



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:45 AM UTC

PDB ID : 5E63 / pdb_00005e63
Title : K262A mutant of I-SmaMI
Authors : Shen, B.; Stoddard, B.
Deposited on : 2015-10-09
Resolution : 2.60 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

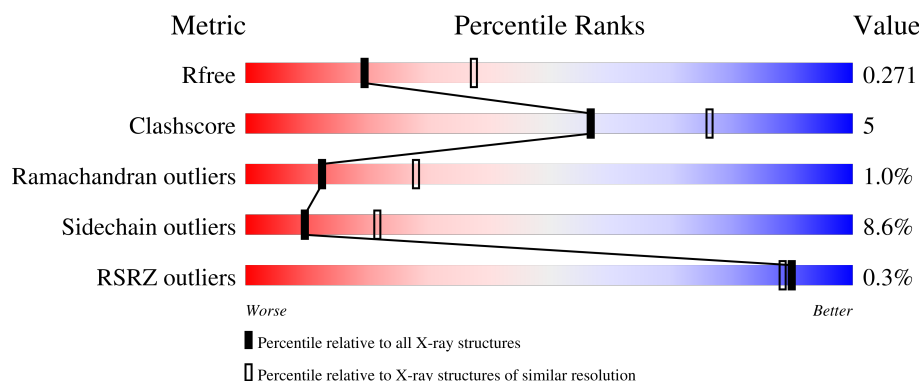
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	302	
2	B	14	
3	C	11	
4	D	15	
5	E	10	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 3428 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 I-SmaMI LAGLIDADG meganuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2334	1523	383	420	8			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	165	ASN	LEU	conflict	UNP F7WD42
A	262	ALA	LYS	engineered mutation	UNP F7WD42
A	267	GLN	MET	conflict	UNP F7WD42

- Molecule 2 is a DNA chain called DNA right half site Bottom strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	14	Total	C	N	O	P	0	0	0
			282	136	53	80	13			

- Molecule 3 is a DNA chain called DNA left half site bottom strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	11	Total	C	N	O	P	0	0	0
			230	108	45	66	11			

- Molecule 4 is a DNA chain called DNA left site top strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	15	Total	C	N	O	P	0	0	0
			300	146	49	91	14			

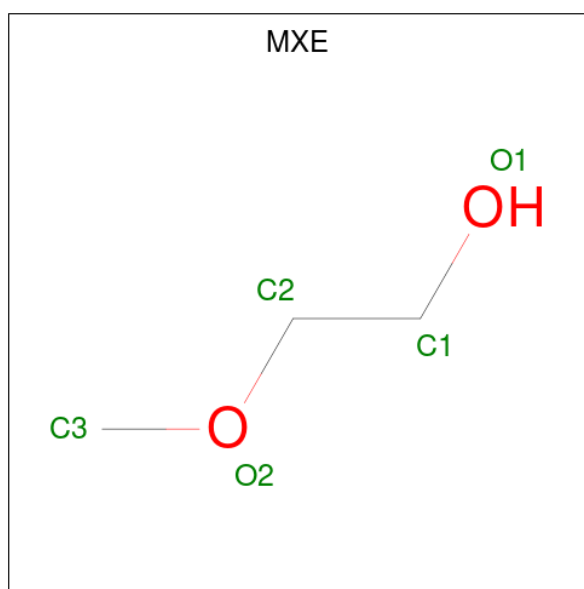
- Molecule 5 is a DNA chain called DNA (5'-D(P*CP*AP*GP*GP*TP*GP*TP*AP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	10	Total	C	N	O	P	0	0	0
			209	98	40	61	10			

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

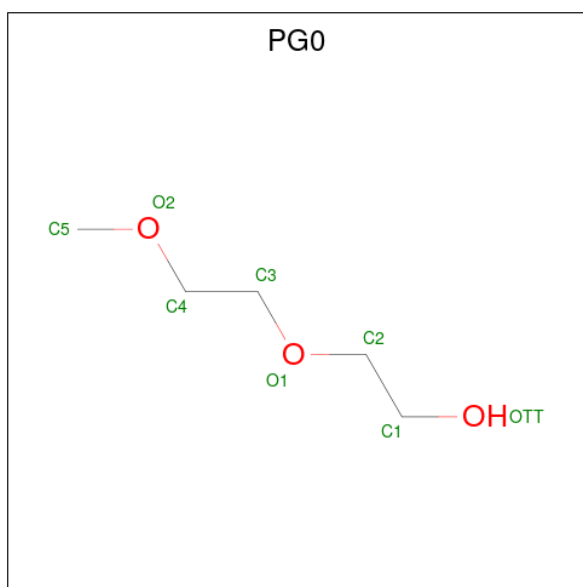
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	Mg	0	0
			3	3		

- Molecule 7 is 2-METHOXYETHANOL (CCD ID: MXE) (formula: C₃H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			5	3	2		

- Molecule 8 is 2-(2-METHOXYETHOXY)ETHANOL (CCD ID: PG0) (formula: C₅H₁₂O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total	C	O	0	1
			16	10	6		

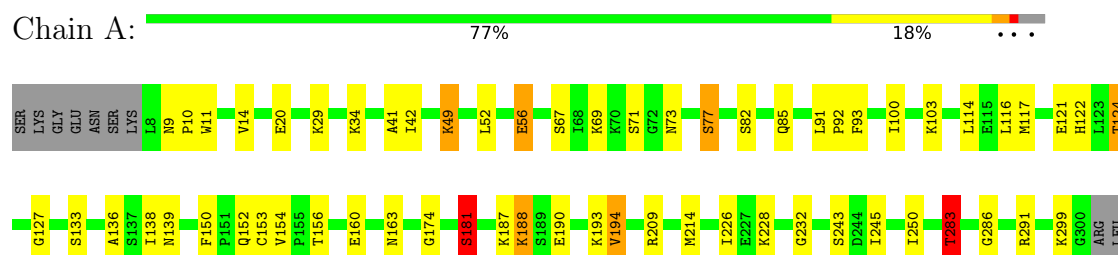
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	36	Total	O	0	0
			36	36		
9	B	2	Total	O	0	0
			2	2		
9	C	2	Total	O	0	0
			2	2		
9	D	5	Total	O	0	0
			5	5		
9	E	4	Total	O	0	0
			4	4		

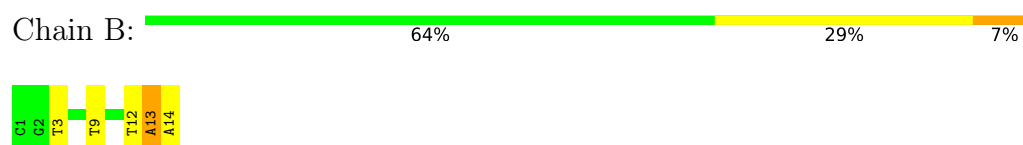
3 Residue-property plots

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.

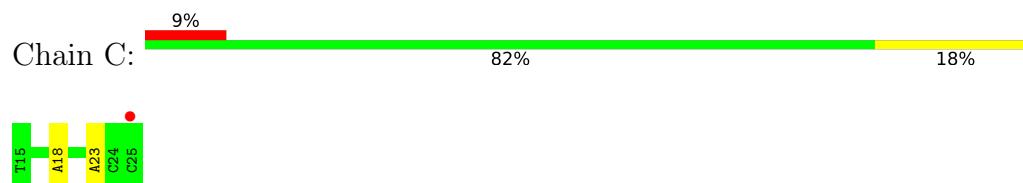
- Molecule 1: I-SmaMI LAGLIDADG meganuclease



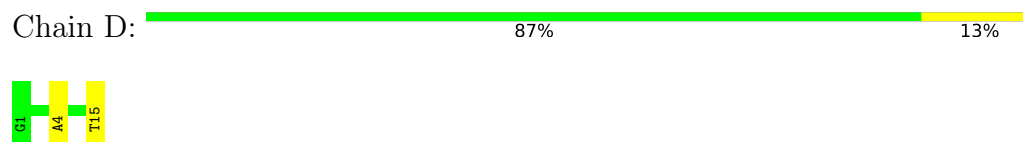
- Molecule 2: DNA right half site Bottom strand



- Molecule 3: DNA left half site bottom strand



- Molecule 4: DNA left site top strand



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.84Å 67.69Å 97.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 30.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.60) 99.9 (30.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.58 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.189 , 0.279 (Not available) , 0.271	Depositor DCC
R_{free} test set	618 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3428	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MXE, PG0, MG

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	1.28	11/2388 (0.5%)	1.29	8/3216 (0.2%)
2	B	0.53	0/316	1.21	3/485 (0.6%)
3	C	0.56	0/258	1.14	1/395 (0.3%)
4	D	0.58	0/334	1.11	0/513
5	E	0.55	0/234	1.24	2/358 (0.6%)
All	All	1.10	11/3530 (0.3%)	1.25	14/4967 (0.3%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	93	PHE	CA-C	6.91	1.61	1.52
1	A	245	ILE	C-O	-6.23	1.17	1.24
1	A	250	ILE	CA-CB	6.20	1.57	1.54
1	A	188	LYS	CA-C	5.54	1.59	1.52
1	A	299	LYS	CA-C	5.54	1.60	1.52
1	A	194	VAL	CA-C	5.48	1.58	1.52
1	A	77	SER	N-CA	-5.40	1.39	1.46
1	A	100	ILE	N-CA	5.17	1.51	1.46
1	A	174	GLY	C-O	-5.17	1.17	1.23
1	A	100	ILE	CA-C	5.11	1.58	1.52
1	A	136	ALA	CA-C	5.07	1.59	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	LYS	N-CA-C	8.82	125.86	114.75
2	B	13	DA	C2'-C3'-O3'	-8.43	98.86	111.50
5	E	23	DA	C4'-C3'-O3'	7.47	121.20	110.00
1	A	283	THR	CB-CA-C	7.35	118.83	108.76
1	A	100	ILE	N-CA-C	6.82	120.36	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	VAL	CB-CA-C	6.15	117.92	110.85
1	A	181	SER	N-CA-C	5.74	117.86	108.55
2	B	3	DT	C2'-C3'-O3'	5.50	119.75	111.50
2	B	9	DT	C2'-C3'-O3'	-5.43	103.36	111.50
1	A	150	PHE	CA-C-N	5.41	125.50	119.87
1	A	150	PHE	C-N-CA	5.41	125.50	119.87
5	E	24	DC	C4'-C3'-O3'	-5.29	102.07	110.00
1	A	250	ILE	O-C-N	5.21	123.75	120.42
3	C	18	DA	C2'-C3'-O3'	-5.07	103.89	111.50

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	2334	0	2388	21	0
2	B	282	0	159	5	0
3	C	230	0	124	1	0
4	D	300	0	173	2	0
5	E	209	0	113	6	0
6	A	3	0	0	0	0
7	A	5	0	8	1	0
8	E	16	0	24	0	0
9	A	36	0	0	0	0
9	B	2	0	0	0	0
9	C	2	0	0	1	0
9	D	5	0	0	0	0
9	E	4	0	0	0	0
All	All	3428	0	2989	29	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 5.

All (29) 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:82:SER:HB3	1:A:85:GLN:HG2	1.63	0.80
2:B:14:DA:OP1	5:E:16:DC:OP2	2.06	0.73
1:A:187:LYS:NZ	5:E:21:DG:N7	2.47	0.62
1:A:121:GLU:O	1:A:124:THR:HB	2.01	0.61
2:B:12:DT:H2''	2:B:13:DA:N7	2.16	0.60
1:A:181:SER:HB3	5:E:17:DA:OP2	2.03	0.59
1:A:283:THR:HG22	1:A:286:GLY:H	1.68	0.59
1:A:117:MET:HA	1:A:122:HIS:CD2	2.40	0.56
1:A:71:SER:HB2	1:A:77:SER:HB2	1.92	0.52
5:E:24:DC:H2''	5:E:25:DG:C8	2.44	0.52
1:A:82:SER:CB	1:A:85:GLN:HG2	2.37	0.52
1:A:82:SER:HB3	1:A:85:GLN:CG	2.38	0.51
1:A:214:MET:HA	1:A:214:MET:HE2	1.94	0.50
1:A:20:GLU:OE1	2:B:14:DA:H3'	2.12	0.50
1:A:103:LYS:NZ	9:C:101:HOH:O	2.45	0.48
1:A:10:PRO:O	1:A:14:VAL:HG23	2.12	0.48
2:B:12:DT:H2''	2:B:13:DA:C8	2.50	0.47
1:A:52:LEU:O	1:A:56:GLU:HG2	2.16	0.46
1:A:228:LYS:NZ	1:A:232:GLY:O	2.49	0.46
1:A:9:ASN:OD1	1:A:11:TRP:N	2.48	0.46
2:B:12:DT:H2''	2:B:13:DA:C5	2.51	0.45
1:A:91:LEU:HB2	1:A:92:PRO:HD3	1.99	0.45
1:A:133:SER:OG	1:A:156:THR:HG23	2.17	0.44
1:A:41:ALA:C	1:A:42:ILE:HG13	2.43	0.44
1:A:49:LYS:HG2	7:A:404:MXE:H22	2.00	0.44
1:A:138:ILE:O	1:A:139:ASN:C	2.59	0.43
3:C:23:DA:C2	4:D:4:DA:C2	3.06	0.43
5:E:18:DG:H2'	5:E:19:DG:O4'	2.20	0.42
4:D:15:DT:H2''	5:E:16:DC:H5''	2.02	0.42

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	291/302 (96%)	273 (94%)	15 (5%)	3 (1%)	12	28

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	ARG
1	A	163	ASN
1	A	127	GLY

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	257/265 (97%)	235 (91%)	22 (9%)	10	22

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

Mol	Chain	Res	Type
1	A	29	LYS
1	A	34	LYS
1	A	49	LYS
1	A	56	GLU
1	A	67	SER
1	A	69	LYS
1	A	73	ASN
1	A	114	LEU
1	A	116	LEU
1	A	124	THR
1	A	152	GLN
1	A	153	CYS
1	A	160	GLU
1	A	181	SER
1	A	188	LYS
1	A	190	GLU
1	A	193	LYS
1	A	194	VAL

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Mol	Chain	Res	Type
1	A	226	ILE
1	A	243	SER
1	A	283	THR
1	A	291	ARG

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

Mol	Chain	Res	Type
1	A	73	ASN
1	A	122	HIS
1	A	280	ASN

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](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\# Z > 2$
8	PG0	E	101[A]	-	7,7,7	0.71	0	6,6,6	0.67	0
8	PG0	E	101[B]	-	7,7,7	0.57	0	6,6,6	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MXE	A	404	-	4,4,4	0.75	0	3,3,3	0.49	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
8	PG0	E	101[A]	-	-	3/5/5/5	-
8	PG0	E	101[B]	-	-	3/5/5/5	-
7	MXE	A	404	-	-	1/2/2/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	E	101[B]	PG0	O1-C3-C4-O2
7	A	404	MXE	O1-C1-C2-O2
8	E	101[B]	PG0	OTT-C1-C2-O1
8	E	101[A]	PG0	C1-C2-O1-C3
8	E	101[B]	PG0	C3-C4-O2-C5
8	E	101[A]	PG0	OTT-C1-C2-O1
8	E	101[A]	PG0	O1-C3-C4-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	404	MXE	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	293/302 (97%)	-0.42	0	100 100	16, 30, 52, 76	0
2	B	14/14 (100%)	-0.49	0	100 100	24, 37, 65, 67	0
3	C	11/11 (100%)	0.11	1 (9%)	15 11	35, 46, 69, 88	0
4	D	15/15 (100%)	-0.60	0	100 100	33, 40, 51, 51	0
5	E	10/10 (100%)	-0.30	0	100 100	36, 40, 51, 53	0
All	All	343/352 (97%)	-0.41	1 (0%)	90 88	16, 31, 56, 88	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	25	DC	2.8

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MXE	A	404	5/5	0.73	0.18	48,51,53,54	0
8	PG0	E	101[A]	8/8	0.81	0.19	21,25,27,27	8
8	PG0	E	101[B]	8/8	0.81	0.19	25,30,32,32	8
6	MG	A	401	1/1	0.94	0.06	32,32,32,32	0
6	MG	A	403	1/1	0.95	0.06	33,33,33,33	0
6	MG	A	402	1/1	0.99	0.02	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.