C:452:HOH:O	2.53	0.60
1:G:176:ASP:N	5:G:403:HOH:O	2.35	0.59
1:E:37:THR:HG22	1:E:67:GLN:HB2	1.83	0.59
1:H:152:ARG:O	1:H:156:GLU:HG2	2.02	0.59
1:A:184:GLU:HG2	5:A:483:HOH:O	2.02	0.59
1:A:26:THR:HG23	1:B:219:GLY:CA	2.32	0.59
1:G:64:ARG:NH2	5:G:401:HOH:O	2.22	0.59
1:D:103:PHE:CD2	3:D:302:GOL:H32	2.39	0.58
1:H:35:HIS:HE1	5:H:367:HOH:O	1.85	0.57
1:F:125:CYS:SG	1:F:192:ILE:HD13	2.44	0.57
1:B:142:ARG:HH11	1:B:142:ARG:HG3	1.70	0.57
1:F:152:ARG:O	1:F:156:GLU:HG2	2.04	0.57
1:B:37:THR:HG22	1:B:67:GLN:HB2	1.85	0.56
1:E:87:MET:SD	5:E:419:HOH:O	2.58	0.56
1:C:175:LEU:HA	1:C:178:ARG:HD3	1.89	0.55
1:B:211:SER:CB	5:B:410:HOH:O	2.39	0.55
1:G:157:ALA:HB2	5:G:428:HOH:O	2.06	0.55
1:B:240:GLY:C	5:B:430:HOH:O	2.44	0.55
1:F:204:MET:HE3	1:F:210:PHE:CE2	2.42	0.54
2:B:301:EDO:O2	2:B:302:EDO:O2	2.24	0.54
1:E:142:ARG:HH11	1:E:142:ARG:HG3	1.73	0.53
2:B:301:EDO:C1	2:B:302:EDO:H22	2.38	0.53
1:A:142:ARG:HH11	1:A:142:ARG:CG	2.18	0.53
1:E:64:ARG:NE	5:E:403:HOH:O	2.40	0.53
1:D:204:MET:HE3	1:D:210:PHE:CE2	2.44	0.53
1:H:35:HIS:CE1	5:H:367:HOH:O	2.61	0.53
1:A:59:LYS:HE2	1:A:63:ARG:HH22	1.74	0.53
1:G:188:GLU:OE2	2:G:302:EDO:C2	2.57	0.53
1:B:28:SER:HB3	5:B:409:HOH:O	2.08	0.52
1:A:85:ARG:HG3	5:A:404:HOH:O	2.09	0.52
1:C:63:ARG:HG2	1:F:86:SER:HB3	1.92	0.51
1:E:131:TRP:HB3	1:H:198:ARG:O	2.11	0.51
1:C:71:LEU:HD13	1:C:196:LEU:HD11	1.92	0.51
1:D:37:THR:HG22	1:D:67:GLN:HB2	1.92	0.51
1:E:39:PHE:HA	1:E:69:THR:O	2.10	0.51
1:H:74:ASP:O	1:H:96:ALA:HB1	2.10	0.51
1:G:64:ARG:NE	5:G:401:HOH:O	2.32	0.51
1:G:159:GLY:O	1:G:160:ARG:CG	2.59	0.51
1:C:152:ARG:HA	5:C:452:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:EDO:O1	2:B:302:EDO:C2	2.58	0.50
1:A:36:ASP:CG	1:A:66:SER:HG	2.14	0.50
1:F:108:GLN:N	1:F:109:PRO:HD2	2.25	0.50
1:A:36:ASP:OD2	1:A:66:SER:OG	2.28	0.50
1:C:145:TYR:CB	5:C:452:HOH:O	2.60	0.50
1:D:82:GLU:OE2	1:D:89:PRO:HA	2.12	0.50
1:H:211:SER:O	1:H:215:GLU:HG3	2.11	0.49
1:F:37:THR:OG1	1:F:200:GLY:O	2.23	0.49
1:A:87:MET:CE	1:A:95:ASP:OD2	2.61	0.49
1:C:145:TYR:CA	5:C:452:HOH:O	2.46	0.49
1:E:17:LYS:HE3	1:E:239:LYS:HD3	1.94	0.49
1:A:37:THR:HG22	1:A:67:GLN:HB2	1.95	0.49
1:D:82:GLU:OE2	1:D:89:PRO:CA	2.61	0.49
1:F:139:GLU:HA	1:F:139:GLU:OE1	2.13	0.49
1:E:204:MET:HE3	1:E:210:PHE:CE2	2.47	0.49
1:H:180:ARG:CD	5:H:359:HOH:O	2.49	0.48
1:D:73:GLY:HA2	1:D:125:CYS:SG	2.53	0.48
1:H:102:GLU:HB3	5:H:357:HOH:O	2.13	0.48
1:B:186:PHE:CZ	2:B:301:EDO:H12	2.49	0.48
1:C:108:GLN:N	1:C:109:PRO:HD2	2.29	0.48
1:G:142:ARG:HG3	2:G:303:EDO:O1	2.13	0.48
1:F:103:PHE:CZ	1:F:107:ARG:HG3	2.49	0.47
1:H:142:ARG:HH11	1:H:142:ARG:CG	2.21	0.47
1:C:204:MET:HE2	1:C:206:TYR:HB2	1.96	0.47
1:A:161:ASP:OD1	1:A:162:TYR:N	2.48	0.47
1:D:204:MET:HE3	1:D:210:PHE:HE2	1.79	0.47
1:C:175:LEU:CA	1:C:178:ARG:HD3	2.45	0.47
1:A:87:MET:HE3	1:A:95:ASP:OD2	2.13	0.47
1:D:103:PHE:CE2	3:D:302:GOL:H32	2.50	0.47
1:H:159:GLY:O	1:H:162:TYR:C	2.54	0.46
1:H:176:ASP:O	1:H:180:ARG:HG3	2.16	0.46
1:B:186:PHE:CE2	2:B:301:EDO:H12	2.51	0.46
1:E:139:GLU:HA	1:E:139:GLU:OE1	2.15	0.46
1:A:156:GLU:OE2	1:A:160:ARG:NH2	2.49	0.46
1:E:130:SER:CB	5:E:467:HOH:O	2.61	0.46
1:E:204:MET:HE3	1:E:210:PHE:HE2	1.81	0.46
1:E:215:GLU:HG2	1:E:220:LYS:CE	2.45	0.46
1:E:108:GLN:N	1:E:109:PRO:HD2	2.31	0.46
1:F:160:ARG:NH1	1:F:179:ILE:HD13	2.31	0.46
1:F:219:GLY:HA3	5:F:423:HOH:O	2.15	0.45
1:G:108:GLN:N	1:G:109:PRO:HD2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:104:VAL:HG22	1:H:122:PHE:CD1	2.52	0.45
1:B:28:SER:CB	5:B:409:HOH:O	2.64	0.45
1:C:57:MET:HG3	1:C:238:LEU:HD21	1.99	0.45
1:G:159:GLY:O	1:G:160:ARG:HG3	2.16	0.45
1:G:73:GLY:HA2	1:G:125:CYS:SG	2.57	0.45
1:E:212:THR:O	1:E:216:ILE:HG13	2.17	0.45
4:D:303:PEG:H31	5:D:471:HOH:O	2.17	0.44
1:E:138:HIS:CE1	5:E:420:HOH:O	2.70	0.44
1:G:176:ASP:HA	5:G:407:HOH:O	2.16	0.44
1:C:220:LYS:HD2	1:G:223:GLY:CA	2.47	0.44
1:G:98:ARG:HA	1:G:101:ARG:NH1	2.33	0.44
2:B:301:EDO:H22	2:B:302:EDO:O2	2.17	0.44
1:E:189:GLU:HG2	1:E:193:PHE:CZ	2.53	0.44
1:B:73:GLY:HA2	1:B:125:CYS:SG	2.58	0.44
1:A:63:ARG:HG2	1:E:86:SER:HB3	1.99	0.44
1:D:108:GLN:N	1:D:109:PRO:HD2	2.33	0.43
1:E:204:MET:HE2	1:E:233:VAL:HG13	2.00	0.43
1:H:212:THR:O	1:H:216:ILE:HG13	2.18	0.43
1:A:212:THR:O	1:A:216:ILE:HG13	2.19	0.43
1:C:220:LYS:HD2	1:G:223:GLY:HA3	1.99	0.43
1:F:58:ALA:O	1:F:62:SER:HB2	2.19	0.43
2:B:301:EDO:O1	2:B:302:EDO:C1	2.66	0.43
1:A:108:GLN:N	1:A:109:PRO:CD	2.82	0.43
1:H:177:HIS:CD2	5:H:335:HOH:O	2.71	0.43
1:A:47:SER:O	1:A:50:LYS:HG3	2.18	0.43
1:A:210:PHE:HB2	1:A:213:LEU:HD12	2.01	0.43
1:B:158:PHE:CE1	2:B:301:EDO:H21	2.54	0.43
1:A:160:ARG:HG2	1:A:179:ILE:HD13	2.00	0.42
1:H:108:GLN:N	1:H:109:PRO:HD2	2.34	0.42
1:A:98:ARG:HA	1:A:101:ARG:NH1	2.34	0.42
1:B:104:VAL:O	1:B:108:GLN:HB2	2.20	0.42
1:E:128:VAL:CG1	5:E:456:HOH:O	2.64	0.42
1:H:39:PHE:CZ	1:H:204:MET:HB2	2.54	0.42
1:G:177:HIS:HD2	1:G:180:ARG:HH21	1.67	0.42
1:G:59:LYS:HE3	1:G:63:ARG:NH2	2.34	0.42
1:H:45:GLU:OE1	1:H:85:ARG:NH2	2.53	0.42
1:B:212:THR:O	1:B:216:ILE:HG13	2.20	0.42
1:G:207:PRO:HA	1:G:236:LEU:O	2.20	0.42
1:A:142:ARG:CG	1:A:142:ARG:NH1	2.80	0.42
1:B:105:GLU:HB3	5:B:473:HOH:O	2.18	0.42
1:C:103:PHE:CZ	1:C:107:ARG:HG3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:74:ASP:OD1	1:H:75:SER:N	2.48	0.42
1:D:82:GLU:HG2	5:D:493:HOH:O	2.20	0.41
1:G:85:ARG:O	1:G:86:SER:C	2.58	0.41
1:B:229:ARG:HD2	5:B:433:HOH:O	2.21	0.41
1:A:152:ARG:NH2	1:D:143:GLN:HA	2.35	0.41
1:F:130:SER:CB	5:F:471:HOH:O	2.69	0.41
1:B:74:ASP:O	1:B:96:ALA:HB1	2.21	0.41
1:B:80:THR:HG23	2:B:302:EDO:H11	2.02	0.41
1:B:204:MET:HE1	1:B:210:PHE:CE2	2.56	0.41
1:E:58:ALA:O	1:E:62:SER:HB2	2.21	0.41
1:A:39:PHE:CZ	1:A:204:MET:HB2	2.55	0.41
1:E:69:THR:CG2	1:E:123:VAL:HG12	2.50	0.41
1:E:185:TYR:CD1	2:E:301:EDO:H11	2.55	0.41
1:F:39:PHE:HA	1:F:69:THR:O	2.21	0.41
1:F:130:SER:HB3	5:F:471:HOH:O	2.21	0.41
1:C:16:TYR:HA	1:C:239:LYS:O	2.21	0.41
1:D:62:SER:HA	1:D:118:THR:OG1	2.21	0.41
1:F:204:MET:HE3	1:F:210:PHE:HE2	1.83	0.41
1:G:62:SER:HA	1:G:118:THR:OG1	2.21	0.41
1:E:180:ARG:O	1:E:184:GLU:HG2	2.21	0.40
1:E:29:ARG:NE	5:E:405:HOH:O	2.51	0.40
2:B:301:EDO:C1	2:B:302:EDO:C2	3.00	0.40
1:H:24:SER:HA	1:H:25:PRO:HA	1.97	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	216/249 (87%)	211 (98%)	5 (2%)	0	100	100
1	B	224/249 (90%)	218 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	208/249 (84%)	202 (97%)	6 (3%)	0	100	100
1	D	207/249 (83%)	205 (99%)	2 (1%)	0	100	100
1	E	209/249 (84%)	205 (98%)	4 (2%)	0	100	100
1	F	208/249 (84%)	206 (99%)	2 (1%)	0	100	100
1	G	207/249 (83%)	204 (99%)	3 (1%)	0	100	100
1	H	210/249 (84%)	207 (99%)	3 (1%)	0	100	100
All	All	1689/1992 (85%)	1658 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	191/215 (89%)	185 (97%)	6 (3%)	35	39
1	B	194/215 (90%)	186 (96%)	8 (4%)	26	27
1	C	182/215 (85%)	172 (94%)	10 (6%)	18	16
1	D	182/215 (85%)	176 (97%)	6 (3%)	33	36
1	E	185/215 (86%)	173 (94%)	12 (6%)	14	12
1	F	184/215 (86%)	177 (96%)	7 (4%)	28	30
1	G	184/215 (86%)	179 (97%)	5 (3%)	40	44
1	H	187/215 (87%)	181 (97%)	6 (3%)	34	37
All	All	1489/1720 (87%)	1429 (96%)	60 (4%)	27	28

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ASP
1	A	90	ARG
1	A	133	LEU
1	A	142	ARG

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Mol	Chain	Res	Type
1	A	161	ASP
1	A	184	GLU
1	B	17	LYS
1	B	62	SER
1	B	90	ARG
1	B	133	LEU
1	B	160	ARG
1	B	166	ARG
1	B	167	SER
1	B	181	LYS
1	C	17	LYS
1	C	22	SER
1	C	28	SER
1	C	47	SER
1	C	62	SER
1	C	90	ARG
1	C	95	ASP
1	C	133	LEU
1	C	178	ARG
1	C	237	HIS
1	D	28	SER
1	D	90	ARG
1	D	101	ARG
1	D	133	LEU
1	D	176	ASP
1	D	178	ARG
1	E	15	ARG
1	E	17	LYS
1	E	28	SER
1	E	62	SER
1	E	90	ARG
1	E	94	ASP
1	E	133	LEU
1	E	175	LEU
1	E	176	ASP
1	E	178	ARG
1	E	211	SER
1	E	239	LYS
1	F	22	SER
1	F	29	ARG
1	F	62	SER
1	F	90	ARG

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Mol	Chain	Res	Type
1	F	94	ASP
1	F	127	GLU
1	F	133	LEU
1	G	15	ARG
1	G	36	ASP
1	G	62	SER
1	G	94	ASP
1	G	133	LEU
1	H	29	ARG
1	H	62	SER
1	H	82	GLU
1	H	90	ARG
1	H	133	LEU
1	H	237	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	177	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

16 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	EDO	G	302	-	3,3,3	0.36	0	2,2,2	0.71	0
2	EDO	F	302	-	3,3,3	0.10	0	2,2,2	0.27	0
2	EDO	F	301	-	3,3,3	0.18	0	2,2,2	0.28	0
2	EDO	B	302	-	3,3,3	0.29	0	2,2,2	0.62	0
2	EDO	D	301	-	3,3,3	0.18	0	2,2,2	0.22	0
2	EDO	A	301	-	3,3,3	0.08	0	2,2,2	0.06	0
3	GOL	D	302	-	5,5,5	0.11	0	5,5,5	0.45	0
2	EDO	C	301	-	3,3,3	0.31	0	2,2,2	0.10	0
2	EDO	E	301	-	3,3,3	0.17	0	2,2,2	0.35	0
4	PEG	D	303	-	6,6,6	0.26	0	5,5,5	0.14	0
3	GOL	B	304	-	5,5,5	0.11	0	5,5,5	0.33	0
2	EDO	B	301	-	3,3,3	0.23	0	2,2,2	0.61	0
2	EDO	B	303	-	3,3,3	0.17	0	2,2,2	0.26	0
2	EDO	G	301	-	3,3,3	0.31	0	2,2,2	0.40	0
2	EDO	G	304	-	3,3,3	0.09	0	2,2,2	0.22	0
2	EDO	G	303	-	3,3,3	0.17	0	2,2,2	0.23	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	EDO	G	302	-	-	0/1/1/1	-
2	EDO	F	302	-	-	0/1/1/1	-
2	EDO	F	301	-	-	1/1/1/1	-
2	EDO	B	302	-	-	1/1/1/1	-
2	EDO	D	301	-	-	1/1/1/1	-
2	EDO	A	301	-	-	1/1/1/1	-
3	GOL	D	302	-	-	0/4/4/4	-
2	EDO	C	301	-	-	1/1/1/1	-
2	EDO	E	301	-	-	1/1/1/1	-
4	PEG	D	303	-	-	3/4/4/4	-
3	GOL	B	304	-	-	2/4/4/4	-
2	EDO	B	301	-	-	1/1/1/1	-
2	EDO	B	303	-	-	1/1/1/1	-
2	EDO	G	301	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	G	304	-	-	0/1/1/1	-
2	EDO	G	303	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	304	GOL	C1-C2-C3-O3
3	B	304	GOL	O2-C2-C3-O3
4	D	303	PEG	O2-C3-C4-O4
2	A	301	EDO	O1-C1-C2-O2
2	B	303	EDO	O1-C1-C2-O2
2	F	301	EDO	O1-C1-C2-O2
2	E	301	EDO	O1-C1-C2-O2
2	G	303	EDO	O1-C1-C2-O2
2	B	301	EDO	O1-C1-C2-O2
2	C	301	EDO	O1-C1-C2-O2
4	D	303	PEG	C4-C3-O2-C2
4	D	303	PEG	C1-C2-O2-C3
2	G	301	EDO	O1-C1-C2-O2
2	B	302	EDO	O1-C1-C2-O2
2	D	301	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	302	EDO	2	0
2	B	302	EDO	11	0
3	D	302	GOL	2	0
2	E	301	EDO	1	0
4	D	303	PEG	1	0
2	B	301	EDO	11	0
2	G	303	EDO	1	0

5.7 Other polymers

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, 95^{th} 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	220/249 (88%)	-0.01	1 (0%)	87	88	25, 40, 63, 87	0
1	B	226/249 (90%)	0.08	1 (0%)	89	90	27, 43, 65, 79	0
1	C	212/249 (85%)	0.42	9 (4%)	41	43	26, 49, 77, 96	0
1	D	211/249 (84%)	-0.01	6 (2%)	55	57	26, 39, 63, 105	0
1	E	213/249 (85%)	0.09	3 (1%)	73	74	26, 41, 67, 105	0
1	F	212/249 (85%)	0.16	9 (4%)	41	43	27, 43, 73, 100	0
1	G	211/249 (84%)	0.09	3 (1%)	73	74	26, 42, 68, 84	0
1	H	214/249 (85%)	0.27	4 (1%)	66	67	28, 48, 71, 82	0
All	All	1719/1992 (86%)	0.13	36 (2%)	63	65	25, 43, 69, 105	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	175	LEU	4.8
1	F	175	LEU	3.9
1	A	159	GLY	3.3
1	C	175	LEU	3.3
1	D	158	PHE	3.1
1	F	158	PHE	3.1
1	E	157	ALA	2.9
1	F	36	ASP	2.9
1	G	158	PHE	2.9
1	F	150	ALA	2.9
1	F	157	ALA	2.7
1	C	177	HIS	2.7
1	H	238	LEU	2.5
1	C	176	ASP	2.5
1	C	240	GLY	2.4
1	F	142	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	178	ARG	2.4
1	D	177	HIS	2.4
1	F	177	HIS	2.3
1	F	180	ARG	2.3
1	C	149	ALA	2.3
1	F	83	SER	2.3
1	H	240	GLY	2.3
1	H	237	HIS	2.3
1	E	113	SER	2.2
1	D	83	SER	2.2
1	D	36	ASP	2.2
1	C	220	LYS	2.2
1	C	18	ALA	2.1
1	H	123	VAL	2.1
1	D	147	GLN	2.1
1	C	237	HIS	2.1
1	G	160	ARG	2.0
1	G	55	ASP	2.0
1	C	150	ALA	2.0
1	D	160	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PEG	D	303	7/7	0.69	0.18	65,68,70,72	0
2	EDO	G	302	4/4	0.73	0.12	45,51,54,58	0
2	EDO	D	301	4/4	0.77	0.20	52,52,54,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	B	302	4/4	0.79	0.20	76,80,83,84	0
2	EDO	C	301	4/4	0.80	0.15	51,52,52,52	0
2	EDO	B	301	4/4	0.83	0.24	76,77,77,79	0
2	EDO	A	301	4/4	0.83	0.14	52,53,54,62	0
2	EDO	G	304	4/4	0.87	0.18	52,52,56,64	0
2	EDO	E	301	4/4	0.87	0.12	53,55,58,61	0
3	GOL	B	304	6/6	0.88	0.11	56,57,57,57	0
3	GOL	D	302	6/6	0.88	0.11	37,41,49,50	0
2	EDO	G	303	4/4	0.88	0.11	54,57,58,60	0
2	EDO	F	302	4/4	0.89	0.14	53,53,59,60	0
2	EDO	F	301	4/4	0.91	0.10	47,48,52,58	0
2	EDO	B	303	4/4	0.92	0.08	35,36,38,42	0
2	EDO	G	301	4/4	0.93	0.14	52,53,61,64	0

6.5 Other polymers (i)

There are no such residues in this entry.