Full wwPDB X-ray Structure Validation Report (i)

Jan 5, 2024 – 12:09 am GMT

PDB ID	:	5G3O
Title	:	Bacillus cereus formamidase (BceAmiF) inhibited with urea.
Authors	:	Gavira, J.A.; Martinez-Rodriguez, S.; Conejero-Muriel, M.
Deposited on	:	2016-04-29
Resolution	:	2.15 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:

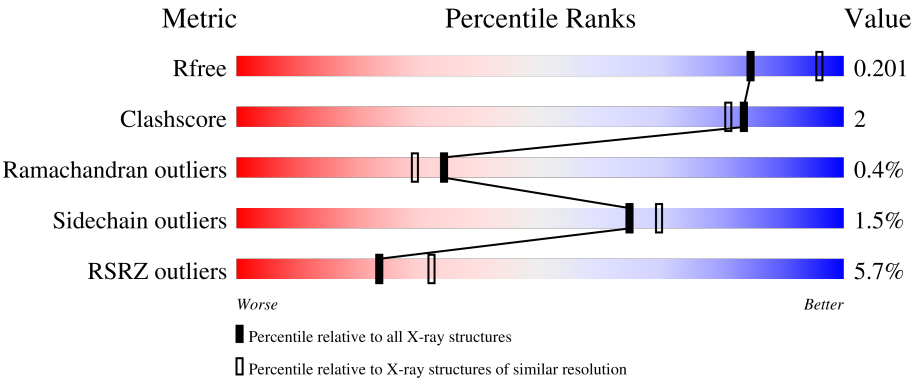
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	346	5% 74% 5% 20%
1	B	346	4% 73% 6% 21%
1	C	346	3% 75% 21%
1	D	346	5% 75% 5% 20%
1	E	346	5% 76% 20%

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Mol	Chain	Length	Quality of chain
1	F	346	5% 73% 7% 20%

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	PEG	A	1309	-	-	-	X
2	PEG	B	1308	-	-	-	X
2	PEG	D	1311	-	-	-	X
2	PEG	E	1308	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14672 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 FORMAMIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	18	0
			2336	1498	381	444	13			
1	B	275	Total	C	N	O	S	0	19	0
			2325	1490	378	444	13			
1	C	274	Total	C	N	O	S	0	17	0
			2296	1473	375	435	13			
1	D	278	Total	C	N	O	S	0	21	0
			2354	1507	384	450	13			
1	E	278	Total	C	N	O	S	0	22	0
			2376	1522	392	450	12			
1	F	277	Total	C	N	O	S	0	20	0
			2351	1504	384	450	13			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	333	TRP	-	expression tag	UNP E5LR94
A	334	PHE	-	expression tag	UNP E5LR94
A	335	ARG	-	expression tag	UNP E5LR94
A	336	VAL	-	expression tag	UNP E5LR94
A	337	ASP	-	expression tag	UNP E5LR94
A	338	PRO	-	expression tag	UNP E5LR94
A	339	LEU	-	expression tag	UNP E5LR94
A	340	GLU	-	expression tag	UNP E5LR94
A	341	HIS	-	expression tag	UNP E5LR94
A	342	HIS	-	expression tag	UNP E5LR94
A	343	HIS	-	expression tag	UNP E5LR94
A	344	HIS	-	expression tag	UNP E5LR94
A	345	HIS	-	expression tag	UNP E5LR94
A	346	HIS	-	expression tag	UNP E5LR94
B	333	TRP	-	expression tag	UNP E5LR94
B	334	PHE	-	expression tag	UNP E5LR94
B	335	ARG	-	expression tag	UNP E5LR94

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Chain	Residue	Modelled	Actual	Comment	Reference
B	336	VAL	-	expression tag	UNP E5LR94
B	337	ASP	-	expression tag	UNP E5LR94
B	338	PRO	-	expression tag	UNP E5LR94
B	339	LEU	-	expression tag	UNP E5LR94
B	340	GLU	-	expression tag	UNP E5LR94
B	341	HIS	-	expression tag	UNP E5LR94
B	342	HIS	-	expression tag	UNP E5LR94
B	343	HIS	-	expression tag	UNP E5LR94
B	344	HIS	-	expression tag	UNP E5LR94
B	345	HIS	-	expression tag	UNP E5LR94
B	346	HIS	-	expression tag	UNP E5LR94
C	333	TRP	-	expression tag	UNP E5LR94
C	334	PHE	-	expression tag	UNP E5LR94
C	335	ARG	-	expression tag	UNP E5LR94
C	336	VAL	-	expression tag	UNP E5LR94
C	337	ASP	-	expression tag	UNP E5LR94
C	338	PRO	-	expression tag	UNP E5LR94
C	339	LEU	-	expression tag	UNP E5LR94
C	340	GLU	-	expression tag	UNP E5LR94
C	341	HIS	-	expression tag	UNP E5LR94
C	342	HIS	-	expression tag	UNP E5LR94
C	343	HIS	-	expression tag	UNP E5LR94
C	344	HIS	-	expression tag	UNP E5LR94
C	345	HIS	-	expression tag	UNP E5LR94
C	346	HIS	-	expression tag	UNP E5LR94
D	333	TRP	-	expression tag	UNP E5LR94
D	334	PHE	-	expression tag	UNP E5LR94
D	335	ARG	-	expression tag	UNP E5LR94
D	336	VAL	-	expression tag	UNP E5LR94
D	337	ASP	-	expression tag	UNP E5LR94
D	338	PRO	-	expression tag	UNP E5LR94
D	339	LEU	-	expression tag	UNP E5LR94
D	340	GLU	-	expression tag	UNP E5LR94
D	341	HIS	-	expression tag	UNP E5LR94
D	342	HIS	-	expression tag	UNP E5LR94
D	343	HIS	-	expression tag	UNP E5LR94
D	344	HIS	-	expression tag	UNP E5LR94
D	345	HIS	-	expression tag	UNP E5LR94
D	346	HIS	-	expression tag	UNP E5LR94
E	333	TRP	-	expression tag	UNP E5LR94
E	334	PHE	-	expression tag	UNP E5LR94
E	335	ARG	-	expression tag	UNP E5LR94

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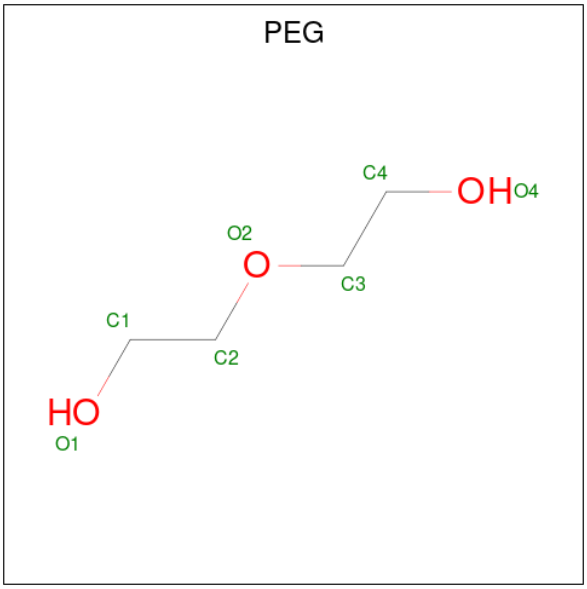
Chain	Residue	Modelled	Actual	Comment	Reference
E	336	VAL	-	expression tag	UNP E5LR94
E	337	ASP	-	expression tag	UNP E5LR94
E	338	PRO	-	expression tag	UNP E5LR94
E	339	LEU	-	expression tag	UNP E5LR94
E	340	GLU	-	expression tag	UNP E5LR94
E	341	HIS	-	expression tag	UNP E5LR94
E	342	HIS	-	expression tag	UNP E5LR94
E	343	HIS	-	expression tag	UNP E5LR94
E	344	HIS	-	expression tag	UNP E5LR94
E	345	HIS	-	expression tag	UNP E5LR94
E	346	HIS	-	expression tag	UNP E5LR94
F	333	TRP	-	expression tag	UNP E5LR94
F	334	PHE	-	expression tag	UNP E5LR94
F	335	ARG	-	expression tag	UNP E5LR94
F	336	VAL	-	expression tag	UNP E5LR94
F	337	ASP	-	expression tag	UNP E5LR94
F	338	PRO	-	expression tag	UNP E5LR94
F	339	LEU	-	expression tag	UNP E5LR94
F	340	GLU	-	expression tag	UNP E5LR94
F	341	HIS	-	expression tag	UNP E5LR94
F	342	HIS	-	expression tag	UNP E5LR94
F	343	HIS	-	expression tag	UNP E5LR94
F	344	HIS	-	expression tag	UNP E5LR94
F	345	HIS	-	expression tag	UNP E5LR94
F	346	HIS	-	expression tag	UNP E5LR94

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

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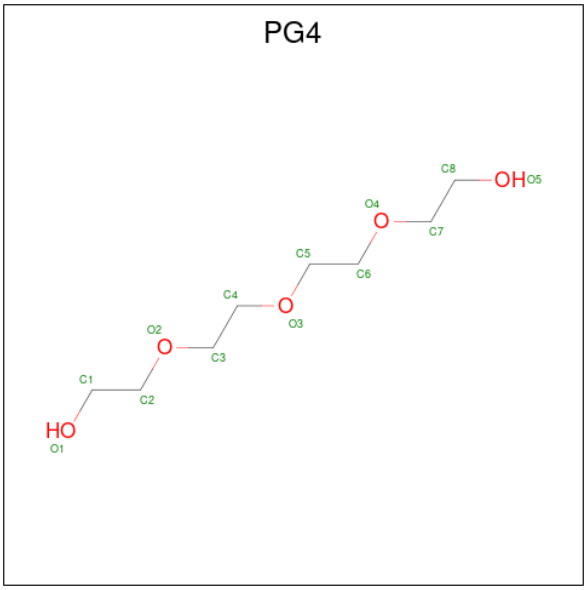
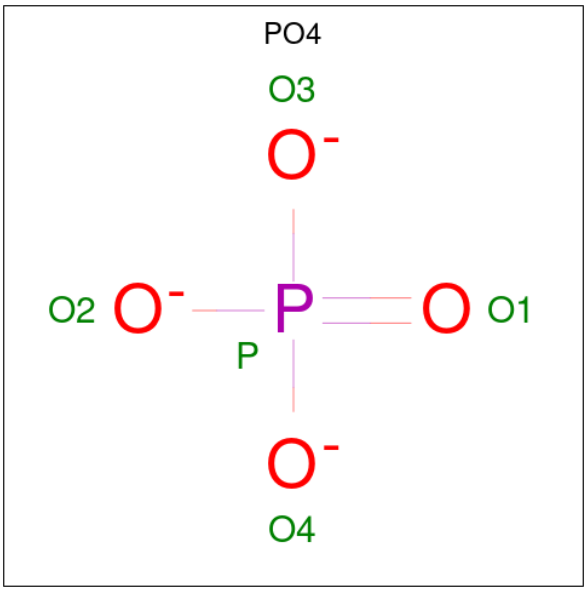
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total C O 7 4 3	0	0

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



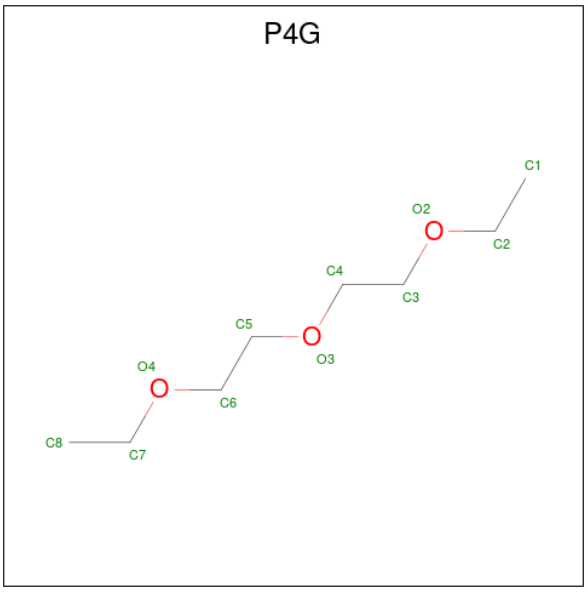
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 8 5	0	0
3	A	1	Total C O 13 8 5	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 5 is 1-ETHOXY-2-(2-ETHOXYETHOXY)ETHANE (three-letter code: P4G) (formula: $C_8H_{18}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 11 8 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	C	O	0	0
			11	8	3		

- Molecule 6 is water.

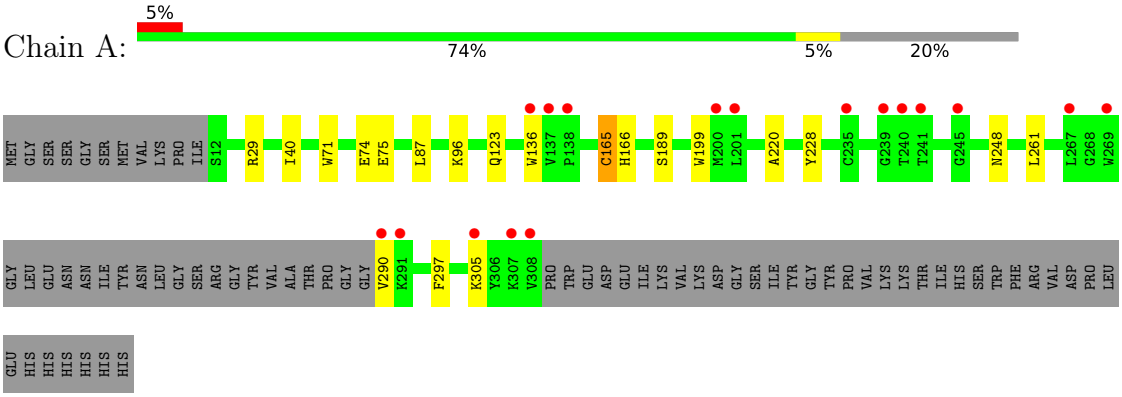
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	95	Total	O	0	0
			95	95		
6	B	74	Total	O	0	0
			74	74		
6	C	70	Total	O	0	0
			70	70		
6	D	69	Total	O	0	0
			69	69		
6	E	61	Total	O	0	0
			61	61		
6	F	46	Total	O	0	0
			46	46		

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.

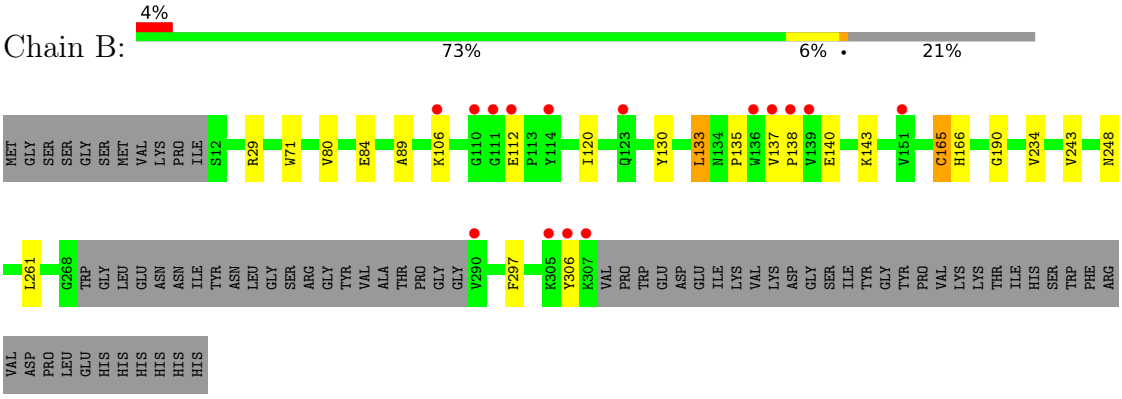
• Molecule 1: FORMAMIDASE

Chain A:



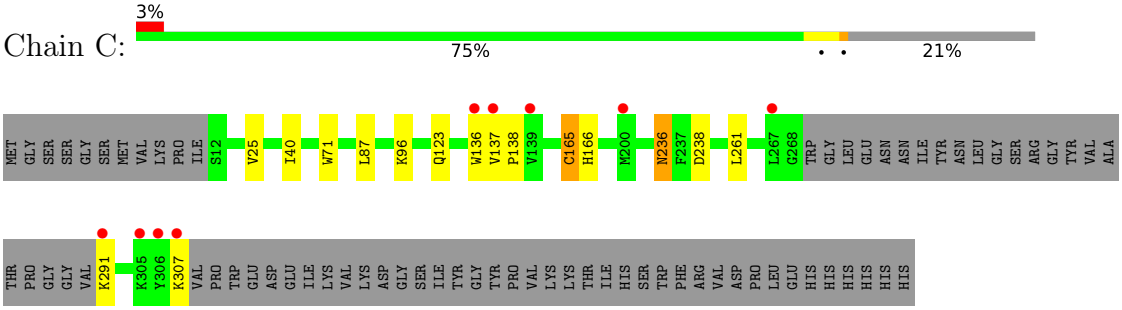
• Molecule 1: FORMAMIDASE

Chain B:



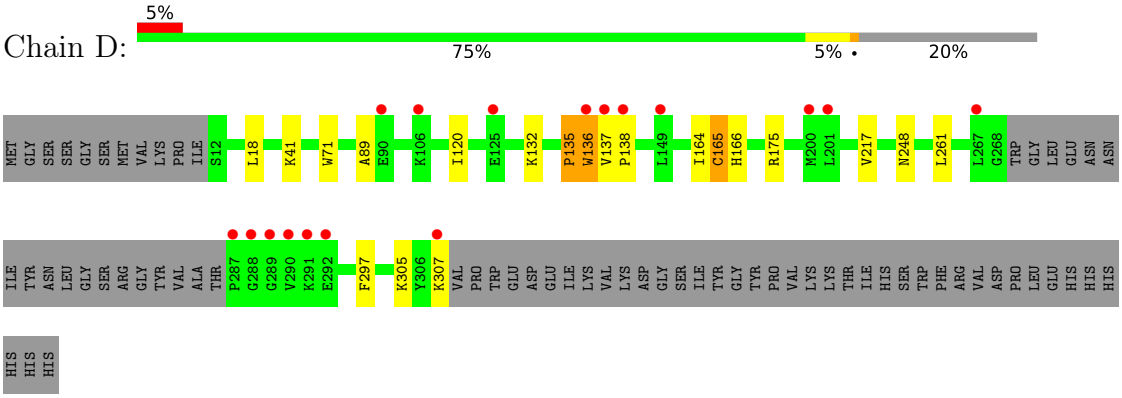
• Molecule 1: FORMAMIDASE

Chain C:



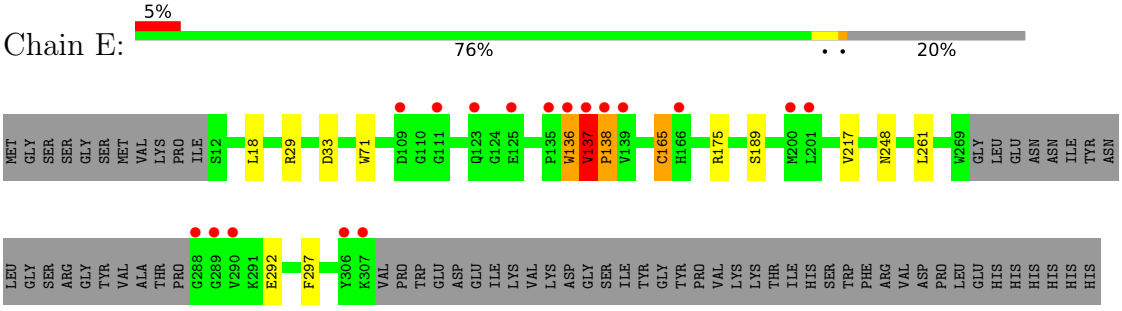
• Molecule 1: FORMAMIDASE

Chain D:



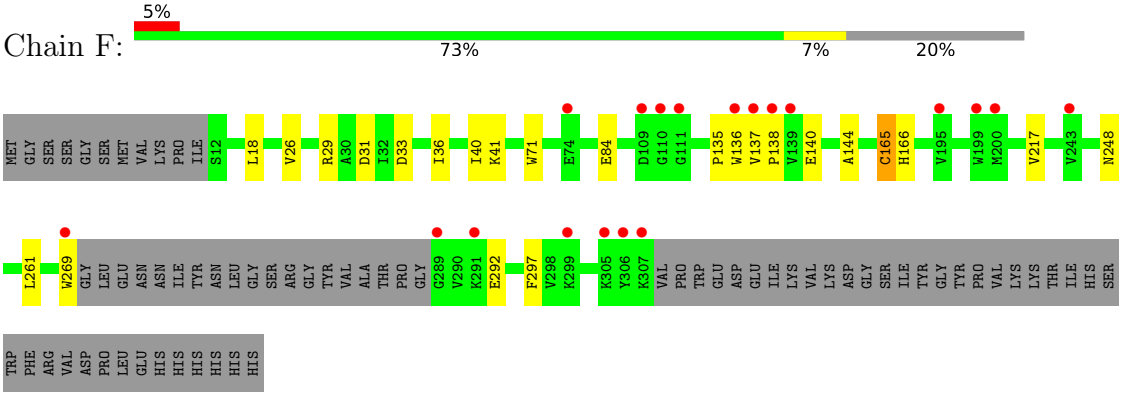
• Molecule 1: FORMAMIDASE

Chain E:



• Molecule 1: FORMAMIDASE

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	142.69Å 149.75Å 97.22Å 90.00° 98.68° 90.00°	Depositor
Resolution (Å)	47.06 – 2.15 59.07 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.06-2.15) 99.2 (59.07-2.15)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 2.14Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.179 , 0.202 0.179 , 0.201	Depositor DCC
R_{free} test set	5444 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	40.0	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 53.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14672	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 3.35% 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: PO4, QCS, PEG, P4G, PG4

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	0.26	0/2380	0.46	0/3237
1	B	0.26	0/2367	0.45	0/3217
1	C	0.26	0/2338	0.45	0/3176
1	D	0.26	0/2397	0.45	0/3254
1	E	0.26	0/2420	0.46	0/3284
1	F	0.26	0/2395	0.45	0/3258
All	All	0.26	0/14297	0.45	0/19426

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	E	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	136[A]	TRP	Peptide
1	E	137[A]	VAL	Peptide

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	2336	0	2253	11	0
1	B	2325	0	2248	15	0
1	C	2296	0	2228	10	0
1	D	2354	0	2273	15	0
1	E	2376	0	2300	10	0
1	F	2351	0	2255	13	0
2	A	21	0	30	0	0
2	B	28	0	40	0	0
2	C	21	0	30	0	0
2	D	28	0	40	1	0
2	E	35	0	50	0	0
2	F	28	0	40	0	0
3	A	26	0	36	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
5	C	11	0	18	1	0
5	F	11	0	18	1	0
6	A	95	0	0	2	0
6	B	74	0	0	3	0
6	C	70	0	0	0	0
6	D	69	0	0	0	0
6	E	61	0	0	0	0
6	F	46	0	0	0	0
All	All	14672	0	13859	69	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 2.

All (69) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165[B]:QCS:SG	1:D:166[B]:HIS:N	2.43	0.91
1:D:41:LYS:NZ	2:D:1311:PEG:O4	2.10	0.83
1:F:29[A]:ARG:NH1	1:F:33:ASP:OD1	2.14	0.81
1:C:165[B]:QCS:SG	1:C:166[B]:HIS:N	2.54	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:29[B]:ARG:NH1	1:E:33:ASP:OD1	2.16	0.79
1:E:165[A]:QCS:NE2	1:E:189[A]:SER:OG	2.16	0.78
6:B:2062:HOH:O	1:F:248:ASN:ND2	2.16	0.78
1:A:189[B]:SER:HG	1:A:199:TRP:HZ3	1.35	0.73
1:F:165[A]:QCS:SG	1:F:166[A]:HIS:N	2.64	0.70
1:B:248:ASN:OD1	6:B:2062:HOH:O	2.08	0.69
1:B:306:TYR:O	1:C:291:LYS:NZ	2.26	0.68
1:F:29[A]:ARG:NH2	1:F:84:GLU:OE2	2.31	0.62
1:B:29:ARG:NH2	1:B:84:GLU:OE2	2.32	0.62
1:B:165[B]:QCS:OE1	1:B:166[B]:HIS:NE2	2.33	0.61
1:A:165[B]:QCS:SG	1:A:166[B]:HIS:N	2.75	0.60
1:A:248:ASN:OD1	6:A:2080:HOH:O	2.16	0.59
1:A:29[B]:ARG:NH1	1:A:75[B]:GLU:O	2.35	0.59
1:B:135[A]:PRO:O	1:B:137[A]:VAL:N	2.36	0.58
1:B:261:LEU:HD11	1:D:261:LEU:HD11	1.85	0.58
1:D:165[B]:QCS:SG	1:D:166[B]:HIS:ND1	2.77	0.58
1:E:136[B]:TRP:HB2	1:E:137[B]:VAL:HA	1.87	0.56
6:B:2062:HOH:O	1:E:248:ASN:OD1	2.18	0.54
1:A:261:LEU:HD11	1:E:261:LEU:HD11	1.89	0.54
1:E:136[B]:TRP:HB3	1:E:138[B]:PRO:HD2	1.91	0.51
1:C:261:LEU:HD11	1:F:261:LEU:HD11	1.91	0.51
1:D:136[B]:TRP:CD1	1:D:138[B]:PRO:HD2	2.46	0.50
1:A:40:ILE:HD11	1:A:87:LEU:HB3	1.94	0.50
1:B:165[A]:QCS:SG	1:B:166[A]:HIS:N	2.85	0.49
1:F:135[B]:PRO:O	1:F:140:GLU:HB2	2.11	0.49
6:A:2080:HOH:O	1:D:248:ASN:OD1	2.20	0.49
1:C:165[B]:QCS:SG	1:C:166[B]:HIS:ND1	2.87	0.47
1:A:305:LYS:O	1:A:305:LYS:HG3	2.13	0.47
1:D:137[B]:VAL:HG12	1:D:138[B]:PRO:HD3	1.96	0.47
1:B:165[A]:QCS:OE1	1:B:190:GLY:N	2.42	0.47
1:C:96[B]:LYS:NZ	1:C:123[B]:GLN:OE1	2.46	0.47
1:A:96:LYS:NZ	1:A:123:GLN:OE1	2.48	0.47
1:E:137[B]:VAL:N	1:E:138[B]:PRO:CD	2.78	0.47
1:B:89:ALA:HA	1:B:120:ILE:HG21	1.97	0.46
1:F:137[B]:VAL:N	1:F:138[B]:PRO:CD	2.78	0.46
1:D:305:LYS:CG	1:D:305:LYS:O	2.65	0.45
1:D:132:LYS:NZ	1:D:165[A]:QCS:OE1	2.44	0.45
1:B:234:VAL:HB	1:B:243:VAL:HG12	1.99	0.45
1:D:135[B]:PRO:O	1:D:136[B]:TRP:HB2	2.17	0.45
1:C:25:VAL:O	1:C:25:VAL:HG23	2.17	0.44
1:B:135[B]:PRO:O	1:B:140:GLU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:ALA:HA	1:D:120:ILE:HG21	2.00	0.43
1:E:137[A]:VAL:HB	1:E:138[A]:PRO:HD3	2.00	0.43
1:C:236:ASN:OD1	5:C:1311:P4G:H62	2.19	0.43
1:D:137[B]:VAL:N	1:D:138[B]:PRO:CD	2.81	0.43
1:E:137[A]:VAL:O	1:E:138[A]:PRO:C	2.57	0.43
1:C:137[B]:VAL:N	1:C:138[B]:PRO:HD3	2.34	0.42
1:A:290:VAL:HG13	1:F:144:ALA:HB3	2.02	0.42
1:D:305:LYS:O	1:D:305:LYS:HG3	2.20	0.42
1:F:36:ILE:O	1:F:40:ILE:HG12	2.19	0.42
1:B:80:VAL:O	1:B:80:VAL:HG23	2.20	0.42
1:D:18:LEU:HB3	1:D:217:VAL:HB	2.02	0.41
1:E:18:LEU:HB3	1:E:217:VAL:HB	2.02	0.41
1:F:269:TRP:CD1	1:F:269:TRP:N	2.87	0.41
1:B:112[B]:GLU:HG2	1:B:143:LYS:HB2	2.01	0.41
1:A:74:GLU:OE1	1:A:74:GLU:N	2.39	0.41
1:B:130:TYR:HE1	1:B:133:LEU:HD22	1.86	0.41
1:C:40:ILE:HD11	1:C:87:LEU:HB3	2.01	0.41
1:F:26:VAL:HG13	1:F:31:ASP:HB2	2.03	0.41
1:B:137[B]:VAL:N	1:B:138[B]:PRO:CD	2.84	0.41
1:F:18:LEU:HB3	1:F:217:VAL:HB	2.03	0.40
1:D:164:ILE:HG22	1:D:165[B]:QCS:H5	2.03	0.40
1:A:220:ALA:HA	1:A:228:TYR:O	2.21	0.40
1:C:236:ASN:HB3	1:C:238[A]:ASP:OD1	2.21	0.40
1:F:41:LYS:HZ1	5:F:1312:P4G:C6	2.34	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	289/346 (84%)	278 (96%)	9 (3%)	2 (1%)	22 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	288/346 (83%)	279 (97%)	9 (3%)	0	100 100
1	C	285/346 (82%)	270 (95%)	13 (5%)	2 (1%)	22 15
1	D	293/346 (85%)	275 (94%)	14 (5%)	4 (1%)	11 5
1	E	294/346 (85%)	281 (96%)	11 (4%)	2 (1%)	22 15
1	F	291/346 (84%)	280 (96%)	9 (3%)	2 (1%)	22 15
All	All	1740/2076 (84%)	1663 (96%)	65 (4%)	12 (1%)	34 15

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	135[A]	PRO
1	D	135[B]	PRO
1	D	136[A]	TRP
1	D	136[B]	TRP
1	F	136[A]	TRP
1	F	136[B]	TRP
1	C	136[A]	TRP
1	C	136[B]	TRP
1	A	136[A]	TRP
1	A	136[B]	TRP
1	E	138[A]	PRO
1	E	138[B]	PRO

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	251/293 (86%)	249 (99%)	2 (1%)	81 86
1	B	250/293 (85%)	246 (98%)	4 (2%)	62 67
1	C	246/293 (84%)	243 (99%)	3 (1%)	71 76
1	D	252/293 (86%)	248 (98%)	4 (2%)	62 67
1	E	254/293 (87%)	248 (98%)	6 (2%)	49 51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	252/293 (86%)	249 (99%)	3 (1%)	71 76
All	All	1505/1758 (86%)	1483 (98%)	22 (2%)	65 69

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	TRP
1	A	297	PHE
1	B	71	TRP
1	B	106	LYS
1	B	133	LEU
1	B	297	PHE
1	C	71	TRP
1	C	236	ASN
1	C	307	LYS
1	D	71	TRP
1	D	175	ARG
1	D	297	PHE
1	D	307	LYS
1	E	71	TRP
1	E	137[A]	VAL
1	E	137[B]	VAL
1	E	175	ARG
1	E	292	GLU
1	E	297	PHE
1	F	71	TRP
1	F	292	GLU
1	F	297	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	QCS	B	165[A]	1	6,8,9	1.86	1 (16%)	3,9,11	1.67	1 (33%)
1	QCS	A	165[A]	1	6,8,9	1.88	1 (16%)	3,9,11	2.02	1 (33%)
1	QCS	C	165[B]	1	6,8,9	1.82	1 (16%)	3,9,11	1.48	1 (33%)
1	QCS	D	165[B]	1	6,8,9	1.82	1 (16%)	3,9,11	1.54	1 (33%)
1	QCS	F	165[B]	1	6,8,9	1.91	1 (16%)	3,9,11	2.06	1 (33%)
1	QCS	C	165[A]	1	6,8,9	1.87	1 (16%)	3,9,11	2.09	1 (33%)
1	QCS	F	165[A]	1	6,8,9	1.84	1 (16%)	3,9,11	1.42	1 (33%)
1	QCS	D	165[A]	1	6,8,9	1.89	1 (16%)	3,9,11	1.92	1 (33%)
1	QCS	E	165[B]	1	6,8,9	1.88	1 (16%)	3,9,11	2.00	1 (33%)
1	QCS	A	165[B]	1	6,8,9	1.91	1 (16%)	3,9,11	1.82	1 (33%)
1	QCS	E	165[A]	1	6,8,9	1.84	1 (16%)	3,9,11	1.62	1 (33%)
1	QCS	B	165[B]	1	6,8,9	1.86	1 (16%)	3,9,11	2.10	1 (33%)

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
1	QCS	B	165[A]	1	-	0/4/7/9	-
1	QCS	A	165[A]	1	-	3/4/7/9	-
1	QCS	C	165[B]	1	-	1/4/7/9	-
1	QCS	D	165[B]	1	-	3/4/7/9	-
1	QCS	F	165[B]	1	-	1/4/7/9	-
1	QCS	C	165[A]	1	-	1/4/7/9	-
1	QCS	F	165[A]	1	-	1/4/7/9	-
1	QCS	D	165[A]	1	-	2/4/7/9	-
1	QCS	E	165[B]	1	-	1/4/7/9	-
1	QCS	A	165[B]	1	-	1/4/7/9	-
1	QCS	E	165[A]	1	-	1/4/7/9	-
1	QCS	B	165[B]	1	-	2/4/7/9	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	165[B]	QCS	CD-NE2	3.75	1.42	1.33
1	A	165[A]	QCS	CD-NE2	3.70	1.42	1.33
1	E	165[B]	QCS	CD-NE2	3.70	1.42	1.33
1	C	165[A]	QCS	CD-NE2	3.69	1.42	1.33
1	D	165[A]	QCS	CD-NE2	3.67	1.42	1.33
1	A	165[B]	QCS	CD-NE2	3.66	1.42	1.33
1	B	165[B]	QCS	CD-NE2	3.61	1.42	1.33
1	E	165[A]	QCS	CD-NE2	3.42	1.41	1.33
1	F	165[A]	QCS	CD-NE2	3.36	1.41	1.33
1	C	165[B]	QCS	CD-NE2	3.31	1.41	1.33
1	B	165[A]	QCS	CD-NE2	3.30	1.41	1.33
1	D	165[B]	QCS	CD-NE2	3.26	1.41	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	165[B]	QCS	OE1-CD-NE2	-3.55	119.78	125.53
1	C	165[A]	QCS	OE1-CD-NE2	-3.50	119.86	125.53
1	F	165[B]	QCS	OE1-CD-NE2	-3.49	119.88	125.53
1	E	165[B]	QCS	OE1-CD-NE2	-3.39	120.04	125.53
1	A	165[A]	QCS	OE1-CD-NE2	-3.38	120.07	125.53
1	D	165[A]	QCS	OE1-CD-NE2	-3.19	120.36	125.53
1	A	165[B]	QCS	OE1-CD-NE2	-3.03	120.63	125.53
1	B	165[A]	QCS	OE1-CD-NE2	-2.85	120.91	125.53
1	E	165[A]	QCS	OE1-CD-NE2	-2.79	121.02	125.53
1	D	165[B]	QCS	OE1-CD-NE2	-2.67	121.21	125.53
1	C	165[B]	QCS	OE1-CD-NE2	-2.56	121.39	125.53
1	F	165[A]	QCS	OE1-CD-NE2	-2.45	121.56	125.53

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	165[A]	QCS	CA-CB-SG-CD
1	A	165[A]	QCS	OE1-CD-SG-CB
1	A	165[B]	QCS	OE1-CD-SG-CB
1	B	165[B]	QCS	OE1-CD-SG-CB
1	C	165[B]	QCS	OE1-CD-SG-CB
1	D	165[A]	QCS	OE1-CD-SG-CB
1	D	165[B]	QCS	C-CA-CB-SG
1	D	165[B]	QCS	OE1-CD-SG-CB

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Mol	Chain	Res	Type	Atoms
1	E	165[A]	QCS	OE1-CD-SG-CB
1	F	165[A]	QCS	OE1-CD-SG-CB
1	A	165[A]	QCS	N-CA-CB-SG
1	B	165[B]	QCS	N-CA-CB-SG
1	D	165[A]	QCS	CA-CB-SG-CD
1	D	165[B]	QCS	N-CA-CB-SG
1	C	165[A]	QCS	N-CA-CB-SG
1	E	165[B]	QCS	N-CA-CB-SG
1	F	165[B]	QCS	N-CA-CB-SG

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	165[A]	QCS	2	0
1	C	165[B]	QCS	2	0
1	D	165[B]	QCS	3	0
1	F	165[A]	QCS	1	0
1	D	165[A]	QCS	1	0
1	A	165[B]	QCS	1	0
1	E	165[A]	QCS	1	0
1	B	165[B]	QCS	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

29 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	$\#\|Z\| > 2$
3	PG4	A	1313	-	12,12,12	0.52	0	11,11,11	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PEG	E	1312	-	6,6,6	0.48	0	5,5,5	0.34	0
2	PEG	B	1310	-	6,6,6	0.49	0	5,5,5	0.30	0
2	PEG	E	1311	-	6,6,6	0.48	0	5,5,5	0.31	0
2	PEG	A	1310	-	6,6,6	0.48	0	5,5,5	0.31	0
2	PEG	C	1309	-	6,6,6	0.47	0	5,5,5	0.35	0
3	PG4	A	1312	-	12,12,12	0.50	0	11,11,11	0.39	0
2	PEG	B	1311	-	6,6,6	0.49	0	5,5,5	0.40	0
2	PEG	B	1308	-	6,6,6	0.47	0	5,5,5	0.40	0
2	PEG	C	1310	-	6,6,6	0.48	0	5,5,5	0.38	0
2	PEG	E	1309	-	6,6,6	0.49	0	5,5,5	0.30	0
2	PEG	B	1309	-	6,6,6	0.49	0	5,5,5	0.33	0
2	PEG	F	1311	-	6,6,6	0.46	0	5,5,5	0.52	0
2	PEG	D	1311	-	6,6,6	0.61	0	5,5,5	1.41	1 (20%)
2	PEG	A	1309	-	6,6,6	0.48	0	5,5,5	0.32	0
2	PEG	D	1308	-	6,6,6	0.47	0	5,5,5	0.42	0
2	PEG	F	1310	-	6,6,6	0.48	0	5,5,5	0.28	0
2	PEG	D	1310	-	6,6,6	0.47	0	5,5,5	0.39	0
2	PEG	E	1310	-	6,6,6	0.49	0	5,5,5	0.26	0
5	P4G	F	1312	-	10,10,10	0.56	0	9,9,9	0.45	0
2	PEG	C	1308	-	6,6,6	0.48	0	5,5,5	0.28	0
2	PEG	F	1309	-	6,6,6	0.48	0	5,5,5	0.30	0
2	PEG	D	1309	-	6,6,6	0.48	0	5,5,5	0.39	0
4	PO4	B	1312	-	4,4,4	0.87	0	6,6,6	0.43	0
5	P4G	C	1311	-	10,10,10	0.55	0	9,9,9	0.52	0
4	PO4	C	1312	-	4,4,4	0.87	0	6,6,6	0.49	0
2	PEG	A	1311	-	6,6,6	0.48	0	5,5,5	0.30	0
2	PEG	E	1308	-	6,6,6	0.46	0	5,5,5	0.45	0
2	PEG	F	1308	-	6,6,6	0.47	0	5,5,5	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
3	PG4	A	1313	-	-	3/10/10/10	-
2	PEG	E	1312	-	-	2/4/4/4	-
2	PEG	B	1310	-	-	1/4/4/4	-
2	PEG	E	1311	-	-	1/4/4/4	-
2	PEG	A	1310	-	-	1/4/4/4	-
2	PEG	C	1309	-	-	2/4/4/4	-
3	PG4	A	1312	-	-	7/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	B	1311	-	-	1/4/4/4	-
2	PEG	B	1308	-	-	1/4/4/4	-
2	PEG	C	1310	-	-	2/4/4/4	-
2	PEG	E	1309	-	-	1/4/4/4	-
2	PEG	B	1309	-	-	2/4/4/4	-
2	PEG	F	1311	-	-	4/4/4/4	-
2	PEG	D	1311	-	-	1/4/4/4	-
2	PEG	A	1309	-	-	2/4/4/4	-
2	PEG	D	1308	-	-	2/4/4/4	-
2	PEG	F	1310	-	-	1/4/4/4	-
2	PEG	D	1310	-	-	3/4/4/4	-
2	PEG	E	1310	-	-	1/4/4/4	-
5	P4G	F	1312	-	-	4/8/8/8	-
2	PEG	C	1308	-	-	1/4/4/4	-
2	PEG	F	1309	-	-	2/4/4/4	-
2	PEG	D	1309	-	-	3/4/4/4	-
5	P4G	C	1311	-	-	3/8/8/8	-
2	PEG	A	1311	-	-	2/4/4/4	-
2	PEG	E	1308	-	-	0/4/4/4	-
2	PEG	F	1308	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1311	PEG	C3-O2-C2	2.90	125.83	113.29

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1312	PG4	O3-C5-C6-O4
2	B	1310	PEG	O1-C1-C2-O2
2	D	1308	PEG	O2-C3-C4-O4
2	D	1309	PEG	O1-C1-C2-O2
2	E	1312	PEG	O1-C1-C2-O2
2	E	1312	PEG	O2-C3-C4-O4
2	F	1309	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
2	F	1310	PEG	O1-C1-C2-O2
3	A	1312	PG4	O2-C3-C4-O3
2	C	1310	PEG	O2-C3-C4-O4
2	D	1310	PEG	O2-C3-C4-O4
5	C	1311	P4G	O2-C3-C4-O3
3	A	1313	PG4	O3-C5-C6-O4
2	A	1309	PEG	O2-C3-C4-O4
2	A	1310	PEG	O1-C1-C2-O2
2	C	1309	PEG	O1-C1-C2-O2
2	E	1311	PEG	O2-C3-C4-O4
2	F	1311	PEG	O2-C3-C4-O4
2	A	1311	PEG	O1-C1-C2-O2
2	A	1311	PEG	O2-C3-C4-O4
2	B	1311	PEG	O2-C3-C4-O4
2	F	1308	PEG	O1-C1-C2-O2
2	F	1311	PEG	O1-C1-C2-O2
2	B	1309	PEG	O2-C3-C4-O4
2	A	1309	PEG	O1-C1-C2-O2
5	F	1312	P4G	C8-C7-O4-C6
5	F	1312	P4G	O3-C5-C6-O4
5	F	1312	P4G	C1-C2-O2-C3
2	D	1309	PEG	C1-C2-O2-C3
2	D	1308	PEG	C1-C2-O2-C3
2	D	1310	PEG	C1-C2-O2-C3
2	B	1308	PEG	C1-C2-O2-C3
3	A	1312	PG4	C1-C2-O2-C3
2	C	1309	PEG	C1-C2-O2-C3
3	A	1312	PG4	C6-C5-O3-C4
3	A	1313	PG4	C6-C5-O3-C4
2	E	1310	PEG	O2-C3-C4-O4
2	F	1311	PEG	C1-C2-O2-C3
3	A	1312	PG4	C8-C7-O4-C6
2	D	1311	PEG	C4-C3-O2-C2
2	D	1310	PEG	O1-C1-C2-O2
2	F	1308	PEG	C4-C3-O2-C2
2	C	1310	PEG	O1-C1-C2-O2
2	E	1309	PEG	C4-C3-O2-C2
2	D	1309	PEG	O2-C3-C4-O4
2	F	1311	PEG	C4-C3-O2-C2
5	F	1312	P4G	C5-C6-O4-C7
3	A	1312	PG4	O4-C7-C8-O5
5	C	1311	P4G	C3-C4-O3-C5

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Mol	Chain	Res	Type	Atoms
2	B	1309	PEG	O1-C1-C2-O2
2	F	1309	PEG	C1-C2-O2-C3
3	A	1312	PG4	C3-C4-O3-C5
3	A	1313	PG4	O4-C7-C8-O5
2	C	1308	PEG	O2-C3-C4-O4
5	C	1311	P4G	O3-C5-C6-O4

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1311	PEG	1	0
5	F	1312	P4G	1	0
5	C	1311	P4G	1	0

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, 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	276/346 (79%)	0.38	17 (6%)	20	27	28, 38, 62, 107	0
1	B	274/346 (79%)	0.50	15 (5%)	25	34	33, 44, 76, 103	0
1	C	273/346 (78%)	0.13	9 (3%)	46	55	29, 39, 56, 103	0
1	D	277/346 (80%)	0.33	17 (6%)	21	28	29, 40, 63, 117	0
1	E	277/346 (80%)	0.44	17 (6%)	21	28	31, 41, 71, 98	0
1	F	276/346 (79%)	0.41	19 (6%)	16	23	31, 42, 77, 104	0
All	All	1653/2076 (79%)	0.37	94 (5%)	23	32	28, 41, 69, 117	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	290	VAL	13.8
1	E	136[A]	TRP	8.3
1	D	287	PRO	7.3
1	B	136[A]	TRP	7.0
1	D	290	VAL	6.6
1	A	291	LYS	6.1
1	D	289	GLY	5.9
1	C	291	LYS	5.8
1	D	307	LYS	5.6
1	D	288	GLY	5.4
1	F	138[A]	PRO	5.0
1	A	307[A]	LYS	4.9
1	F	306	TYR	4.9
1	B	306	TYR	4.7
1	E	137[A]	VAL	4.6
1	F	136[A]	TRP	4.5
1	A	269	TRP	4.4
1	B	290	VAL	4.4
1	B	305[A]	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	308	VAL	4.1
1	E	138[A]	PRO	4.0
1	D	136[A]	TRP	4.0
1	F	269	TRP	3.9
1	A	136[A]	TRP	3.7
1	B	111	GLY	3.7
1	E	289	GLY	3.7
1	C	267	LEU	3.7
1	B	123	GLN	3.7
1	D	291	LYS	3.7
1	B	137[A]	VAL	3.6
1	E	290	VAL	3.6
1	F	137[A]	VAL	3.6
1	B	110	GLY	3.6
1	B	114	TYR	3.6
1	C	136[A]	TRP	3.5
1	A	138[A]	PRO	3.4
1	C	305	LYS	3.4
1	B	139[A]	VAL	3.3
1	F	110	GLY	3.2
1	B	138[A]	PRO	3.2
1	F	289	GLY	3.2
1	F	307	LYS	3.1
1	D	292[A]	GLU	3.0
1	E	306	TYR	3.0
1	B	307	LYS	2.9
1	F	200[A]	MET	2.9
1	C	307	LYS	2.9
1	A	200[A]	MET	2.9
1	A	267	LEU	2.9
1	D	200[A]	MET	2.9
1	E	200	MET	2.8
1	E	307	LYS	2.8
1	D	137[A]	VAL	2.7
1	E	288	GLY	2.7
1	A	241	THR	2.7
1	F	111	GLY	2.6
1	C	200[A]	MET	2.6
1	F	305	LYS	2.5
1	E	135[A]	PRO	2.5
1	A	137[A]	VAL	2.5
1	C	139[A]	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	109	ASP	2.5
1	E	201	LEU	2.5
1	D	201	LEU	2.4
1	E	109	ASP	2.4
1	A	235	CYS	2.4
1	E	166[A]	HIS	2.4
1	C	137[A]	VAL	2.4
1	E	139	VAL	2.4
1	C	306	TYR	2.4
1	F	299	LYS	2.4
1	A	201	LEU	2.3
1	A	240	THR	2.3
1	D	125[A]	GLU	2.3
1	D	90[A]	GLU	2.3
1	D	106[A]	LYS	2.2
1	D	138[A]	PRO	2.2
1	E	111	GLY	2.2
1	F	291	LYS	2.2
1	D	267	LEU	2.1
1	F	139[A]	VAL	2.1
1	A	305	LYS	2.1
1	A	239	GLY	2.1
1	A	245	GLY	2.1
1	B	151	VAL	2.1
1	F	74[A]	GLU	2.1
1	D	149	LEU	2.1
1	F	195	VAL	2.1
1	E	125[A]	GLU	2.0
1	B	106	LYS	2.0
1	B	112[A]	GLU	2.0
1	F	199	TRP	2.0
1	E	123	GLN	2.0
1	F	243	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
1	QCS	E	165[A]	9/10	0.90	0.24	47,49,52,53	9
1	QCS	E	165[B]	9/10	0.90	0.24	47,49,53,54	9
1	QCS	D	165[A]	9/10	0.92	0.17	46,47,52,53	9
1	QCS	D	165[B]	9/10	0.92	0.17	46,47,51,52	9
1	QCS	A	165[A]	9/10	0.92	0.18	44,45,50,51	9
1	QCS	A	165[B]	9/10	0.92	0.18	44,45,49,50	9
1	QCS	F	165[A]	9/10	0.92	0.17	46,47,52,53	9
1	QCS	F	165[B]	9/10	0.92	0.17	46,47,53,53	9
1	QCS	C	165[A]	9/10	0.94	0.20	40,41,46,47	9
1	QCS	C	165[B]	9/10	0.94	0.20	40,41,45,47	9
1	QCS	B	165[A]	9/10	0.96	0.21	46,47,50,50	9
1	QCS	B	165[B]	9/10	0.96	0.21	46,46,51,54	9

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PEG	D	1311	7/7	0.41	0.69	131,132,134,134	0
2	PEG	F	1310	7/7	0.44	0.36	85,86,87,87	0
5	P4G	F	1312	11/11	0.64	0.26	63,64,65,65	0
2	PEG	E	1308	7/7	0.69	0.55	69,69,71,71	0
3	PG4	A	1313	13/13	0.70	0.39	109,112,114,114	0
2	PEG	B	1311	7/7	0.74	0.21	86,87,88,88	0
2	PEG	A	1309	7/7	0.78	0.47	70,71,72,73	0
2	PEG	B	1308	7/7	0.78	0.51	66,66,67,67	0
3	PG4	A	1312	13/13	0.79	0.31	85,88,92,92	0
2	PEG	E	1310	7/7	0.79	0.27	73,73,74,74	0
2	PEG	D	1308	7/7	0.79	0.22	64,64,64,64	0
2	PEG	B	1310	7/7	0.80	0.18	109,110,110,110	0
2	PEG	D	1309	7/7	0.82	0.16	72,72,73,73	0
2	PEG	B	1309	7/7	0.82	0.19	76,77,79,79	0
2	PEG	C	1309	7/7	0.83	0.17	74,74,75,75	0
2	PEG	E	1311	7/7	0.83	0.23	88,88,89,89	0
2	PEG	C	1308	7/7	0.84	0.17	73,73,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	P4G	C	1311	11/11	0.84	0.19	56,57,58,58	0
2	PEG	E	1312	7/7	0.84	0.17	74,75,76,76	0
2	PEG	D	1310	7/7	0.85	0.69	79,79,79,79	0
2	PEG	F	1311	7/7	0.85	0.17	73,73,73,73	0
2	PEG	F	1308	7/7	0.86	0.53	65,65,65,66	0
2	PEG	A	1311	7/7	0.87	0.15	68,68,69,69	0
2	PEG	A	1310	7/7	0.89	0.15	84,85,87,87	0
2	PEG	E	1309	7/7	0.90	0.24	76,77,79,79	0
2	PEG	C	1310	7/7	0.91	0.48	70,70,72,73	0
2	PEG	F	1309	7/7	0.91	0.15	79,79,80,80	0
4	PO4	B	1312	5/5	0.99	0.22	31,32,33,34	0
4	PO4	C	1312	5/5	0.99	0.23	28,30,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.