



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:25 PM UTC

PDB ID : 7M66 / pdb_00007m66
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 ⓘ 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

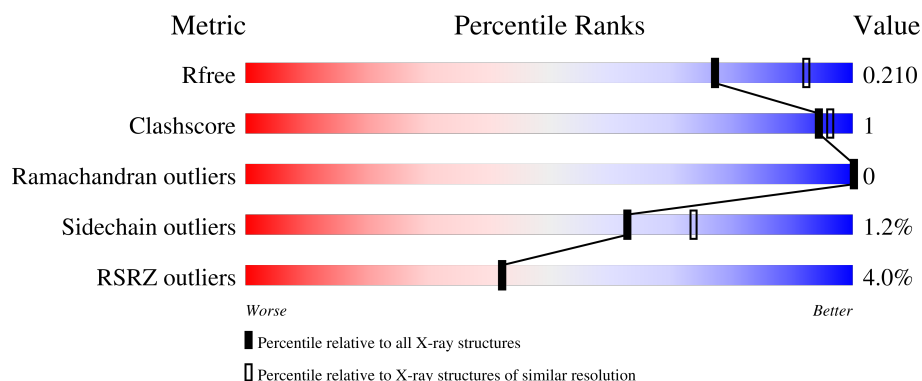
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (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 $\leq 5\%$. 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	423	4% 81% 15%
1	B	423	3% 82% 15%
1	C	423	6% 83% 15%
1	D	423	% 82% 16%

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.

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	360	Total	C	H	N	O	S	0	4	0
			5560	1741	2790	473	543	13			
1	B	360	Total	C	H	N	O	S	0	12	0
			5651	1766	2846	482	545	12			
1	C	360	Total	C	H	N	O	S	0	8	0
			5580	1745	2801	477	545	12			
1	D	357	Total	C	H	N	O	S	0	17	0
			5635	1761	2836	478	546	14			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
3	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
3	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
3	D	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
3	D	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			17	4	10	3		
4	A	1	Total	C	H	O	0	0
			17	4	10	3		
4	A	1	Total	C	H	O	0	0
			17	4	10	3		
4	C	1	Total	C	H	O	0	0
			17	4	10	3		
4	C	1	Total	C	H	O	0	0
			17	4	10	3		
4	D	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Ca	0	0
			3	3		
5	B	2	Total	Ca	0	0
			2	2		
5	C	2	Total	Ca	0	0
			2	2		
5	D	3	Total	Ca	0	0
			3	3		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

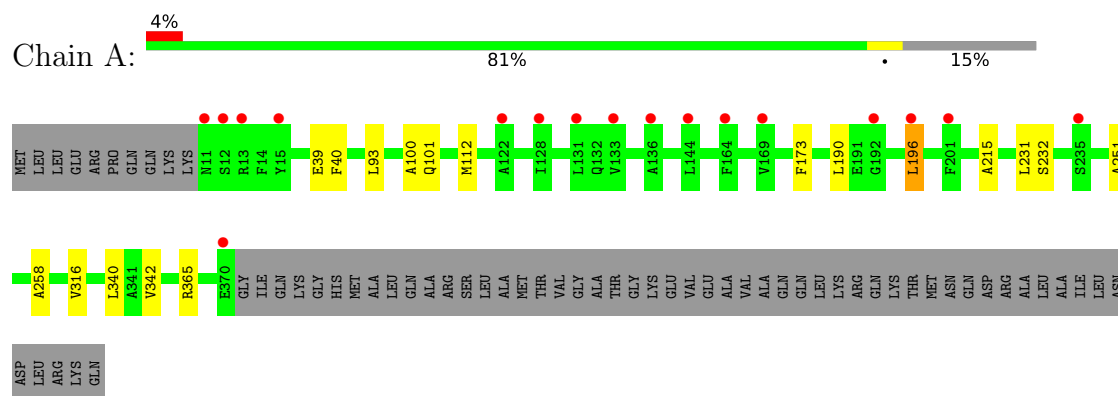
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	153	Total	O	0	0
			153	153		
7	B	156	Total	O	0	0
			156	156		
7	C	158	Total	O	0	0
			158	158		
7	D	179	Total	O	0	2
			181	181		

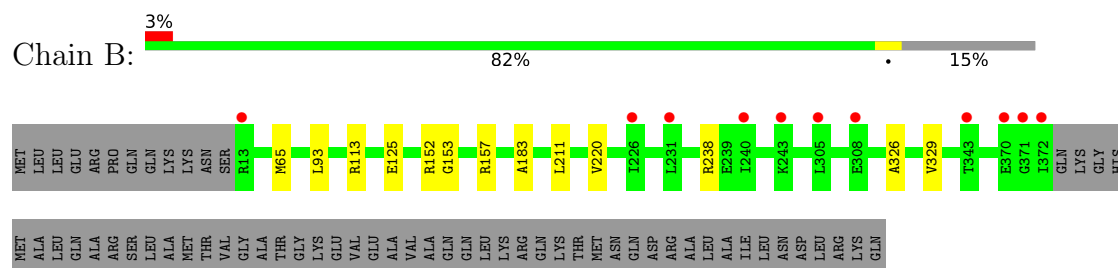
3 Residue-property plots

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.

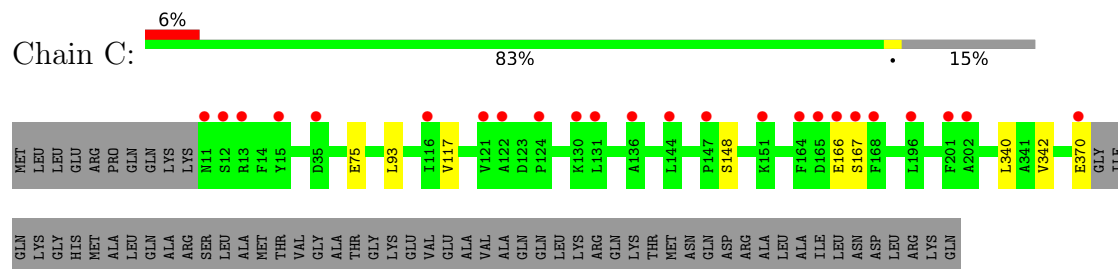
- Molecule 1: Hydroxymethylglutaryl-CoA reductase, degradative



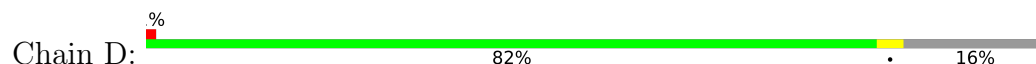
- Molecule 1: Hydroxymethylglutaryl-CoA reductase, degradative

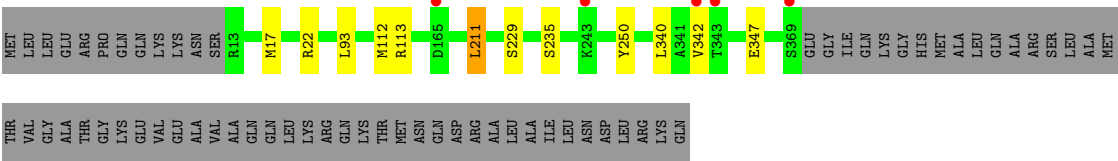


- Molecule 1: Hydroxymethylglutaryl-CoA reductase, degradative



- Molecule 1: Hydroxymethylglutaryl-CoA reductase, degradative





4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	168.66Å 168.66Å 120.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.13 – 2.25 45.13 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.13-2.25) 99.7 (45.13-2.25)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.175 , 0.209 0.176 , 0.210	Depositor DCC
R_{free} test set	4593 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PEG, EDO, CA, MES

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	0.11	0/2808	0.27	0/3801
1	B	0.15	0/2875	0.29	0/3892
1	C	0.12	0/2851	0.29	0/3858
1	D	0.12	0/2886	0.29	0/3907
All	All	0.13	0/11420	0.28	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	A	2770	2790	2786	11	0
1	B	2805	2846	2799	7	0
1	C	2779	2801	2765	4	0
1	D	2799	2836	2782	9	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0
3	A	12	13	13	0	0
3	B	24	26	25	0	0
3	D	24	26	26	0	0

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

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:D:112[A]:MET:HE3	1:D:211[A]:LEU:HD21	1.71	0.71
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:A:93:LEU:C	1:A:93:LEU:HD13	2.39	0.47
1:B:152:ARG:NH2	7:B:606:HOH:O	2.49	0.46
1:A:40:PHE:CE1	1:B:65[B]:MET:HE1	2.52	0.45
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:B:93:LEU:C	1:B:93:LEU:HD13	2.42	0.45
1:D:342[A]:VAL:HG13	1:D:347:GLU:HB3	1.98	0.45
1:C:93:LEU:C	1:C:93:LEU:HD13	2.42	0.44
1:A:112:MET:HE1	1:A:215:ALA:HB2	2.00	0.43
1:B:326:ALA:HA	1:B:329:VAL:HG12	2.01	0.42
1:A:100:ALA:O	1:A:101:GLN:HB2	2.19	0.42
1:D:17:MET:HE2	1:D:22:ARG:HA	2.01	0.42
1:A:342:VAL:HG22	7:A:647:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:LEU:C	1:A:196:LEU:HD23	2.45	0.41
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:D:93:LEU:C	1:D:93:LEU:HD13	2.45	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

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	362/423 (86%)	354 (98%)	8 (2%)	0	100	100
1	B	370/423 (88%)	360 (97%)	10 (3%)	0	100	100
1	C	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	A	297/344 (86%)	294 (99%)	3 (1%)	68	77
1	B	304/344 (88%)	300 (99%)	4 (1%)	61	72
1	C	301/344 (88%)	295 (98%)	6 (2%)	48	59
1	D	306/344 (89%)	302 (99%)	4 (1%)	61	72
All	All	1208/1376 (88%)	1191 (99%)	17 (1%)	63	70

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

Mol	Chain	Res	Type
1	A	196	LEU
1	A	232	SER
1	A	316	VAL
1	B	125	GLU
1	B	220[A]	VAL
1	B	220[B]	VAL
1	B	238	ARG
1	C	75	GLU
1	C	148	SER
1	C	166	GLU
1	C	167[A]	SER
1	C	167[B]	SER
1	C	370	GLU
1	D	211[A]	LEU
1	D	211[B]	LEU
1	D	229	SER
1	D	235	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	31	GLN
1	B	141	GLN
1	B	334	GLN
1	C	11	ASN
1	D	334	GLN

5.3.3 RNA ⓘ

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 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	PEG	A	505	-	6,6,6	0.62	0	5,5,5	1.11	0
3	MES	D	501	-	12,12,12	2.12	1 (8%)	15,16,16	1.82	4 (26%)
3	MES	B	501	-	12,12,12	2.27	1 (8%)	15,16,16	1.46	2 (13%)
2	SO4	A	501	-	4,4,4	0.24	0	6,6,6	0.10	0
6	EDO	B	504	-	3,3,3	0.44	0	2,2,2	0.35	0
3	MES	D	502	-	12,12,12	2.23	1 (8%)	15,16,16	1.62	4 (26%)
3	MES	B	502	-	12,12,12	2.22	1 (8%)	15,16,16	1.41	2 (13%)
6	EDO	C	502	-	3,3,3	0.44	0	2,2,2	0.34	0
4	PEG	D	503	-	6,6,6	0.62	0	5,5,5	1.07	0
6	EDO	B	503	-	3,3,3	0.43	0	2,2,2	0.33	0
2	SO4	C	501	-	4,4,4	0.23	0	6,6,6	0.08	0
4	PEG	A	503	-	6,6,6	0.64	0	5,5,5	1.03	0
4	PEG	A	504	-	6,6,6	0.67	0	5,5,5	1.08	0
4	PEG	C	503	-	6,6,6	0.67	0	5,5,5	1.08	0
4	PEG	C	504	-	6,6,6	0.65	0	5,5,5	1.06	0
6	EDO	B	505	-	3,3,3	0.44	0	2,2,2	0.37	0
3	MES	A	502	-	12,12,12	2.27	1 (8%)	15,16,16	1.52	3 (20%)

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	A	505	-	-	2/4/4/4	-
3	MES	D	501	-	-	2/6/14/14	0/1/1/1
3	MES	B	501	-	-	0/6/14/14	0/1/1/1
6	EDO	B	504	-	-	1/1/1/1	-
3	MES	D	502	-	-	1/6/14/14	0/1/1/1
3	MES	B	502	-	-	5/6/14/14	0/1/1/1
6	EDO	C	502	-	-	1/1/1/1	-
4	PEG	D	503	-	-	1/4/4/4	-
6	EDO	B	503	-	-	0/1/1/1	-
4	PEG	A	503	-	-	1/4/4/4	-
4	PEG	A	504	-	-	3/4/4/4	-
4	PEG	C	503	-	-	2/4/4/4	-
4	PEG	C	504	-	-	3/4/4/4	-
6	EDO	B	505	-	-	1/1/1/1	-
3	MES	A	502	-	-	2/6/14/14	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	MES	C8-S	-7.59	1.66	1.77
3	A	502	MES	C8-S	-7.58	1.67	1.77
3	D	502	MES	C8-S	-7.42	1.67	1.77
3	B	502	MES	C8-S	-7.40	1.67	1.77
3	D	501	MES	C8-S	-7.02	1.67	1.77

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	MES	C5-N4-C3	3.70	116.81	108.84
3	D	501	MES	O2S-S-C8	3.44	111.92	106.73
3	D	502	MES	O3S-S-C8	3.09	112.04	106.00
3	D	502	MES	C2-C3-N4	-2.73	105.97	110.12
3	A	502	MES	C6-C5-N4	-2.72	105.99	110.12
3	D	501	MES	C2-C3-N4	-2.69	106.03	110.12
3	B	502	MES	O3S-S-C8	2.62	111.13	106.00
3	D	501	MES	O1-C6-C5	2.49	117.13	111.77
3	A	502	MES	C5-N4-C3	2.41	114.04	108.84
3	D	502	MES	C5-N4-C3	2.39	114.00	108.84
3	D	502	MES	C6-C5-N4	-2.36	106.54	110.12
3	B	502	MES	C5-N4-C3	2.26	113.72	108.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	MES	C6-O1-C2	2.16	116.86	109.88
3	A	502	MES	O1S-S-C8	2.14	109.97	106.73
3	B	501	MES	O2S-S-C8	2.14	109.97	106.73

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	MES	C7-C8-S-O1S
3	B	502	MES	C7-C8-S-O2S
3	B	502	MES	C7-C8-S-O3S
4	D	503	PEG	O2-C3-C4-O4
4	A	503	PEG	O1-C1-C2-O2
6	B	504	EDO	O1-C1-C2-O2
6	C	502	EDO	O1-C1-C2-O2
4	C	504	PEG	O1-C1-C2-O2
3	B	502	MES	N4-C7-C8-S
4	C	504	PEG	O2-C3-C4-O4
3	A	502	MES	C8-C7-N4-C3
3	D	501	MES	C7-C8-S-O1S
4	C	503	PEG	O2-C3-C4-O4
4	C	504	PEG	C4-C3-O2-C2
6	B	505	EDO	O1-C1-C2-O2
4	A	505	PEG	C1-C2-O2-C3
4	A	504	PEG	O2-C3-C4-O4
4	A	505	PEG	C4-C3-O2-C2
3	A	502	MES	C8-C7-N4-C5
3	B	502	MES	C8-C7-N4-C3
4	A	504	PEG	O1-C1-C2-O2
4	A	504	PEG	C1-C2-O2-C3
3	D	502	MES	C8-C7-N4-C3
3	D	501	MES	C7-C8-S-O3S
4	C	503	PEG	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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

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, 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	360/423 (85%)	0.14	17 (4%) 36 35	18, 46, 93, 103	14 (3%)
1	B	360/423 (85%)	-0.02	11 (3%) 51 51	18, 45, 80, 120	15 (4%)
1	C	360/423 (85%)	0.07	24 (6%) 24 22	18, 44, 92, 111	17 (4%)
1	D	357/423 (84%)	-0.10	5 (1%) 73 74	17, 43, 79, 99	17 (4%)
All	All	1437/1692 (84%)	0.02	57 (3%) 42 42	17, 44, 89, 120	63 (4%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	343[A]	THR	6.2
1	A	11	ASN	5.9
1	B	370	GLU	4.3
1	B	372	ILE	4.0
1	C	166	GLU	3.8
1	C	202	ALA	3.5
1	D	369	SER	3.5
1	C	11	ASN	3.3
1	C	165	ASP	3.3
1	C	15	TYR	3.3
1	C	167[A]	SER	3.2
1	A	164	PHE	3.1
1	C	201	PHE	3.1
1	B	308	GLU	3.1
1	A	370	GLU	3.0
1	D	165	ASP	3.0
1	A	12	SER	2.9
1	D	342[A]	VAL	2.9
1	B	371	GLY	2.6
1	C	13	ARG	2.6
1	A	201	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	128	ILE	2.5
1	B	305	LEU	2.5
1	B	226	ILE	2.4
1	A	122	ALA	2.4
1	B	343	THR	2.4
1	C	151	LYS	2.4
1	C	116	ILE	2.4
1	A	131	LEU	2.4
1	A	192	GLY	2.3
1	C	164	PHE	2.3
1	C	121	VAL	2.3
1	C	196	LEU	2.3
1	B	13	ARG	2.3
1	A	169	VAL	2.3
1	B	240	ILE	2.3
1	C	124	PRO	2.2
1	A	13	ARG	2.2
1	A	15	TYR	2.2
1	C	131	LEU	2.2
1	A	196	LEU	2.2
1	A	235	SER	2.1
1	C	12	SER	2.1
1	C	122	ALA	2.1
1	C	35	ASP	2.1
1	A	133	VAL	2.1
1	C	147	PRO	2.1
1	B	243	LYS	2.1
1	C	136	ALA	2.0
1	A	144	LEU	2.0
1	B	231	LEU	2.0
1	C	144	LEU	2.0
1	C	168[A]	PHE	2.0
1	C	130	LYS	2.0
1	D	243	LYS	2.0
1	C	370	GLU	2.0
1	A	136	ALA	2.0

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

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(Å ²)	Q<0.9
4	PEG	A	504	7/7	0.67	0.18	56,69,84,85	0
4	PEG	C	504	7/7	0.69	0.19	59,73,80,86	0
6	EDO	B	505	4/4	0.69	0.17	54,65,70,76	10
6	EDO	C	502	4/4	0.77	0.14	59,71,79,82	0
3	MES	A	502	12/12	0.78	0.24	47,56,68,70	25
3	MES	B	502	12/12	0.78	0.22	53,70,87,89	25
4	PEG	D	503	7/7	0.80	0.21	39,48,57,65	17
4	PEG	A	505	7/7	0.81	0.22	35,54,63,65	0
6	EDO	B	503	4/4	0.81	0.18	63,76,81,82	0
6	EDO	B	504	4/4	0.84	0.14	54,65,67,76	0
4	PEG	C	503	7/7	0.84	0.14	53,65,84,84	0
4	PEG	A	503	7/7	0.84	0.16	49,63,75,76	0
2	SO4	A	501	5/5	0.85	0.11	68,73,80,90	0
2	SO4	C	501	5/5	0.86	0.18	52,55,64,66	5
3	MES	D	502	12/12	0.91	0.12	48,70,93,108	0
3	MES	D	501	12/12	0.93	0.10	36,45,53,57	0
3	MES	B	501	12/12	0.94	0.12	39,54,63,64	25
5	CA	D	506	1/1	0.94	0.16	71,71,71,71	0
5	CA	D	504	1/1	0.95	0.05	51,51,51,51	0
5	CA	B	507	1/1	0.96	0.07	74,74,74,74	0
5	CA	A	508	1/1	0.97	0.06	68,68,68,68	0
5	CA	A	507	1/1	0.98	0.04	42,42,42,42	0
5	CA	A	506	1/1	0.98	0.06	34,34,34,34	0
5	CA	D	505	1/1	0.98	0.04	35,35,35,35	0
5	CA	B	506	1/1	0.98	0.05	51,51,51,51	0
5	CA	C	506	1/1	0.99	0.04	64,64,64,64	0
5	CA	C	505	1/1	0.99	0.03	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.