

Full wwPDB X-ray Structure Validation Report (i)

Sep 22, 2022 – 02:12 PM EDT

PDB ID	:	7M66
Title	:	Targeting Enterococcus faecalis HMG-CoA reductase with a novel non-statin
		inhibitor
Authors	:	Bose, S.; Steussy, C.N.
Deposited on	:	2021-03-25
Resolution	:	2.25 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	:	2.29
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)	:	2.29

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.25 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.



Motrie	Whole archive	Similar resolution
Meth	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R _{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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		
			15%		
1	А	423	82%	•	15%
			7%		
1	В	423	82%	•	15%
			15%		
1	С	423	83%	•	15%
			6%		
1	D	423	82%	•	16%



7M66

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 23361 atoms, of which 11422 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.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace	
1	Δ	360	Total	С	Η	Ν	0	\mathbf{S}	0	4	0
1	Л	300	5560	1741	2790	473	543	13	0	4	0
1	В	360	Total	С	Η	Ν	0	S	0	12	0
1	I D	300	5651	1766	2846	482	545	12	0		0
1	С	360	Total	С	Η	Ν	0	S	0	8	0
1			5580	1745	2801	477	545	12			0
1	1 D	257	Total	С	Η	Ν	0	S	0	17	0
	397	5635	1761	2836	478	546	14	0	11	0	

• Molecule 1 is a protein called Hydroxymethylglutaryl-CoA reductase, degradative.

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0



• Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Λ	1	Total C H N O S	0	0
J	A	1	25 6 13 1 4 1	0	0
2	В	1	Total C H N O S	0	0
0	D	I	25 6 13 1 4 1	0	0
3	В	B 1	Total C H N O S	0	0
5	D		25 6 13 1 4 1		0
3	Л	1	Total C H N O S	0	0
5 D	1	25 6 13 1 4 1	0	0	
2	Л	1	Total C H N O S	0	0
5	D		25 6 13 1 4 1	0	0

• Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	Λ	1	Total	С	Η	0	0	0
4	A	L	17	4	10	3	0	0
4	Λ	1	Total	С	Η	Ο	0	0
4	Л	T	17	4	10	3	0	0
4	Δ	1	Total	С	Η	Ο	0	0
4	Π	T	17	4	10	3	0	0
4	С	1	Total	С	Η	Ο	0	0
4	U	L	17	4	10	3	0	0
1	С	1	Total	С	Η	Ο	0	0
T	4 0	1	17	4	10	3	0	0
1	П	1	Total	C	Η	O	0	0
		1 I	17	4	10	3	0	

• Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	3	Total Ca 3 3	0	0
5	В	2	Total Ca 2 2	0	0
5	С	2	Total Ca 2 2	0	0
5	D	3	Total Ca 3 3	0	0

• Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	В	1	Total C H O 10 2 6 2	0	0
6	В	1	Total C H O 10 2 6 2	0	0
6	В	1	Total C H O 10 2 6 2	0	0
6	С	1	Total C H O 10 2 6 2	0	0

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	153	Total O	0	0
			153 153		
7	В	156	Total O	0	0
•	2	100	156 156	Ŭ	Ŭ
7	C	159	Total O	0	0
(C	156	158 158	0	0
7	П	170	Total O	0	2
(D	179	181 181	U	



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.

- 15% Chain A: 82% 15% MET LEU LEU GLU PRO GLN GLN GLN LYS • Molecule 1: Hydroxymethylglutaryl-CoA reductase, degradative Chain B: 82% 15% MET LEU LEU LEU ARG PRO PRO CLVS
- Molecule 1: Hydroxymethylglutaryl-CoA reductase, degradative

ALA ILEU LEU ASP ASP LEU ARG LYS GLN

• Molecule 1: Hydroxymethylglutaryl-CoA reductase, degradative





• Molecule 1: Hydroxymethylglutaryl-CoA reductase, degradative





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants	168.66Å 168.66Å 120.19Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	45.13 - 2.25	Depositor
Resolution (A)	45.13 - 2.25	EDS
% Data completeness	99.7 (45.13-2.25)	Depositor
(in resolution range)	$99.8 \ (45.13 - 2.25)$	EDS
R _{merge}	0.12	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.39 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
D D.	0.175 , 0.209	Depositor
Π, Π_{free}	0.173 , 0.206	DCC
R_{free} test set	4593 reflections $(5.02%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	38.7	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	0.40 , 42.0	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.026 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	23361	wwPDB-VP
Average B, all atoms $(Å^2)$	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 21.07 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.5905e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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.



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: EDO, MES, PEG, SO4, CA

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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.26	0/2808	0.48	0/3801	
1	В	0.27	0/2875	0.51	0/3892	
1	С	0.26	0/2851	0.49	0/3858	
1	D	0.26	0/2886	0.50	0/3907	
All	All	0.26	0/11420	0.50	0/15458	

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 (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	А	2770	2790	2786	8	0
1	В	2805	2846	2799	6	0
1	С	2779	2801	2765	3	0
1	D	2799	2836	2782	6	0
2	А	5	0	0	0	0
2	С	5	0	0	0	0
3	А	12	13	13	0	0
3	В	24	26	25	0	0
3	D	24	26	26	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	А	21	30	30	0	0
4	С	14	20	20	0	0
4	D	7	10	10	0	0
5	А	3	0	0	0	0
5	В	2	0	0	0	0
5	С	2	0	0	0	0
5	D	3	0	0	0	0
6	В	12	18	18	0	0
6	С	4	6	6	0	0
7	А	153	0	0	2	0
7	В	156	0	0	1	0
7	С	158	0	0	1	0
7	D	181	0	0	0	0
All	All	11939	11422	11280	22	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 1.

All (22) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:113:ARG:O	1:B:211[A]:LEU:HD22	2.06	0.55	
1:D:112[B]:MET:SD	1:D:211[B]:LEU:HD11	2.46	0.55	
1:D:113:ARG:O	1:D:211[A]:LEU:HD22	2.07	0.55	
1:B:183:ALA:HA	1:B:211[B]:LEU:HD22	1.91	0.54	
1:C:342:VAL:HG22	7:C:658:HOH:O	2.10	0.52	
1:C:340:LEU:HG	1:C:342:VAL:HG13	1.91	0.51	
1:B:152:ARG:NH2	7:B:606:HOH:O	2.49	0.46	
1:D:340:LEU:HG	1:D:342[B]:VAL:HG23	1.98	0.45	
1:A:231:LEU:O	1:A:365:ARG:NE	2.49	0.45	
1:D:342[A]:VAL:HG13	1:D:347:GLU:HB3	1.98	0.45	
1:B:326:ALA:HA	1:B:329:VAL:HG12	2.01	0.42	
1:A:93:LEU:C	1:A:93:LEU:HD13	2.39	0.42	
1:A:100:ALA:O	1:A:101:GLN:HB2	2.19	0.42	
1:A:342:VAL:HG22	7:A:647:HOH:O	2.19	0.42	
1:A:251:ALA:O	1:A:258:ALA:HB2	2.21	0.41	
1:A:39:GLU:OE1	7:A:601:HOH:O	2.22	0.41	
1:C:117:VAL:HG21	1:D:250:TYR:CE2	2.56	0.40	
1:B:153:GLY:O	1:B:157[A]:ARG:NH2	2.54	0.40	
1:A:173:PHE:CG	1:A:190:LEU:HD11	2.56	0.40	
1:A:340:LEU:HG	1:A:342:VAL:HG13	2.03	0.40	



Clash

overlap (Å)

0.40

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Atom-1	Atom-2	Interatomic distance (Å)

1:B:93:LEU:C 1:B:93:LEU:HD13 2.42

There are no symmetry-related clashes.

5.3 Torsion angles (i)

<u>O</u>______ f_____ f______

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	ntiles
1	А	362/423~(86%)	354~(98%)	8 (2%)	0	100	100
1	В	370/423~(88%)	360~(97%)	10 (3%)	0	100	100
1	С	366/423~(86%)	358~(98%)	8 (2%)	0	100	100
1	D	372/423~(88%)	363~(98%)	9(2%)	0	100	100
All	All	1470/1692~(87%)	1435~(98%)	35~(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	А	297/344~(86%)	294 (99%)	3~(1%)	76 84		
1	В	304/344~(88%)	298~(98%)	6(2%)	55 64		
1	С	301/344~(88%)	294 (98%)	7 (2%)	50 59		
1	D	306/344~(89%)	303~(99%)	3 (1%)	76 84		



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1208/1376~(88%)	1189~(98%)	19 (2%)	65	73

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	232	SER
1	А	281	ARG
1	А	316	VAL
1	В	125	GLU
1	В	220[A]	VAL
1	В	220[B]	VAL
1	В	227	PRO
1	В	238	ARG
1	В	281	ARG
1	С	120	ASP
1	С	148	SER
1	С	166	GLU
1	С	167[A]	SER
1	С	167[B]	SER
1	С	281	ARG
1	С	370	GLU
1	D	229	SER
1	D	235	SER
1	D	281	ARG

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 27 ligands modelled in this entry, 10 are monoatomic - leaving 17 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).

Mal	Tuno	Chain	Dog	Tink	Bo	ond leng	ths	Bond angles			
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
4	PEG	А	504	-	6,6,6	0.66	0	$5,\!5,\!5$	1.08	0	
4	PEG	С	503	-	6,6,6	0.66	0	$5,\!5,\!5$	1.08	0	
2	SO4	А	501	-	4,4,4	0.14	0	$6,\!6,\!6$	0.06	0	
6	EDO	С	502	-	3,3,3	0.48	0	2,2,2	0.30	0	
6	EDO	В	504	-	3,3,3	0.47	0	$2,\!2,\!2$	0.31	0	
3	MES	А	502	-	12,12,12	2.22	1 (8%)	$14,\!16,\!16$	1.60	4 (28%)	
2	SO4	С	501	-	4,4,4	0.14	0	6,6,6	0.06	0	
4	PEG	А	505	-	6,6,6	0.61	0	$5,\!5,\!5$	1.12	0	
4	PEG	А	503	-	6,6,6	0.63	0	$5,\!5,\!5$	1.03	0	
4	PEG	D	503	-	6,6,6	0.60	0	$5,\!5,\!5$	1.08	0	
6	EDO	В	505	-	3,3,3	0.47	0	2,2,2	0.33	0	
3	MES	В	502	-	12,12,12	2.17	1 (8%)	14,16,16	1.54	3 (21%)	
3	MES	В	501	-	12,12,12	2.22	1 (8%)	14,16,16	1.56	3 (21%)	
3	MES	D	502	-	12,12,12	2.18	1 (8%)	14,16,16	1.80	5 (35%)	
4	PEG	С	504	-	6,6,6	0.64	0	$5,\!5,\!5$	1.07	0	
3	MES	D	501	-	12,12,12	2.07	1 (8%)	14,16,16	2.01	6 (42%)	
6	EDO	В	503	-	3,3,3	0.46	0	2,2,2	0.28	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
4	PEG	А	504	-	-	3/4/4/4	-
4	PEG	С	503	-	-	1/4/4/4	-
6	EDO	С	502	-	-	1/1/1/1	-
6	EDO	В	504	-	-	1/1/1/1	-
3	MES	А	502	-	-	2/6/14/14	0/1/1/1
4	PEG	А	505	-	-	2/4/4/4	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	А	503	-	-	1/4/4/4	-
4	PEG	D	503	-	-	1/4/4/4	-
6	EDO	В	505	-	-	1/1/1/1	-
3	MES	В	502	-	-	5/6/14/14	0/1/1/1
3	MES	В	501	-	-	0/6/14/14	0/1/1/1
3	MES	D	502	-	-	1/6/14/14	0/1/1/1
4	PEG	С	504	-	-	3/4/4/4	-
3	MES	D	501	-	-	1/6/14/14	0/1/1/1
6	EDO	B	503	-	-	0/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	В	501	MES	C8-S	-7.43	1.66	1.77
3	А	502	MES	C8-S	-7.42	1.67	1.77
3	D	502	MES	C8-S	-7.26	1.67	1.77
3	В	502	MES	C8-S	-7.24	1.67	1.77
3	D	501	MES	C8-S	-6.87	1.67	1.77

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	D	501	MES	O2S-S-C8	4.16	111.92	106.92
3	D	502	MES	O3S-S-C8	3.88	112.04	105.77
3	В	501	MES	C5-N4-C3	3.55	116.81	108.83
3	В	502	MES	O3S-S-C8	3.31	111.13	105.77
3	D	502	MES	C2-C3-N4	-2.73	105.97	110.10
3	А	502	MES	C6-C5-N4	-2.71	105.99	110.10
3	D	501	MES	C2-C3-N4	-2.69	106.03	110.10
3	А	502	MES	O1S-S-C8	2.54	109.97	106.92
3	В	501	MES	O2S-S-C8	2.54	109.97	106.92
3	D	501	MES	O1-C6-C5	2.42	117.13	111.80
3	D	502	MES	C6-C5-N4	-2.35	106.54	110.10
3	А	502	MES	C5-N4-C3	2.31	114.04	108.83
3	D	502	MES	C5-N4-C3	2.30	114.00	108.83
3	В	502	MES	C5-N4-C3	2.17	113.72	108.83
3	D	501	MES	O1S-S-C8	2.16	109.51	106.92
3	А	502	MES	O3S-S-C8	2.15	109.25	105.77
3	D	501	MES	C6-O1-C2	2.09	116.86	109.89
3	D	501	MES	O3S-S-C8	2.08	109.14	105.77
3	D	502	MES	O1S-S-C8	2.04	109.37	106.92
3	В	501	MES	$\overline{O3S-S-C8}$	2.01	109.02	105.77



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	В	502	MES	O1S-S-C8	2.01	109.33	106.92

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
3	В	502	MES	C7-C8-S-O1S
3	В	502	MES	C7-C8-S-O2S
3	В	502	MES	C7-C8-S-O3S
4	D	503	PEG	O2-C3-C4-O4
4	А	503	PEG	O1-C1-C2-O2
4	С	504	PEG	O1-C1-C2-O2
6	В	504	EDO	O1-C1-C2-O2
6	С	502	EDO	O1-C1-C2-O2
4	С	504	PEG	O2-C3-C4-O4
3	В	502	MES	N4-C7-C8-S
3	А	502	MES	C8-C7-N4-C3
4	С	503	PEG	O2-C3-C4-O4
4	С	504	PEG	C4-C3-O2-C2
6	В	505	EDO	O1-C1-C2-O2
3	D	501	MES	C7-C8-S-O1S
4	А	505	PEG	C1-C2-O2-C3
4	А	505	PEG	C4-C3-O2-C2
4	А	504	PEG	O2-C3-C4-O4
4	А	504	PEG	O1-C1-C2-O2
4	А	504	PEG	C1-C2-O2-C3
3	А	502	MES	C8-C7-N4-C5
3	В	502	MES	C8-C7-N4-C3
3	D	502	MES	C8-C7-N4-C3

There are no ring outliers.

No monomer is involved in short contacts.

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	Analysed	< RSRZ >	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	360/423~(85%)	0.68	62 (17%) 1 1	27, 42, 85, 97	10 (2%)
1	В	360/423~(85%)	0.18	30 (8%) 11 12	29, 41, 75, 107	9 (2%)
1	С	360/423~(85%)	0.64	63 (17%) 1 1	26, 41, 87, 100	14 (3%)
1	D	357/423~(84%)	0.12	25 (7%) 16 17	28, 39, 72, 88	7 (1%)
All	All	1437/1692~(84%)	0.41	180 (12%) 3 3	26, 41, 82, 107	40 (2%)

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	201	PHE	7.2
1	С	166	GLU	6.6
1	А	166	GLU	5.8
1	А	11	ASN	5.6
1	С	133	VAL	5.3
1	В	372	ILE	5.3
1	С	144	LEU	5.2
1	В	308	GLU	5.1
1	С	202	ALA	4.9
1	В	370	GLU	4.9
1	А	12	SER	4.8
1	С	11	ASN	4.8
1	А	280	THR	4.7
1	С	205	LYS	4.4
1	D	308	GLU	4.4
1	А	164	PHE	4.3
1	A	235	SER	4.3
1	А	131	LEU	4.2
1	А	122	ALA	4.2
1	С	131	LEU	4.2
1	С	280	THR	4.2



Mol	Chain	Res	Type	RSRZ
1	С	124	PRO	4.0
1	D	235	SER	4.0
1	А	133	VAL	4.0
1	А	196	LEU	4.0
1	С	12	SER	4.0
1	В	226	ILE	3.9
1	А	282	ALA	3.9
1	С	15	TYR	3.9
1	В	233	LYS	3.9
1	С	197	PHE	3.9
1	В	235	SER	3.9
1	D	232	SER	3.9
1	А	202	ALA	3.8
1	А	13	ARG	3.8
1	В	271	ALA	3.8
1	А	126	SER	3.8
1	D	233	LYS	3.7
1	С	200	TRP	3.7
1	С	283	VAL	3.7
1	А	15	TYR	3.7
1	А	283	VAL	3.7
1	С	199	GLU	3.6
1	В	306	ASP	3.6
1	В	305	LEU	3.6
1	А	144	LEU	3.6
1	А	273	VAL	3.5
1	А	200	TRP	3.5
1	А	128	ILE	3.5
1	А	138	ILE	3.4
1	С	138	ILE	3.4
1	С	196	LEU	3.4
1	A	124	PRO	3.3
1	A	284	SER	3.3
1	C	198	ARG	3.3
1	D	$284[\overline{A}]$	SER	3.2
1	C	284	SER	3.2
1	D	234	GLY	3.2
1	D	306	ASP	3.2
1	C	13	ARG	3.2
1	D	343[A]	THR	3.1
1	C	272	VAL	3.1
1	D	307	GLY	3.1



Mol	Chain	Res	Type	RSRZ
1	А	16	GLN	3.0
1	С	122	ALA	3.0
1	С	151	LYS	3.0
1	А	201	PHE	3.0
1	С	130	LYS	3.0
1	А	127	LEU	2.9
1	С	126	SER	2.9
1	В	280	THR	2.9
1	D	231	LEU	2.8
1	А	199	GLU	2.8
1	А	130	LYS	2.8
1	С	194	ALA	2.8
1	D	271	ALA	2.8
1	С	273	VAL	2.8
1	В	264	GLY	2.8
1	С	282	ALA	2.8
1	D	273	VAL	2.8
1	С	123	ASP	2.8
1	С	165	ASP	2.7
1	В	307	GLY	2.7
1	В	260	THR	2.7
1	В	269	ILE	2.7
1	С	125	GLU	2.7
1	В	274	LEU	2.7
1	A	121	VAL	2.7
1	С	140	GLN	2.7
1	A	271	ALA	2.7
1	A	272	VAL	2.7
1	A	195	GLU	2.7
1	A	204	GLN	2.7
1	C	320	LEU	2.7
1	B	266	MET	2.7
1	С	147	PRO	2.6
1	В	371	GLY	2.6
1	B	227	PRO	2.6
1	D	240	ILE	2.6
1	A	84	THR	2.6
1	B	234	GLY	2.6
1	A	266	MET	2.6
1	C	145	SER	2.6
1	В	83	ALA	2.6
1	C	271	ALA	2.6



Mol	Chain	Res	Type	RSRZ
1	С	16	GLN	2.6
1	D	228	VAL	2.6
1	В	273	VAL	2.6
1	С	146	TYR	2.6
1	А	198	ARG	2.6
1	С	281	ARG	2.5
1	С	128	ILE	2.5
1	В	236	ASN	2.5
1	С	269	ILE	2.5
1	С	203	GLU	2.5
1	С	204	GLN	2.5
1	D	283	VAL	2.5
1	А	285	ALA	2.5
1	А	134	ARG	2.5
1	D	266[A]	MET	2.5
1	А	145	SER	2.5
1	С	285	ALA	2.5
1	D	238	ARG	2.4
1	А	269	ILE	2.4
1	В	267	ASN	2.4
1	А	319	ALA	2.4
1	D	267[A]	ASN	2.4
1	А	279	ASP	2.4
1	В	283	VAL	2.4
1	С	121	VAL	2.4
1	А	151	LYS	2.4
1	А	192	GLY	2.4
1	С	266	MET	2.4
1	С	319	ALA	2.4
1	А	286	SER	2.4
1	В	311	ILE	2.4
1	A	123	ASP	2.3
1	С	193	VAL	2.3
1	D	269	ILE	2.3
1	С	267	ASN	2.3
1	A	281	ARG	2.3
1	А	318	LEU	2.3
1	A	205	LYS	2.3
1	С	343	THR	2.3
1	A	203	GLU	2.3
1	В	238	ARG	2.3
1	А	321	ALA	2.3



Mol	Chain	Res	Type	RSRZ
1	С	134	ARG	2.2
1	С	129	ASP	2.2
1	А	140	GLN	2.2
1	С	278	ASN	2.2
1	В	281	ARG	2.2
1	С	306	ASP	2.2
1	D	243	LYS	2.2
1	В	284	SER	2.2
1	А	275	ALA	2.2
1	В	285	ALA	2.2
1	C	195	GLU	2.2
1	А	147	PRO	2.2
1	А	197	PHE	2.1
1	С	279	ASP	2.1
1	D	268	GLY	2.1
1	А	119	TYR	2.1
1	D	263	LYS	2.1
1	С	164	PHE	2.1
1	С	141	GLN	2.1
1	А	345	ALA	2.1
1	А	270	GLU	2.1
1	А	139	PHE	2.1
1	А	320	LEU	2.1
1	D	288	HIS	2.1
1	С	268	GLY	2.1
1	С	137	GLU	2.0
1	A	233	LYS	2.0
1	D	270	GLU	2.0
1	В	268	GLY	2.0
1	D	227	PRO	2.0
1	С	48	GLN	2.0
1	А	165	ASP	2.0
1	С	286	SER	2.0

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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	\mathbf{Res}	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
6	EDO	С	502	4/4	0.63	0.18	59,71,79,82	0
6	EDO	В	505	4/4	0.65	0.30	54,65,70,76	10
4	PEG	С	503	7/7	0.70	0.20	53,65,84,84	0
6	EDO	В	503	4/4	0.75	0.23	63,76,81,82	0
3	MES	А	502	12/12	0.78	0.27	47,56,68,70	25
4	PEG	А	505	7/7	0.78	0.25	35,54,63,65	0
4	PEG	А	503	7/7	0.79	0.15	49,63,75,76	0
4	PEG	А	504	7/7	0.80	0.29	56,69,84,85	0
6	EDO	В	504	4/4	0.82	0.27	54,65,67,76	0
3	MES	В	502	12/12	0.84	0.28	53,70,87,89	25
4	PEG	С	504	7/7	0.85	0.45	59,73,80,86	0
2	SO4	С	501	5/5	0.87	0.23	52,55,64,66	5
4	PEG	D	503	7/7	0.88	0.21	39,48,57,65	17
2	SO4	А	501	5/5	0.92	0.16	68,73,80,90	0
3	MES	D	502	12/12	0.94	0.14	48,70,93,108	0
5	CA	D	505	1/1	0.94	0.07	35,35,35,35	0
3	MES	D	501	12/12	0.94	0.11	36,45,53,57	0
5	CA	С	506	1/1	0.95	0.03	64,64,64,64	0
5	CA	D	504	1/1	0.97	0.05	51,51,51,51	0
5	CA	А	507	1/1	0.97	0.12	42,42,42,42	0
5	CA	А	508	1/1	0.97	0.03	68,68,68,68	0
5	CA	В	506	1/1	0.97	0.05	51,51,51,51	0
5	CA	В	507	1/1	0.97	0.11	74,74,74,74	0
3	MES	В	501	12/12	0.97	0.18	39,54,63,64	25
5	CA	А	506	1/1	0.98	0.21	34,34,34,34	0
5	CA	D	506	1/1	0.98	0.21	71,71,71,71	0
5	CA	С	505	1/1	0.98	0.09	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.

