Full wwPDB X-ray Structure Validation Report (i)

Aug 21, 2023 – 04:22 PM EDT

PDB ID	:	8F6B
Title	:	Crystal structure of murine PolG2 hexamer bound to DNA
Authors	:	Wojtaszek, J.L.; Hoff, K.E.; Williams, R.S.
Deposited on	:	2022-11-16
Resolution	:	2.75 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 (1)) were used in the production of this report:

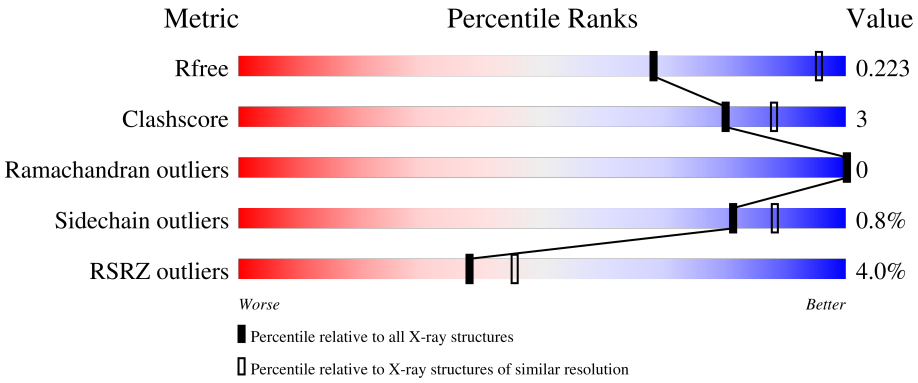
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	455	3% 82% 8% 10%
1	B	455	2% 83% 7% 10%
1	C	455	4% 83% 6% 11%
1	D	455	4% 84% 7% 9%
1	E	455	4% 83% 5% 12%

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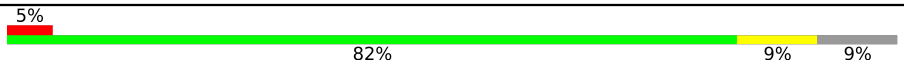
Mol	Chain	Length	Quality of chain
1	F	455	
2	G	18	
2	H	18	
2	I	18	
2	J	18	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 20672 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 PolG2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	0	0
			3118	1995	538	571	14			
1	B	411	Total	C	N	O	S	0	1	0
			3169	2023	550	581	15			
1	C	404	Total	C	N	O	S	0	1	0
			3120	1991	545	571	13			
1	D	414	Total	C	N	O	S	0	3	0
			3223	2054	565	589	15			
1	E	401	Total	C	N	O	S	0	1	0
			3091	1971	539	567	14			
1	F	416	Total	C	N	O	S	0	2	0
			3248	2071	569	593	15			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	MET	-	initiating methionine	UNP Q0VES3
A	460	ALA	-	expression tag	UNP Q0VES3
A	461	ALA	-	expression tag	UNP Q0VES3
A	462	ALA	-	expression tag	UNP Q0VES3
A	463	LEU	-	expression tag	UNP Q0VES3
A	464	GLU	-	expression tag	UNP Q0VES3
A	465	HIS	-	expression tag	UNP Q0VES3
A	466	HIS	-	expression tag	UNP Q0VES3
A	467	HIS	-	expression tag	UNP Q0VES3
A	468	HIS	-	expression tag	UNP Q0VES3
A	469	HIS	-	expression tag	UNP Q0VES3
A	470	HIS	-	expression tag	UNP Q0VES3
B	16	MET	-	initiating methionine	UNP Q0VES3
B	460	ALA	-	expression tag	UNP Q0VES3
B	461	ALA	-	expression tag	UNP Q0VES3
B	462	ALA	-	expression tag	UNP Q0VES3
B	463	LEU	-	expression tag	UNP Q0VES3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	464	GLU	-	expression tag	UNP Q0VES3
B	465	HIS	-	expression tag	UNP Q0VES3
B	466	HIS	-	expression tag	UNP Q0VES3
B	467	HIS	-	expression tag	UNP Q0VES3
B	468	HIS	-	expression tag	UNP Q0VES3
B	469	HIS	-	expression tag	UNP Q0VES3
B	470	HIS	-	expression tag	UNP Q0VES3
C	16	MET	-	initiating methionine	UNP Q0VES3
C	460	ALA	-	expression tag	UNP Q0VES3
C	461	ALA	-	expression tag	UNP Q0VES3
C	462	ALA	-	expression tag	UNP Q0VES3
C	463	LEU	-	expression tag	UNP Q0VES3
C	464	GLU	-	expression tag	UNP Q0VES3
C	465	HIS	-	expression tag	UNP Q0VES3
C	466	HIS	-	expression tag	UNP Q0VES3
C	467	HIS	-	expression tag	UNP Q0VES3
C	468	HIS	-	expression tag	UNP Q0VES3
C	469	HIS	-	expression tag	UNP Q0VES3
C	470	HIS	-	expression tag	UNP Q0VES3
D	16	MET	-	initiating methionine	UNP Q0VES3
D	460	ALA	-	expression tag	UNP Q0VES3
D	461	ALA	-	expression tag	UNP Q0VES3
D	462	ALA	-	expression tag	UNP Q0VES3
D	463	LEU	-	expression tag	UNP Q0VES3
D	464	GLU	-	expression tag	UNP Q0VES3
D	465	HIS	-	expression tag	UNP Q0VES3
D	466	HIS	-	expression tag	UNP Q0VES3
D	467	HIS	-	expression tag	UNP Q0VES3
D	468	HIS	-	expression tag	UNP Q0VES3
D	469	HIS	-	expression tag	UNP Q0VES3
D	470	HIS	-	expression tag	UNP Q0VES3
E	16	MET	-	initiating methionine	UNP Q0VES3
E	460	ALA	-	expression tag	UNP Q0VES3
E	461	ALA	-	expression tag	UNP Q0VES3
E	462	ALA	-	expression tag	UNP Q0VES3
E	463	LEU	-	expression tag	UNP Q0VES3
E	464	GLU	-	expression tag	UNP Q0VES3
E	465	HIS	-	expression tag	UNP Q0VES3
E	466	HIS	-	expression tag	UNP Q0VES3
E	467	HIS	-	expression tag	UNP Q0VES3
E	468	HIS	-	expression tag	UNP Q0VES3
E	469	HIS	-	expression tag	UNP Q0VES3

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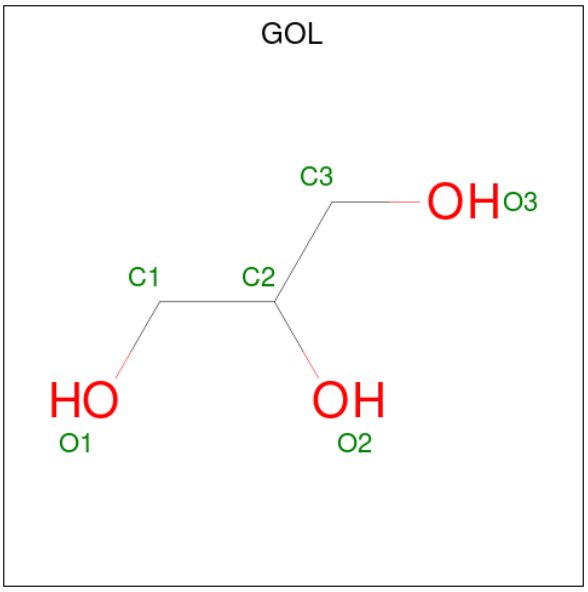
Chain	Residue	Modelled	Actual	Comment	Reference
E	470	HIS	-	expression tag	UNP Q0VES3
F	16	MET	-	initiating methionine	UNP Q0VES3
F	460	ALA	-	expression tag	UNP Q0VES3
F	461	ALA	-	expression tag	UNP Q0VES3
F	462	ALA	-	expression tag	UNP Q0VES3
F	463	LEU	-	expression tag	UNP Q0VES3
F	464	GLU	-	expression tag	UNP Q0VES3
F	465	HIS	-	expression tag	UNP Q0VES3
F	466	HIS	-	expression tag	UNP Q0VES3
F	467	HIS	-	expression tag	UNP Q0VES3
F	468	HIS	-	expression tag	UNP Q0VES3
F	469	HIS	-	expression tag	UNP Q0VES3
F	470	HIS	-	expression tag	UNP Q0VES3

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*TP*GP*GP*TP*AP*GP*GP*CP*GP*CP*CP*TP*AP*CP*CP*AP*G)-3').

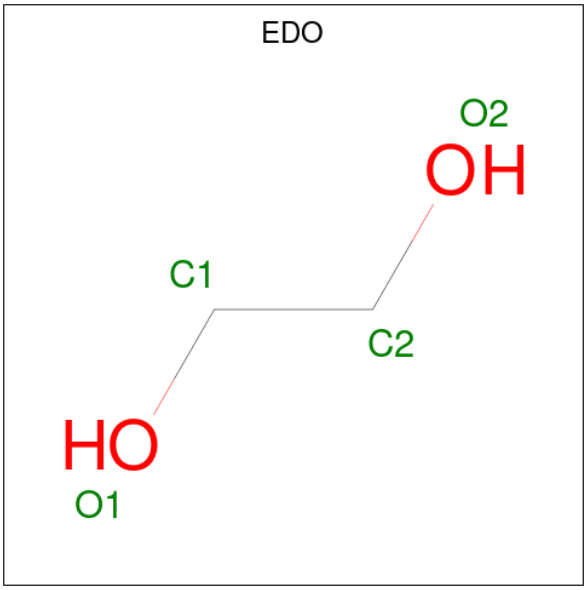
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	18	Total	C	N	O	P	0	0	0
			366	174	69	106	17			
2	H	18	Total	C	N	O	P	0	0	0
			366	174	69	106	17			
2	I	18	Total	C	N	O	P	0	0	0
			366	174	69	106	17			
2	J	18	Total	C	N	O	P	0	0	0
			366	174	69	106	17			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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



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

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

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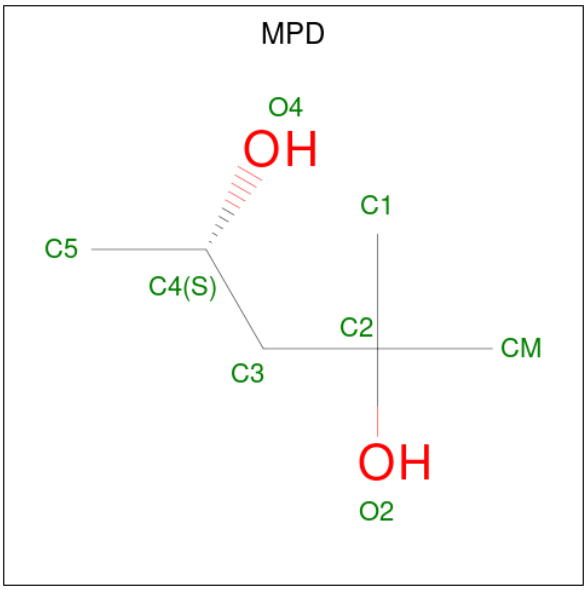
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 8 6 2	0	0
5	B	1	Total C O 8 6 2	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total Na 1 1	0	0
6	I	1	Total Na 1 1	0	0

- Molecule 7 is water.

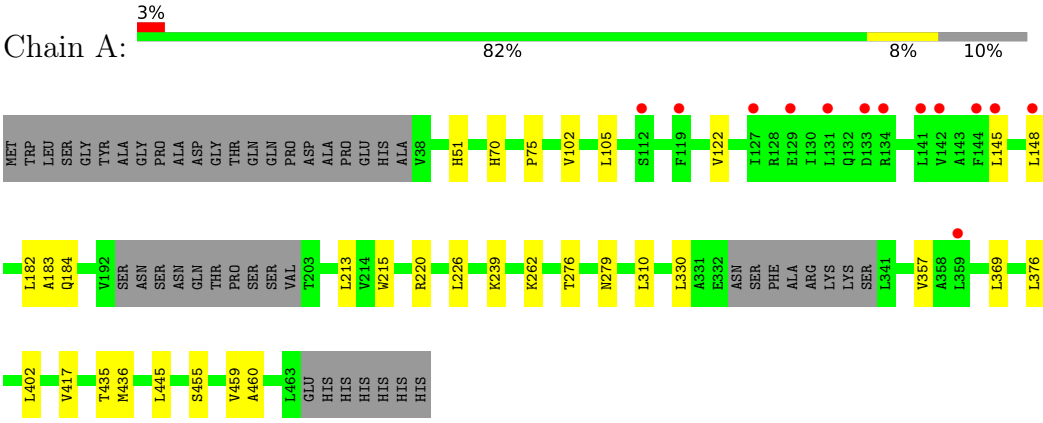
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	15	Total O 15 15	0	0
7	B	21	Total O 21 21	0	0
7	C	13	Total O 13 13	0	0
7	D	6	Total O 6 6	0	0
7	E	4	Total O 4 4	0	0
7	F	11	Total O 11 11	0	0
7	G	1	Total O 1 1	0	0
7	H	4	Total O 4 4	0	0
7	I	6	Total O 6 6	0	0

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.

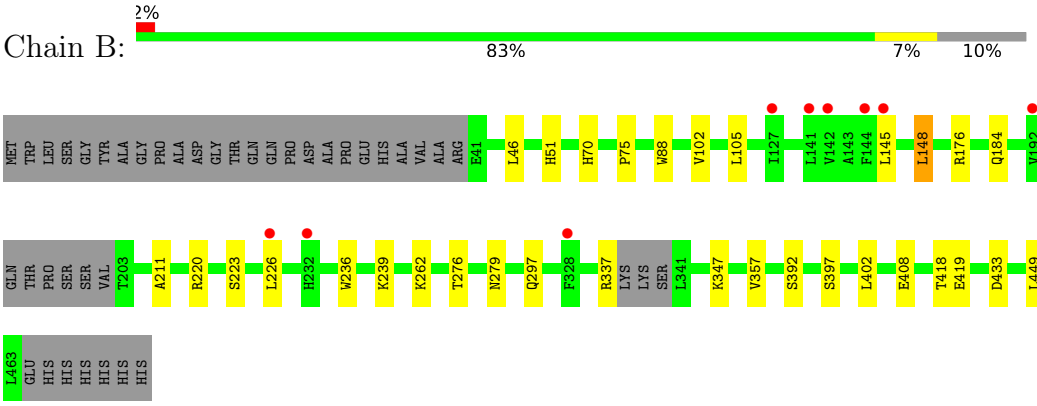
• Molecule 1: PolG2

Chain A:



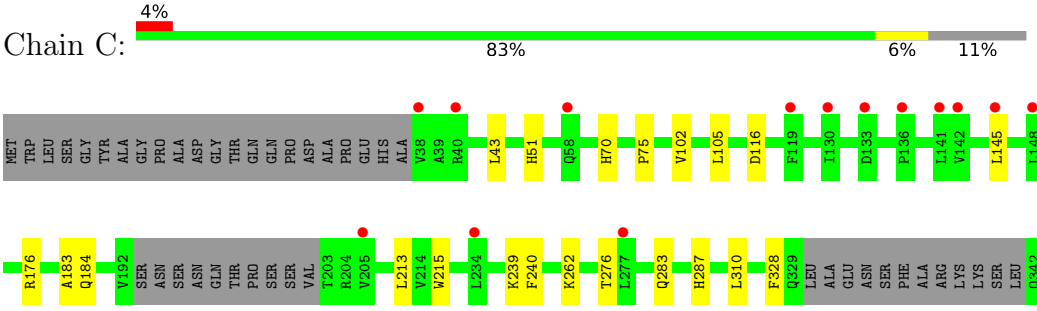
• Molecule 1: PolG2

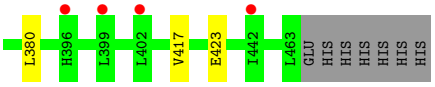
Chain B:



• Molecule 1: PolG2

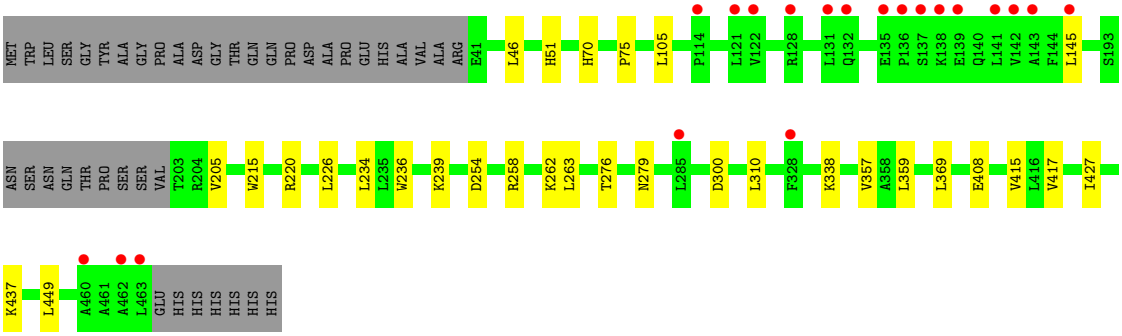
Chain C:





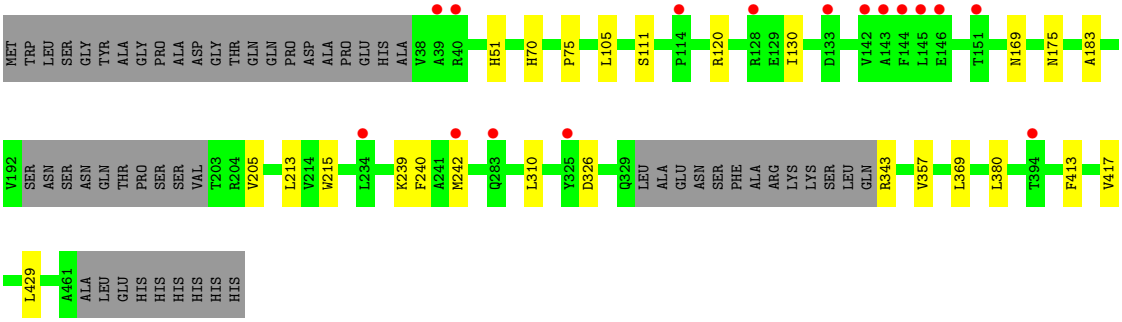
• Molecule 1: PolG2

Chain D:



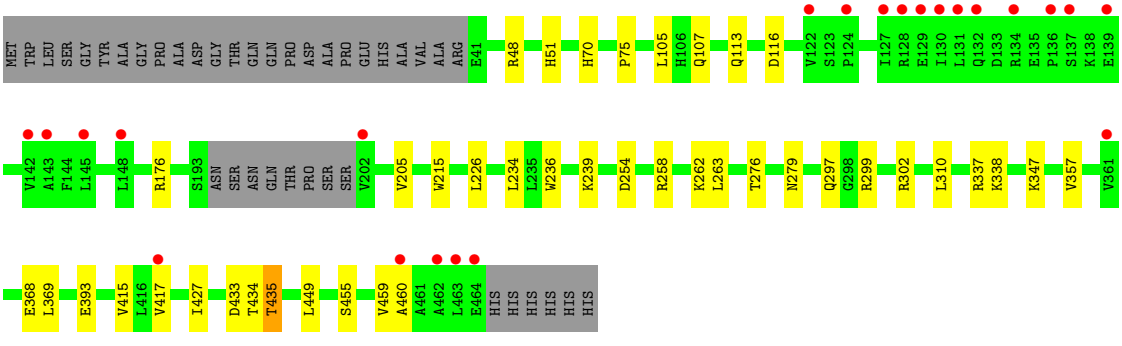
• Molecule 1: PolG2

Chain E:



• Molecule 1: PolG2

Chain F:

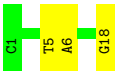


• Molecule 2: DNA (5'-D(*CP*TP*GP*GP*TP*AP*GP*GP*CP*GP*CP*CP*TP*AP*CP*CP*AP*G)-3')

Chain G:

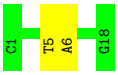
• Molecule 2: DNA (5'-D(*CP*TP*GP*GP*TP*AP*GP*GP*CP*GP*CP*CP*TP*AP*CP*CP *AP*G)-3')

Chain H:



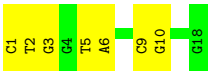
• Molecule 2: DNA (5'-D(*CP*TP*GP*GP*TP*AP*GP*GP*CP*GP*CP*CP*TP*AP*CP*CP *AP*G)-3')

Chain I:



• Molecule 2: DNA (5'-D(*CP*TP*GP*GP*TP*AP*GP*GP*CP*GP*CP*CP*TP*AP*CP*CP *AP*G)-3')

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	116.22Å 116.22Å 250.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.04 – 2.75 38.04 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.04-2.75) 99.8 (38.04-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.196 , 0.222 0.198 , 0.223	Depositor DCC
R_{free} test set	1976 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	82.2	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 46.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.011 for -h,-k,l 0.468 for h,-h-k,-l 0.015 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	20672	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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: GOL, MPD, EDO, NA

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	0.24	0/3190	0.44	0/4342
1	B	0.23	0/3244	0.45	0/4409
1	C	0.24	0/3195	0.44	0/4346
1	D	0.24	0/3306	0.45	0/4492
1	E	0.23	0/3166	0.44	0/4308
1	F	0.24	0/3328	0.45	0/4519
2	G	0.50	0/410	0.87	0/631
2	H	0.48	0/410	0.86	0/631
2	I	0.47	0/410	0.84	0/631
2	J	0.49	0/410	0.87	0/631
All	All	0.26	0/21069	0.49	0/28940

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3118	0	3038	18	0
1	B	3169	0	3104	18	0
1	C	3120	0	3058	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3223	0	3174	16	0
1	E	3091	0	3012	15	0
1	F	3248	0	3218	25	0
2	G	366	0	203	7	0
2	H	366	0	203	3	0
2	I	366	0	203	1	0
2	J	366	0	203	4	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
4	A	20	0	30	0	0
4	B	16	0	24	0	0
4	C	12	0	18	0	0
4	D	36	0	54	0	0
4	E	16	0	24	0	0
4	F	28	0	42	0	0
5	A	8	0	14	1	0
5	B	8	0	14	1	0
6	H	1	0	0	0	0
6	I	1	0	0	0	0
7	A	15	0	0	0	0
7	B	21	0	0	0	0
7	C	13	0	0	0	0
7	D	6	0	0	0	0
7	E	4	0	0	0	0
7	F	11	0	0	0	0
7	G	1	0	0	0	0
7	H	4	0	0	0	0
7	I	6	0	0	0	0
All	All	20672	0	19652	109	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 3.

All (109) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:LYS:HB2	1:A:460:ALA:HB1	1.80	0.62
2:J:5:DT:H2"	2:J:6:DA:C8	2.37	0.59
1:E:175:ASN:ND2	1:F:393:GLU:OE1	2.35	0.59
1:F:337:ARG:NH2	2:H:18:DG:N7	2.47	0.58
1:F:337:ARG:NH1	2:H:18:DG:O6	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:LEU:HA	1:B:148:LEU:HD23	1.86	0.57
1:E:105:LEU:HD11	1:F:70:HIS:HA	1.88	0.56
1:E:111:SER:O	1:E:120:ARG:NH2	2.39	0.56
1:D:262:LYS:HG2	1:D:276:THR:HG22	1.88	0.55
1:D:226:LEU:HD22	1:D:279:ASN:HB2	1.87	0.55
1:B:226:LEU:HD22	1:B:279:ASN:HB2	1.88	0.55
1:F:262:LYS:HG2	1:F:276:THR:HG22	1.88	0.55
1:B:223:SER:OG	1:C:423:GLU:O	2.24	0.55
1:C:105:LEU:HD11	1:D:70:HIS:HA	1.89	0.55
1:F:226:LEU:HD22	1:F:279:ASN:HB2	1.88	0.54
1:F:239:LYS:HB2	1:F:460:ALA:HB1	1.90	0.54
1:A:122:VAL:HB	1:A:148:LEU:HD11	1.90	0.53
2:G:5:DT:H2"	2:G:6:DA:C8	2.44	0.53
1:A:226:LEU:HD22	1:A:279:ASN:HB2	1.90	0.52
1:A:357:VAL:HG11	1:A:380:LEU:HD13	1.90	0.52
1:C:283:GLN:O	1:C:287:HIS:ND1	2.37	0.52
1:D:215:TRP:HB3	1:D:310:LEU:HB2	1.92	0.52
1:F:347:LYS:HE2	1:F:433:ASP:HA	1.91	0.52
1:D:51:HIS:HB3	1:D:75:PRO:HD2	1.93	0.51
2:J:2:DT:H2"	2:J:3:DG:C8	2.45	0.51
1:B:347:LYS:HE2	1:B:433:ASP:HA	1.93	0.50
1:A:215:TRP:HB3	1:A:310:LEU:HB2	1.94	0.50
1:F:234:LEU:HD13	1:F:263:LEU:HD22	1.95	0.49
1:A:397:SER:HB2	1:A:402:LEU:HD13	1.94	0.49
2:G:15:DC:H2'	2:G:16:DC:C6	2.47	0.48
1:C:51:HIS:HB3	1:C:75:PRO:HD2	1.94	0.48
1:F:415:VAL:HG13	1:F:427:ILE:HD13	1.95	0.48
1:F:299:ARG:HH21	1:F:302:ARG:HA	1.79	0.48
1:F:254:ASP:OD1	1:F:258:ARG:N	2.45	0.48
2:H:5:DT:H2"	2:H:6:DA:C8	2.49	0.48
1:C:171:LEU:HG	1:C:176:ARG:HG2	1.96	0.48
1:C:70:HIS:HA	1:D:105:LEU:HD11	1.96	0.48
1:E:70:HIS:HA	1:F:105:LEU:HD11	1.96	0.48
1:D:234:LEU:HD13	1:D:263:LEU:HD22	1.96	0.47
1:E:183:ALA:HB2	1:E:213:LEU:HD23	1.96	0.47
1:C:145:LEU:HD21	1:D:145:LEU:HD21	1.96	0.47
1:E:357:VAL:HG11	1:E:380:LEU:HD13	1.96	0.47
1:C:357:VAL:HG11	1:C:380:LEU:HD13	1.97	0.47
1:A:455:SER:O	1:A:459:VAL:HG23	2.15	0.47
1:D:254:ASP:OD1	1:D:258:ARG:N	2.46	0.47
1:D:369:LEU:HD22	1:D:417:VAL:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:HIS:HB3	1:E:75:PRO:HD2	1.97	0.47
1:F:357:VAL:HG21	1:F:449:LEU:HD13	1.96	0.47
1:B:51:HIS:HB3	1:B:75:PRO:HD2	1.96	0.46
1:D:46:LEU:HD11	1:D:408:GLU:HB3	1.97	0.46
1:F:455:SER:O	1:F:459:VAL:HG23	2.15	0.46
1:A:102:VAL:HG23	1:A:184:GLN:HB2	1.97	0.46
1:C:43:LEU:HD13	1:C:328:PHE:HB2	1.98	0.46
1:E:242:MET:N	1:E:326:ASP:OD2	2.40	0.46
2:G:9:DC:H2"	2:G:10:DG:C8	2.51	0.46
2:G:4:DG:H2"	2:G:5:DT:O5'	2.16	0.45
1:D:357:VAL:HG21	1:D:449:LEU:HD13	1.97	0.45
1:F:369:LEU:HD22	1:F:417:VAL:HG12	1.98	0.45
1:A:183:ALA:HB2	1:A:213:LEU:HD23	1.98	0.45
2:J:9:DC:H2"	2:J:10:DG:C8	2.51	0.45
1:A:102:VAL:HG11	1:A:182:LEU:HD13	1.99	0.45
1:A:177:LYS:NZ	1:B:392:SER:O	2.50	0.45
1:C:183:ALA:HB2	1:C:213:LEU:HD23	1.99	0.45
1:F:215:TRP:HB3	1:F:310:LEU:HB2	1.99	0.45
1:A:262:LYS:HG2	1:A:276:THR:HG22	1.99	0.45
1:E:239:LYS:HE3	1:E:240:PHE:CZ	2.53	0.44
2:I:5:DT:H2"	2:I:6:DA:C8	2.53	0.44
2:G:8:DG:H4'	2:G:9:DC:OP1	2.18	0.44
2:G:17:DA:H2"	2:G:18:DG:C8	2.51	0.44
1:C:239:LYS:HE3	1:C:240:PHE:CZ	2.53	0.44
1:B:397:SER:HB2	1:B:402:LEU:HD13	1.99	0.44
1:F:113:GLN:HB2	1:F:116:ASP:HB2	1.99	0.44
1:C:262:LYS:HG2	1:C:276:THR:HG22	1.99	0.44
1:A:70:HIS:HA	1:B:105:LEU:HD11	2.00	0.43
1:B:262:LYS:HG2	1:B:276:THR:HG22	2.00	0.43
2:J:1:DC:H2'	2:J:2:DT:C6	2.52	0.43
1:B:236:TRP:HA	1:B:239:LYS:HD3	1.99	0.43
2:G:16:DC:H2"	2:G:17:DA:C8	2.54	0.43
1:A:369:LEU:HD22	1:A:417:VAL:HG12	1.99	0.43
1:E:215:TRP:HB3	1:E:310:LEU:HB2	1.99	0.43
1:A:105:LEU:HD11	1:B:70:HIS:HA	1.99	0.43
1:B:357:VAL:HG21	1:B:449:LEU:HD13	2.01	0.43
1:F:236:TRP:O	1:F:239:LYS:HG2	2.19	0.43
1:E:413:PHE:HB3	1:E:429:LEU:HD11	2.00	0.43
1:B:418:THR:OG1	1:B:419:GLU:N	2.52	0.43
1:D:415:VAL:HG13	1:D:427:ILE:HD13	2.00	0.43
1:F:176:ARG:NH1	1:F:297:GLN:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:434:THR:O	1:F:435:THR:HG22	2.19	0.42
5:A:507:MPD:HM1	5:A:507:MPD:H4	1.66	0.42
1:D:236:TRP:O	1:D:239:LYS:HG2	2.19	0.42
1:F:368:GLU:N	1:F:368:GLU:OE1	2.52	0.42
1:E:205:VAL:HB	1:F:107:GLN:HE22	1.84	0.42
1:A:51:HIS:HB3	1:A:75:PRO:HD2	2.02	0.42
1:E:169:ASN:OD1	1:F:48:ARG:NH2	2.53	0.42
1:B:176:ARG:NH1	1:B:297:GLN:O	2.52	0.42
1:B:46:LEU:HD11	1:B:408:GLU:HG2	2.01	0.41
1:B:88:TRP:CE2	1:B:211:ALA:HB1	2.55	0.41
5:B:505:MPD:HM1	5:B:505:MPD:H4	1.71	0.41
1:B:102:VAL:HG13	1:B:184:GLN:HB2	2.00	0.41
1:C:215:TRP:HB3	1:C:310:LEU:HB2	2.02	0.41
1:A:145:LEU:HD21	1:B:145:LEU:HD21	2.03	0.41
1:D:220:ARG:HD3	1:D:300:ASP:OD2	2.20	0.41
1:D:359:LEU:HD23	1:D:415:VAL:HB	2.02	0.41
1:A:376:LEU:HD11	1:A:445:LEU:HD23	2.03	0.41
1:F:51:HIS:HB3	1:F:75:PRO:HD2	2.03	0.41
1:C:369:LEU:HD22	1:C:417:VAL:HG12	2.03	0.40
1:E:369:LEU:HD22	1:E:417:VAL:HG12	2.03	0.40
1:C:102:VAL:HG13	1:C:184:GLN:HB2	2.03	0.40
1:E:239:LYS:HE3	1:E:240:PHE:CE2	2.56	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	402/455 (88%)	394 (98%)	8 (2%)	0	100	100
1	B	406/455 (89%)	399 (98%)	7 (2%)	0	100	100
1	C	399/455 (88%)	393 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	413/455 (91%)	407 (98%)	6 (2%)	0	100	100
1	E	396/455 (87%)	389 (98%)	7 (2%)	0	100	100
1	F	414/455 (91%)	405 (98%)	9 (2%)	0	100	100
All	All	2430/2730 (89%)	2387 (98%)	43 (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	331/398 (83%)	327 (99%)	4 (1%)	71	82
1	B	340/398 (85%)	336 (99%)	4 (1%)	71	82
1	C	335/398 (84%)	334 (100%)	1 (0%)	92	95
1	D	349/398 (88%)	346 (99%)	3 (1%)	78	87
1	E	331/398 (83%)	329 (99%)	2 (1%)	86	90
1	F	354/398 (89%)	351 (99%)	3 (1%)	81	88
All	All	2040/2388 (85%)	2023 (99%)	17 (1%)	81	88

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	220	ARG
1	A	330	LEU
1	A	435	THR
1	A	436	MET
1	B	148	LEU
1	B	220	ARG
1	B	337	ARG
1	B	459	VAL
1	C	116	ASP
1	D	205	VAL

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Mol	Chain	Res	Type
1	D	338	LYS
1	D	437	LYS
1	E	130	ILE
1	E	343	ARG
1	F	205	VAL
1	F	338	LYS
1	F	435	THR

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)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 38 ligands modelled in this entry, 2 are monoatomic - leaving 36 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	MPD	B	505	-	7,7,7	0.29	0	9,10,10	0.37	0
4	EDO	E	502	-	3,3,3	0.45	0	2,2,2	0.34	0
4	EDO	F	505	-	3,3,3	0.46	0	2,2,2	0.32	0
4	EDO	D	505	-	3,3,3	0.46	0	2,2,2	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	EDO	E	503	-	3,3,3	0.47	0	2,2,2	0.34	0
4	EDO	F	501	-	3,3,3	0.45	0	2,2,2	0.36	0
4	EDO	A	506	-	3,3,3	0.47	0	2,2,2	0.31	0
4	EDO	E	504	-	3,3,3	0.46	0	2,2,2	0.33	0
4	EDO	B	501	-	3,3,3	0.47	0	2,2,2	0.34	0
4	EDO	E	501	-	3,3,3	0.47	0	2,2,2	0.34	0
4	EDO	D	504	-	3,3,3	0.46	0	2,2,2	0.33	0
5	MPD	A	507	-	7,7,7	0.28	0	9,10,10	0.39	0
4	EDO	D	506	-	3,3,3	0.46	0	2,2,2	0.32	0
4	EDO	B	503	-	3,3,3	0.46	0	2,2,2	0.35	0
4	EDO	C	502	-	3,3,3	0.47	0	2,2,2	0.33	0
4	EDO	A	505	-	3,3,3	0.46	0	2,2,2	0.35	0
4	EDO	D	509	-	3,3,3	0.47	0	2,2,2	0.34	0
4	EDO	D	501	-	3,3,3	0.46	0	2,2,2	0.33	0
4	EDO	B	504	-	3,3,3	0.45	0	2,2,2	0.34	0
4	EDO	A	503	-	3,3,3	0.46	0	2,2,2	0.34	0
4	EDO	F	506	-	3,3,3	0.46	0	2,2,2	0.33	0
4	EDO	F	504	-	3,3,3	0.46	0	2,2,2	0.34	0
4	EDO	C	501	-	3,3,3	0.45	0	2,2,2	0.33	0
4	EDO	A	504	-	3,3,3	0.46	0	2,2,2	0.35	0
4	EDO	B	502	-	3,3,3	0.46	0	2,2,2	0.34	0
4	EDO	D	503	-	3,3,3	0.46	0	2,2,2	0.34	0
4	EDO	F	502	-	3,3,3	0.46	0	2,2,2	0.34	0
4	EDO	F	503	-	3,3,3	0.46	0	2,2,2	0.34	0
4	EDO	A	502	-	3,3,3	0.46	0	2,2,2	0.34	0
3	GOL	B	506	-	5,5,5	0.88	0	5,5,5	1.28	1 (20%)
4	EDO	D	508	-	3,3,3	0.45	0	2,2,2	0.34	0
4	EDO	F	507	-	3,3,3	0.47	0	2,2,2	0.34	0
4	EDO	D	507	-	3,3,3	0.47	0	2,2,2	0.33	0
4	EDO	C	503	-	3,3,3	0.45	0	2,2,2	0.33	0
3	GOL	A	501	-	5,5,5	0.90	0	5,5,5	1.00	0
4	EDO	D	502	-	3,3,3	0.45	0	2,2,2	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPD	B	505	-	-	0/5/5/5	-
4	EDO	E	502	-	-	0/1/1/1	-
4	EDO	F	505	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	505	-	-	0/1/1/1	-
4	EDO	E	503	-	-	0/1/1/1	-
4	EDO	F	501	-	-	1/1/1/1	-
4	EDO	A	506	-	-	0/1/1/1	-
4	EDO	E	504	-	-	0/1/1/1	-
4	EDO	B	501	-	-	0/1/1/1	-
4	EDO	E	501	-	-	0/1/1/1	-
4	EDO	D	504	-	-	0/1/1/1	-
5	MPD	A	507	-	-	1/5/5/5	-
4	EDO	D	506	-	-	0/1/1/1	-
4	EDO	B	503	-	-	0/1/1/1	-
4	EDO	C	502	-	-	0/1/1/1	-
4	EDO	A	505	-	-	0/1/1/1	-
4	EDO	D	509	-	-	0/1/1/1	-
4	EDO	D	501	-	-	0/1/1/1	-
4	EDO	B	504	-	-	0/1/1/1	-
4	EDO	A	503	-	-	0/1/1/1	-
4	EDO	F	506	-	-	0/1/1/1	-
4	EDO	F	504	-	-	0/1/1/1	-
4	EDO	C	501	-	-	0/1/1/1	-
4	EDO	A	504	-	-	0/1/1/1	-
4	EDO	B	502	-	-	0/1/1/1	-
4	EDO	D	503	-	-	0/1/1/1	-
4	EDO	F	502	-	-	0/1/1/1	-
4	EDO	F	503	-	-	0/1/1/1	-
4	EDO	A	502	-	-	0/1/1/1	-
3	GOL	B	506	-	-	0/4/4/4	-
4	EDO	D	508	-	-	0/1/1/1	-
4	EDO	F	507	-	-	0/1/1/1	-
4	EDO	D	507	-	-	0/1/1/1	-
4	EDO	C	503	-	-	0/1/1/1	-
3	GOL	A	501	-	-	0/4/4/4	-
4	EDO	D	502	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	506	GOL	C3-C2-C1	-2.17	103.26	111.70

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	501	EDO	O1-C1-C2-O2
4	F	505	EDO	O1-C1-C2-O2
5	A	507	MPD	C2-C3-C4-C5

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	505	MPD	1	0
5	A	507	MPD	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	408/455 (89%)	0.22	14 (3%) 45 53	54, 86, 169, 235	0
1	B	411/455 (90%)	0.20	10 (2%) 59 68	56, 86, 170, 233	0
1	C	404/455 (88%)	0.30	19 (4%) 31 37	65, 95, 173, 216	0
1	D	414/455 (90%)	0.28	20 (4%) 30 36	58, 87, 168, 223	0
1	E	401/455 (88%)	0.29	16 (3%) 38 45	64, 95, 169, 203	0
1	F	416/455 (91%)	0.32	23 (5%) 25 30	58, 87, 168, 233	0
2	G	18/18 (100%)	-0.48	0 100 100	85, 103, 124, 127	0
2	H	18/18 (100%)	-0.40	0 100 100	93, 103, 126, 126	0
2	I	18/18 (100%)	-0.34	0 100 100	90, 100, 116, 120	0
2	J	18/18 (100%)	-0.55	0 100 100	85, 101, 113, 117	0
All	All	2526/2802 (90%)	0.25	102 (4%) 38 45	54, 91, 170, 235	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	130	ILE	8.2
1	D	136	PRO	7.9
1	F	128	ARG	6.8
1	F	136	PRO	6.5
1	F	462	ALA	6.4
1	A	112	SER	5.4
1	A	145	LEU	5.1
1	B	127	ILE	5.0
1	D	131	LEU	4.7
1	F	143	ALA	4.7
1	D	122	VAL	4.7
1	B	142	VAL	4.5
1	A	141	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	396	HIS	4.4
1	D	460	ALA	4.4
1	A	142	VAL	4.3
1	D	141	LEU	4.3
1	A	131	LEU	4.2
1	D	145	LEU	4.2
1	C	142	VAL	4.1
1	D	132	GLN	4.0
1	F	460	ALA	4.0
1	F	142	VAL	3.8
1	E	133	ASP	3.8
1	B	141	LEU	3.7
1	E	151	THR	3.7
1	F	463	LEU	3.7
1	F	464	GLU	3.6
1	C	133	ASP	3.5
1	E	114	PRO	3.5
1	E	283	GLN	3.4
1	E	143	ALA	3.4
1	A	144	PHE	3.3
1	F	134	ARG	3.3
1	F	122	VAL	3.2
1	F	127	ILE	3.2
1	E	128	ARG	3.2
1	E	39	ALA	3.2
1	A	148	LEU	3.2
1	D	142	VAL	3.2
1	E	146	GLU	3.2
1	C	40	ARG	3.2
1	F	132	GLN	3.2
1	F	139	GLU	3.1
1	A	151	THR	3.1
1	B	144	PHE	3.1
1	A	129	GLU	3.0
1	F	145	LEU	3.0
1	D	137	SER	3.0
1	F	131	LEU	3.0
1	C	402	LEU	2.9
1	A	134	ARG	2.9
1	D	128	ARG	2.9
1	E	144	PHE	2.8
1	C	58	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	361	VAL	2.7
1	C	442	ILE	2.7
1	B	145	LEU	2.7
1	D	285	LEU	2.6
1	D	463	LEU	2.6
1	C	38	VAL	2.6
1	E	142	VAL	2.5
1	D	328	PHE	2.5
1	B	328	PHE	2.5
1	C	141	LEU	2.5
1	C	155	LEU	2.5
1	C	130	ILE	2.4
1	E	145	LEU	2.4
1	E	325	TYR	2.4
1	C	148	LEU	2.4
1	F	129	GLU	2.3
1	D	135	GLU	2.3
1	F	417	VAL	2.3
1	F	202	VAL	2.3
1	A	359	LEU	2.2
1	D	121	LEU	2.2
1	C	119	PHE	2.2
1	E	394	THR	2.2
1	C	145	LEU	2.2
1	C	136	PRO	2.2
1	C	399	LEU	2.2
1	F	124	PRO	2.2
1	F	148	LEU	2.2
1	E	234	LEU	2.2
1	E	242	MET	2.2
1	C	205	VAL	2.2
1	D	139	GLU	2.2
1	D	114	PRO	2.1
1	D	138	LYS	2.1
1	D	462	ALA	2.1
1	A	119	PHE	2.1
1	E	40	ARG	2.1
1	B	192	VAL	2.1
1	D	143	ALA	2.1
1	B	226	LEU	2.1
1	C	234	LEU	2.0
1	F	137	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	127	ILE	2.0
1	A	133	ASP	2.0
1	B	460	ALA	2.0
1	C	277	LEU	2.0
1	B	232	HIS	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
6	NA	I	101	1/1	0.24	0.11	215,215,215,215	0
3	GOL	A	501	6/6	0.60	0.25	80,102,106,112	0
4	EDO	F	501	4/4	0.62	0.29	123,123,124,146	0
4	EDO	D	506	4/4	0.65	0.20	69,87,103,105	0
5	MPD	A	507	8/8	0.76	0.32	80,122,130,138	0
4	EDO	D	507	4/4	0.77	0.29	68,75,82,99	0
6	NA	H	101	1/1	0.77	0.14	178,178,178,178	0
4	EDO	B	502	4/4	0.77	0.22	94,95,104,107	0
4	EDO	A	506	4/4	0.78	0.17	69,81,96,116	0
4	EDO	A	504	4/4	0.78	0.29	75,84,85,90	0
3	GOL	B	506	6/6	0.79	0.27	121,124,167,190	0
4	EDO	F	505	4/4	0.81	0.41	73,82,105,118	0
4	EDO	A	503	4/4	0.81	0.20	94,103,103,109	0
4	EDO	D	503	4/4	0.81	0.18	120,121,124,132	0
4	EDO	D	504	4/4	0.81	0.15	91,94,101,118	0
4	EDO	B	501	4/4	0.83	0.42	75,79,94,100	0
4	EDO	D	505	4/4	0.84	0.35	91,96,105,126	0
5	MPD	B	505	8/8	0.84	0.14	79,114,123,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	A	505	4/4	0.85	0.22	81,88,102,108	0
4	EDO	F	503	4/4	0.87	0.14	73,84,86,100	0
4	EDO	C	501	4/4	0.88	0.18	85,90,102,110	0
4	EDO	F	507	4/4	0.88	0.15	72,79,80,91	0
4	EDO	E	504	4/4	0.89	0.38	77,93,99,106	0
4	EDO	C	502	4/4	0.89	0.15	80,88,97,97	0
4	EDO	A	502	4/4	0.89	0.17	82,98,99,113	0
4	EDO	B	504	4/4	0.90	0.19	75,77,86,91	0
4	EDO	D	502	4/4	0.90	0.12	101,101,103,116	0
4	EDO	D	509	4/4	0.91	0.14	66,82,82,85	0
4	EDO	F	504	4/4	0.92	0.21	79,83,85,90	0
4	EDO	E	501	4/4	0.92	0.26	71,86,90,117	0
4	EDO	F	506	4/4	0.92	0.10	81,92,102,105	0
4	EDO	C	503	4/4	0.92	0.24	63,83,89,102	0
4	EDO	D	501	4/4	0.94	0.17	77,80,83,83	0
4	EDO	D	508	4/4	0.94	0.21	80,82,87,92	0
4	EDO	F	502	4/4	0.94	0.21	78,82,86,86	0
4	EDO	B	503	4/4	0.95	0.12	82,84,84,107	0
4	EDO	E	503	4/4	0.95	0.14	80,87,89,101	0
4	EDO	E	502	4/4	0.98	0.26	86,92,102,103	0

6.5 Other polymers (i)

There are no such residues in this entry.