

wwPDB X-ray Structure Validation Summary Report (i)

May 22, 2020 – 01:47 am BST

PDB ID : 5SV0

Title : Structure of the ExbB/ExbD complex from E. coli at pH 7.0 Authors : Celia, H.; Botos, I.; Lloubes, R.; Buchanan, S.K.; Noinaj, N.

Deposited on : 2016-08-04

Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 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 : 2.11

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)

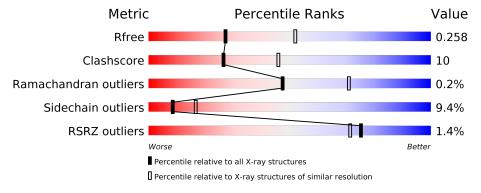
Validation Pipeline (wwPDB-VP) : 2.11

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 2.60 Å.

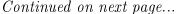
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive	Similar resolution
Metric	$(\# { m Entries})$	$(\# ext{Entries}, ext{resolution range}(ext{Å}))$
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 on 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	244	69%	23%		• 5%
1	В	244	70%	18%		• 8%
1	С	244	70%	17%	•	9%
1	D	244	65%	18%	5%	12%
1	Е	244	65%	20%		11%
1	F	244	71%	18%		• 9%





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Mol	Chain	Length	Quality of chain			
1	G	244	70%	20%		6%
1	Н	244	70%	20%	•	8%
1	I	244	64%	24%	•	9%
1	J	244	66%	19%	• 3	12%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16861 atoms, of which 0 are hydrogens and 0 are deuteriums.

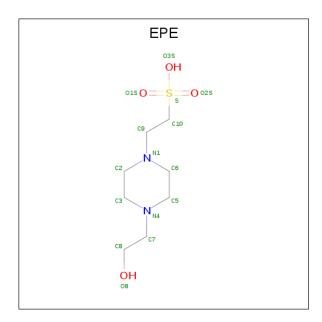
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called Biopolymer transport protein ExbB.

Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	Trace
1	В	225	Total	С	N	О	S	0	0	0
1	Ъ	229	1692	1080	295	311	6	0	U	U
1	С	222	Total	С	N	О	S	0	0	0
1		222	1651	1050	289	306	6	0	U	U
1	D	215	Total	С	N	О	S	0	0	0
1	D	210	1615	1028	282	300	5	0	U	U
1	E	216	Total	$^{\mathrm{C}}$	N	Ο	S	0	0	0
1	L	210	1609	1025	279	300	5		U	U
1	F	223	Total	$^{\mathrm{C}}$	N	Ο	S	0	0	
	1	223	1651	1050	290	306	5	O	0	
1	G	229	Total	$^{\mathrm{C}}$	N	О	S	0	2	
1	<u> </u>	220	1731	1104	301	320	6	0	2	0
1	Н	225	Total	С	N	О	S	0	0	
	11	220	1700	1085	296	313	6	0	U	0
1	I	223	Total	С	N	О	S	0	0	
	1	220	1678	1068	294	310	6	0	U	0
1	J	214	Total	\mathbf{C}	N	О	S	0	0	
	9	214	1596	1017	279	295	5		U	U
1	A	233	Total	\mathbf{C}	N	О	\mathbf{S}	0	0	
1	11	200	1749	1111	308	324	6		U	

• Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
2	D	1	Total	С	N	О	S	0	0	
	D	1	15	8	2	4	1	0	U	
2	L.	1	Total	С	N	О	S	0	0	
	Г	1	15	8	2	4	1	U	U	
2	Т	1	Total	С	N	О	S	0	0	
	1	1	15	8	2	4	1	0	0	

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	I	1	Total Ca 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	14	Total O 14 14	0	0
4	С	11	Total O 11 11	0	0
4	D	12	Total O 12 12	0	0
4	E	16	Total O 16 16	0	0



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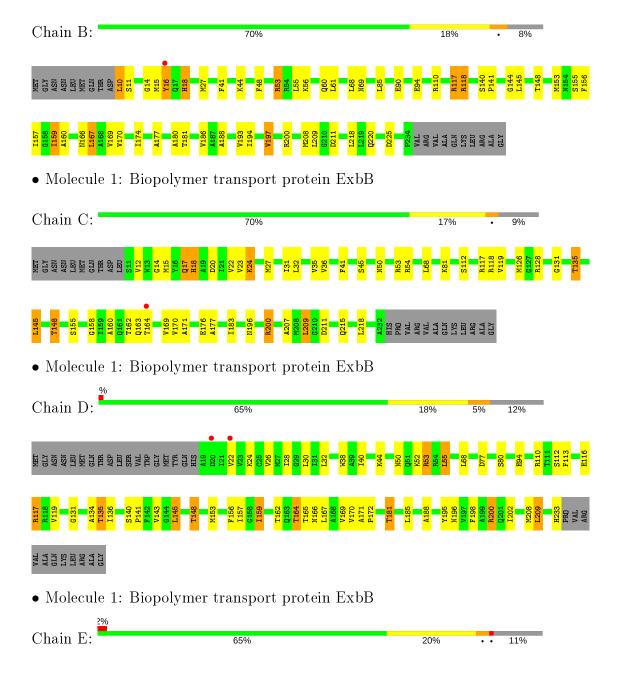
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	16	Total O 16 16	0	0
4	G	15	Total O 15 15	0	0
4	Н	13	Total O 13 13	0	0
4	I	15	Total O 15 15	0	0
4	J	20	Total O 20 20	0	0
4	A	10	Total O 10 10	0	0



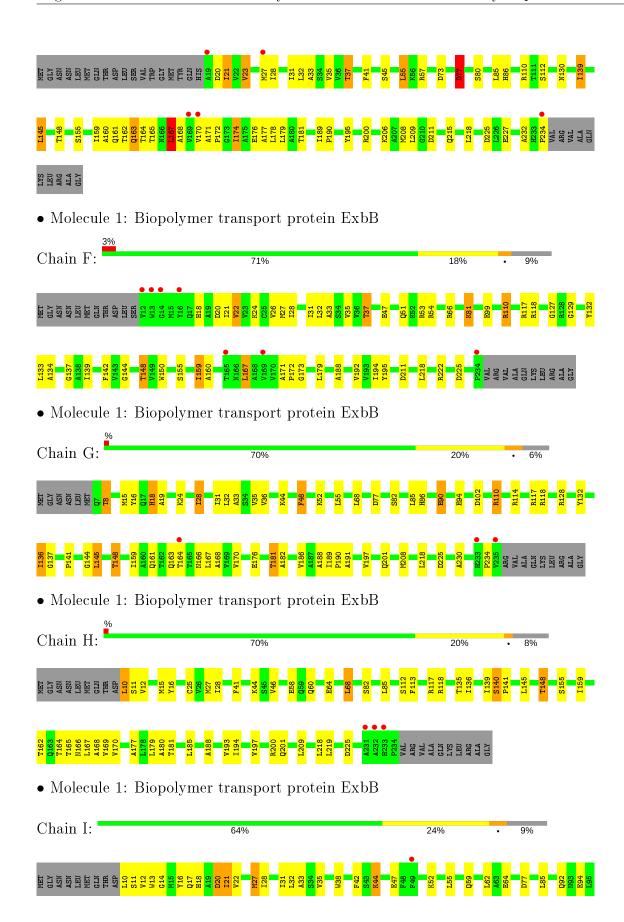
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Biopolymer transport protein ExbB



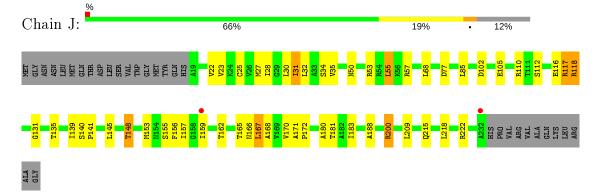




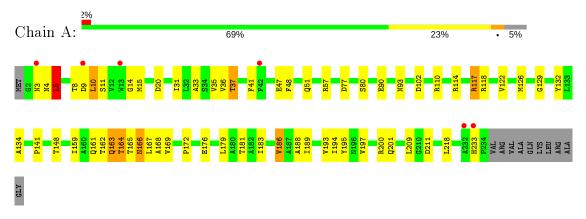




• Molecule 1: Biopolymer transport protein ExbB



• Molecule 1: Biopolymer transport protein ExbB





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	137.17Å 104.78Å 149.36Å	Depositor
a, b, c, α , β , γ	90.00° 91.77° 90.00°	Depositor
Resolution (Å)	46.00 - 2.60	Depositor
Resolution (A)	49.76 - 2.58	EDS
% Data completeness	94.4 (46.00-2.60)	Depositor
(in resolution range)	89.3 (49.76-2.58)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) > 1$	1.08 (at 2.58Å)	Xtriage
Refinement program	PHENIX (1.10_2142: ???)	Depositor
D D.	0.211 , 0.258	Depositor
R, R_{free}	0.210 , 0.258	DCC
R_{free} test set	2008 reflections (1.59%)	wwPDB-VP
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.30 , 59.7	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16861	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, EPE, MLY

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	Во	ond angles
MIOI	Chain	RMSZ	# Z >5	RMSZ	# Z > 5
1	A	0.47	0/1764	0.63	0/2392
1	В	0.44	0/1707	0.68	0/2315
1	С	0.44	0/1661	0.61	0/2249
1	D	0.50	0/1625	0.62	0/2200
1	E	0.44	0/1619	0.64	2/2195~(0.1%)
1	F	0.48	0/1662	0.62	$1/2253 \ (0.0\%)$
1	G	0.46	0/1747	0.66	1/2370~(0.0%)
1	Н	0.46	0/1715	0.63	0/2324
1	I	0.48	0/1690	0.64	0/2289
1	J	0.52	0/1605	0.68	0/2174
All	All	0.47	0/16795	0.64	$4/22761 \ (0.0\%)$

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 maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	С	0	2
1	D	0	1
1	E	0	1
1	G	0	3
All	All	0	8

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	${f Atoms}$	\mathbf{Z}	$Observed(^o)$	$\mathbf{Ideal}(^o)$
1	Ε	167	LEU	C-N-CA	6.74	138.55	121.70



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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
1	Ε	77	ASP	C-N-CA	6.27	137.37	121.70
1	F	110	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	G	110	ARG	NE-CZ-NH2	-5.45	117.58	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	С	17	GLN	Peptide
1	С	18	HIS	Peptide
1	D	162	THR	Peptide
1	E	167	LEU	Peptide
1	G	161	GLN	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	1749	0	1759	45	0
1	В	1692	0	1714	40	0
1	С	1651	0	1679	28	0
1	D	1615	0	1651	36	0
1	E	1609	0	1636	40	0
1	F	1651	0	1663	41	0
1	G	1731	0	1734	41	0
1	Н	1700	0	1729	30	0
1	I	1678	0	1708	53	0
1	J	1596	0	1630	42	0
2	D	15	0	17	0	0
2	F	15	0	17	1	0
2	I	15	0	17	1	0
3	A	1	0	0	0	0
3	I	1	0	0	0	0
4	A	10	0	0	0	0
4	В	14	0	0	4	0
4	С	11	0	0	0	0
4	D	12	0	0	1	0



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Mol	Chain	Non-H	H(model)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
4	Ε	16	0	0	0	0
4	F	16	0	0	1	0
4	G	15	0	0	1	0
4	Н	13	0	0	1	0
4	I	15	0	0	1	0
4	J	20	0	0	0	0
All	All	16861	0	16954	348	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 10.

The worst 5 of 348 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{ll} ext{Interatomic} \ ext{distance} \ (ext{\AA}) \end{array}$	$egin{array}{c} ext{Clash} \ ext{overlap } (ext{Å}) \end{array}$
1:B:117:ARG:NH1	1:C:211:ASP:OD1	1.88	1.06
1:H:136:ILE:O	1:H:140:SER:HB3	1.68	0.93
1:B:90:GLU:HG3	1:B:118:ARG:HH22	1.33	0.92
1:C:196:ASN:HB3	1:C:200:ARG:HH11	1.39	0.87
1:A:141:PRO:HD3	1:A:188:ALA:HB2	1.54	0.87

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	Perce	\mathbf{ntiles}
1	A	230/244~(94%)	216 (94%)	12 (5%)	2 (1%)	17	35
1	В	222/244 (91%)	215 (97%)	7 (3%)	0	100	100
1	С	219/244 (90%)	217 (99%)	2 (1%)	0	100	100
1	D	212/244 (87%)	206 (97%)	6 (3%)	0	100	100
1	E	213/244 (87%)	206 (97%)	7 (3%)	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	F	220/244~(90%)	214 (97%)	6 (3%)	0	100	100
1	G	228/244~(93%)	222 (97%)	6 (3%)	0	100	100
1	Н	222/244 (91%)	214 (96%)	7 (3%)	1 (0%)	29	52
1	I	220/244~(90%)	215 (98%)	3 (1%)	2 (1%)	17	35
1	J	211/244 (86%)	207 (98%)	4 (2%)	0	100	100
All	All	2197/2440 (90%)	2132 (97%)	60 (3%)	5 (0%)	47	71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	12	VAL
1	A	168	ALA
1	Н	68	LEU
1	I	21	ILE
1	A	166	ASN

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	Perce	$_{ m ntiles}$
1	A	$176/189 \ (93\%)$	161 (92%)	15 (8%)	10	21
1	В	171/189 (90%)	156 (91%)	15 (9%)	10	19
1	С	166/189~(88%)	149 (90%)	17 (10%)	7	14
1	D	$164/189 \; (87\%)$	147 (90%)	17 (10%)	7	13
1	E	162/189~(86%)	140 (86%)	22 (14%)	3	6
1	F	163/189~(86%)	155 (95%)	8 (5%)	25	48
1	G	173/189~(92%)	159 (92%)	14 (8%)	11	23
1	Н	$173/189 \ (92\%)$	156 (90%)	17 (10%)	8	15
1	I	170/189 (90%)	156 (92%)	14 (8%)	11	22
1	J	$160/189 \; (85\%)$	142 (89%)	18 (11%)	6	10



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1678/1890 (89%)	1521 (91%)	157 (9%)	8 17

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	22	VAL
1	G	102	ASP
1	A	37	THR
1	F	37	THR
1	G	8	THR

Some 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)

10 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	Tune	Chain	Res	Link	В	ond leng	gths	Bond angles		
MIOI	Type	Chain	nes	DillK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	F	108	1	9,10,11	0.66	0	6,11,13	0.82	0
1	MLY	D	108	1	9,10,11	0.81	0	6,11,13	0.77	0
1	MLY	I	108	1	9,10,11	0.77	0	6,11,13	0.66	0
1	MLY	G	108	1	9,10,11	0.81	0	6,11,13	0.79	0
1	MLY	A	108	1	9,10,11	0.60	0	6,11,13	0.82	0
1	MLY	Е	108	1	9,10,11	0.82	0	6,11,13	0.81	0
1	MLY	С	108	1	9,10,11	0.88	0	6,11,13	0.80	0
1	MLY	J	108	1	9,10,11	0.68	0	6,11,13	0.74	0
1	MLY	Н	108	1	9,10,11	0.94	0	6,11,13	0.97	0
1	MLY	В	108	1	9,10,11	0.79	0	6,11,13	0.83	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
1	MLY	F	108	1	-	1/8/9/11	-
1	MLY	D	108	1	-	2/8/9/11	_
1	MLY	I	108	1	-	0/8/9/11	_
1	MLY	G	108	1	-	0/8/9/11	-
1	MLY	A	108	1	-	0/8/9/11	_
1	MLY	Е	108	1	-	1/8/9/11	_
1	MLY	С	108	1	-	1/8/9/11	_
1	MLY	J	108	1	-	0/8/9/11	_
1	MLY	Н	108	1	-	1/8/9/11	-
1	MLY	В	108	1	-	1/8/9/11	_

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	108	MLY	CD-CE-NZ-CH2
1	Е	108	MLY	CD-CE-NZ-CH2
1	F	108	MLY	CD-CE-NZ-CH2
1	С	108	MLY	CD-CE-NZ-CH2
1	D	108	MLY	CD-CE-NZ-CH1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 2 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 Ty	Trino	Chain	Chain Res	Link	Во	nd leng	ths	Bond angles		
MIOI	Type	Chain		55 LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EPE	D	301	-	15,15,15	0.95	1 (6%)	18,20,20	1.86	7 (38%)
2	EPE	F	301	-	15,15,15	0.93	1 (6%)	18,20,20	2.17	5 (27%)
2	EPE	I	302	-	15,15,15	0.91	1 (6%)	18,20,20	2.03	7 (38%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EPE	D	301	_	-	3/9/19/19	0/1/1/1
2	EPE	F	301	_	-	4/9/19/19	0/1/1/1
2	EPE	I	302	-	-	4/9/19/19	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	${ m Observed}({ m \AA})$	$\operatorname{Ideal}(ext{\AA})$
2	F	301	EPE	C10-S	3.27	1.82	1.77
2	I	302	EPE	C10-S	3.11	1.81	1.77
2	D	301	EPE	C10-S	2.89	1.81	1.77

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\mathbf{Ideal}(^o)$
2	F	301	EPE	C5-N4-C3	5.67	121.58	108.83
2	I	302	EPE	C7-N4-C5	4.09	121.69	111.23
2	I	302	EPE	C5-N4-C3	4.08	118.01	108.83
2	F	301	EPE	O1S-S-C10	3.93	111.64	106.92
2	D	301	EPE	C5-N4-C3	3.69	117.13	108.83

There are no chirality outliers.

5 of 11 torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
2	D	301	EPE	C9-C10-S-O2S
2	D	301	EPE	C9-C10-S-O3S
2	F	301	EPE	C8-C7-N4-C5
2	F	301	EPE	C9-C10-S-O2S
2	F	301	EPE	C9-C10-S-O3S

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	EPE	1	0
2	I	302	EPE	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 (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, 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	${f Analysed}$	<rsrz></rsrz>	#RSR2	Z>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	A	$232/244\ (95\%)$	-0.11	6 (2%) 56	50	42, 74, 134, 191	0
1	В	224/244~(91%)	-0.31	1 (0%) 92	91	46, 76, 121, 164	0
1	С	221/244~(90%)	-0.26	1 (0%) 91	89	42, 77, 115, 160	0
1	D	214/244~(87%)	-0.21	2 (0%) 84	82	41, 68, 128, 200	0
1	E	215/244~(88%)	-0.12	5 (2%) 60	54	42, 76, 134, 164	0
1	F	222/244~(90%)	-0.13	7 (3%) 47	40	43, 73, 147, 218	0
1	G	228/244~(93%)	-0.27	3 (1%) 77	73	44, 76, 132, 214	0
1	Н	224/244~(91%)	-0.36	3 (1%) 77	73	46, 75, 116, 197	0
1	I	222/244~(90%)	-0.32	1 (0%) 91	89	45, 77, 123, 155	0
1	J	213/244~(87%)	-0.32	2 (0%) 84	82	40, 70, 142, 181	0
All	All	$2215/2440 \ (90\%)$	-0.24	31 (1%) 75	5 71	40, 75, 132, 218	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	13	TRP	5.8
1	J	232	ALA	5.8
1	A	3	ASN	4.8
1	F	12	VAL	4.2
1	E	234	PRO	4.1

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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	MLY	С	108	11/12	0.97	0.14	38,44,60,61	0
1	MLY	В	108	11/12	0.97	0.17	38,43,50,53	0
1	MLY	I	108	11/12	0.98	0.11	33,39,65,67	0
1	MLY	G	108	11/12	0.98	0.12	32,43,52,53	0
1	MLY	E	108	11/12	0.98	0.19	52,56,68,73	0
1	MLY	F	108	11/12	0.98	0.16	44,49,62,66	0
1	MLY	J	108	11/12	0.98	0.13	31,40,59,65	0
1	MLY	D	108	11/12	0.98	0.14	36,40,49,56	0
1	MLY	Н	108	11/12	0.99	0.11	35,45,57,60	0
1	MLY	A	108	11/12	0.99	0.13	33,37,55,65	0

6.3 Carbohydrates (i)

There are no carbohydrates 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	${f B-factors}({f \AA}^2)$	Q < 0.9
2	EPE	D	301	15/15	0.76	0.15	95,119,159,163	0
3	CA	I	301	1/1	0.81	0.16	104,104,104,104	0
2	EPE	I	302	15/15	0.82	0.14	85,127,167,169	0
2	EPE	F	301	15/15	0.86	0.29	88,114,157,161	0
3	CA	A	301	1/1	0.97	0.16	97,97,97,97	0

6.5 Other polymers (i)

There are no such residues in this entry.

