

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	7B1S
Title	:	Crystal structure of the ethyl-coenzyme M reductase from Candidatus
		Ethanoperedens thermophilum at 0.994-A resolution
Authors	:	Wagner, T.; Lemaire, O.N.; Engilberge, S.
Deposited on	:	2020-11-25
Resolution	:	0.99 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 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
EDŚ	:	2.22
buster-report	:	1.1.7 (2018)
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)	:	2.22

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 0.99 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.



Motrio	Whole archive	Similar resolution
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	130704	$1050 \ (1.06-0.94)$
Clashscore	141614	1117 (1.06-0.94)
Ramachandran outliers	138981	$1043 \ (1.06-0.94)$
Sidechain outliers	138945	1045 (1.06-0.94)
RSRZ outliers	127900	1023 (1.06-0.94)

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	А	595	94%	
1	D	595	% 95%	••
2	В	467	% 97%	•
2	Е	467	97%	•
3	С	266	3% 96%	•



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Mol	Chain	Length	Quality of chain	
			3%	
3	F	266	95%	5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density	
10	USN	С	301	Х	-	-	-	
10	USN	D	1101	Х	_	-	-	



2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 25172 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 Ethyl-Coenzyme M reductase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	591	Total 4862	C 3061	N 841	O 925	S 35	0	33	0
1	D	593	Total 4879	C 3081	N 846	O 918	S 34	0	35	0

• Molecule 2 is a protein called Ethyl-Coenzyme M reductase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	В	466	Total	С	Ν	Ο	\mathbf{S}	0	33	0
	D	400	3737	2367	637	715	18	0		
2	F	466	Total	С	Ν	Ο	\mathbf{S}	0	37	0
		400	3731	2374	630	709	18	0	51	0

• Molecule 3 is a protein called Ethyl-Coenzyme M reductase gamma subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	С	265	Total 2299	C 1427	N 414	0 437	S 21	0	23	0
3	F	265	Total 2317	C 1432	N 416	O 448	S 21	0	24	0

• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} {\rm Total} & {\rm C} & {\rm O} \\ 6 & 3 & 3 \end{array}$	0	0
4	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
4	Ε	1	$\begin{array}{ccc} {\rm Total} & {\rm C} & {\rm O} \\ 6 & 3 & 3 \end{array}$	0	0
4	Ε	1	$\begin{array}{ccc} {\rm Total} & {\rm C} & {\rm O} \\ 6 & 3 & 3 \end{array}$	0	1

• Molecule 5 is Coenzyme B (three-letter code: TP7) (formula: $C_{11}H_{22}NO_7PS$) (labeled as "Ligand of Interest" by depositor).





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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	Δ	1	Total	С	Ν	Ο	Р	\mathbf{S}	0	0
5	D A		21	11	1	7	1	1	0	
5	п	1	Total	С	Ν	Ο	Р	S	0	0
	D		21	11	1	7	1	1		0

• Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	Total Mn 1 1	0	0

• Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	2	Total K 2 2	0	1
7	С	1	Total K 1 1	0	0
7	D	1	Total K 1 1	0	1

• Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	В	2	Total Cl 2 2	0	0
8	С	1	Total Cl 1 1	0	0
8	Е	2	$\begin{array}{cc} \text{Total} & \text{Cl} \\ 2 & 2 \end{array}$	0	0
8	F	1	Total Cl 1 1	0	0

• Molecule 9 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	В	1	Total 8	С 4	N 1	O 3	0	1
9	Е	1	Total 8	С 4	N 1	O 3	0	1

• Molecule 10 is Dimethylated-F430 cofactor (three-letter code: USN) (formula: $C_{44}H_{55}N_6NiO_{13}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
10	С	1	Total 64	С 44	N 6	Ni 1	O 13	0	0



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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
10	р	1	Total	С	Ν	Ni	Ο	0	Ο
10	D	L L	64	44	6	1	13	0	0

• Molecule 11 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula: C₂H₆O₃S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	С	1	Total 7	$\begin{array}{c} \mathrm{C} \\ \mathrm{2} \end{array}$	$O \\ 3$	${ m S} { m 2}$	0	0
11	F	1	Total 7	С 2	O 3	$\frac{S}{2}$	0	0

• Molecule 12 is (2S)-2-{[(2S)-2-{[(2S)-2-hydroxypropyl]oxy}propyl]oxy}propan-1-ol (three-letter code: UUT) (formula: $C_9H_{20}O_4$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	С	1	Total C O 13 9 4	0	0
12	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 13 9 4 \end{array}$	0	0

• Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	А	628	Total O 628 628	0	63
13	В	574	Total O 574 574	0	96
13	С	345	Total O 345 345	0	26
13	D	642	Total O 642 642	0	84
13	Е	555	Total O 555 555	0	75
13	F	342	Total O 342 342	0	47



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: Ethyl-Coenzyme M reductase alpha subunit





• Molecule 3: Ethyl-Coenzyme M reductase gamma subunit





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	83.74Å 146.93Å 113.13Å	Depositor
a, b, c, α , β , γ	90.00° 106.98° 90.00°	Depositor
Bosolution (Å)	39.76 - 0.99	Depositor
	80.09 - 0.99	EDS
% Data completeness	73.4(39.76-0.99)	Depositor
(in resolution range)	$72.4 \ (80.09 - 0.99)$	EDS
R _{merge}	0.12	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.64 (at 0.99 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
D D.	0.112 , 0.128	Depositor
Π, Π_{free}	0.128 , 0.141	DCC
R_{free} test set	52848 reflections $(5.05%)$	wwPDB-VP
Wilson B-factor (Å ²)	6.2	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.37 , 47.7	EDS
L-test for $twinning^2$	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	25172	wwPDB-VP
Average B, all atoms $(Å^2)$	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.

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.



 $^{^1 {\}rm Intensities}$ 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: MGN, USN, CL, GOL, SMC, HIC, MN, I2M, TP7, TRS, UUT, COM, K, GL3, MHS, AGM

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).

Mal	Mol Chain		nd lengths	Bond angles		
	Cham	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.44	0/4950	0.70	2/6681~(0.0%)	
1	D	0.41	1/4989~(0.0%)	0.72	7/6729~(0.1%)	
2	В	0.39	0/3847	0.67	0/5212	
2	Е	0.42	0/3875	0.68	0/5250	
3	С	0.41	0/2368	0.71	0/3190	
3	F	0.45	2/2374~(0.1%)	0.78	0/3201	
All	All	0.42	3/22403~(0.0%)	0.70	9/30263~(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 mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	1
1	D	0	1
2	Е	0	2
3	С	0	1
3	F	0	4
All	All	0	9

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
1	D	594	PRO	C-N	7.62	1.51	1.34
3	F	178[A]	CYS	CB-SG	-5.43	1.73	1.81
3	F	178[B]	CYS	CB-SG	-5.43	1.73	1.81

All (9) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	D	594	PRO	O-C-N	11.83	141.63	122.70
1	D	304	ARG	NE-CZ-NH2	-8.89	115.86	120.30
1	D	594	PRO	CA-C-N	-8.11	99.35	117.20
1	D	489	TYR	CB-CG-CD1	6.05	124.63	121.00
1	А	304	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	D	489	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	А	485	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	D	243	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	D	485	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

Mol	Chain	\mathbf{Res}	\mathbf{Type}	Group
1	А	304	ARG	Sidechain
3	С	180[A]	MET	Mainchain
1	D	304	ARG	Sidechain
2	Е	429[A]	VAL	Mainchain
2	Е	429[B]	VAL	Mainchain
3	F	186[A]	VAL	Mainchain
3	F	186[B]	VAL	Mainchain
3	F	71[A]	GLU	Mainchain
3	F	71[B]	GLU	Mainchain

All (9) planarity outliers are listed below:

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	4862	0	4669	12	0
1	D	4879	0	4731	14	0
2	В	3737	0	3724	10	0
2	Е	3731	0	3763	7	0
3	С	2299	0	2280	3	0
3	F	2317	0	2264	5	0
4	A	6	0	8	0	0
4	D	6	0	8	0	0
4	Е	12	0	16	1	0
5	A	21	0	19	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	21	0	19	0	0
6	А	1	0	0	0	0
7	А	2	0	0	0	0
7	С	1	0	0	0	0
7	D	1	0	0	0	0
8	В	2	0	0	0	0
8	С	1	0	0	0	0
8	Ε	2	0	0	0	0
8	F	1	0	0	0	0
9	В	8	0	12	0	0
9	Ε	8	0	12	0	0
10	С	64	0	0	0	0
10	D	64	0	0	0	0
11	С	7	0	5	0	0
11	F	7	0	4	0	0
12	С	13	0	0	0	0
12	D	13	0	0	0	0
13	А	628	0	0	0	0
13	В	574	0	0	2	0
13	C	345	0	0	1	0
13	D	642	0	0	2	0
13	E	555	0	0	3	0
13	F	342	0	0	0	0
All	All	25172	0	21534	49	0

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

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
2:B:433[A]:GLU:H	2:B:433[A]:GLU:CD	2.01	0.62
3:C:152:GLN:HE21	3:C:154:ARG:HH21	1.52	0.58
3:C:152:GLN:NE2	3:C:154:ARG:HH21	2.05	0.55
2:E:466[A]:LYS:HG2	2:E:467:PHE:CE1	2.43	0.53
1:A:145:ILE:HG23	2:E:429[A]:VAL:HG11	1.91	0.51
2:B:55[A]:LYS:HD2	2:B:59:THR:HG23	1.93	0.51
2:B:55[A]:LYS:HE3	2:B:59:THR:HG21	1.92	0.50
2:B:55[B]:LYS:HG2	13:B:955[B]:HOH:O	2.12	0.50
4:E:502:GOL:O3	4:E:502:GOL:O1	2.19	0.50
1:D:323[A]:CYS:SG	1:D:567:PHE:CE2	3.06	0.49



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:E:233[A]:LEU:HD22	3:F:69[A]:ILE:HG13	1.95	0.49
2:E:431:GLY:HA2	13:E:655[B]:HOH:O	2.14	0.48
3:F:20[A]:LYS:HG3	3:F:26:VAL:HG11	1.96	0.48
2:B:55[A]:LYS:HD2	2:B:59:THR:CG2	2.44	0.47
1:D:217:ASP:O	1:D:221[B]:MET:HG2	2.14	0.47
1:A:149[A]:THR:OG1	1:A:153:ARG:HD3	2.16	0.46
1:D:270:LEU:HD13	13:D:1495[B]:HOH:O	2.15	0.46
1:D:494:GLN:HA	1:D:497[A]:GLN:HE21	1.80	0.46
2:E:7[B]:LYS:HE2	13:E:663:HOH:O	2.16	0.46
1:D:45[B]:LYS:HE3	1:D:46:ARG:NH1	2.31	0.46
1:A:494:GLN:HA	1:A:497[A]:GLN:HE21	1.81	0.46
3:F:20[B]:LYS:HG3	3:F:26:VAL:HG11	1.97	0.46
1:A:104[A]:LYS:CA	1:A:104[A]:LYS:HZ3	2.30	0.45
1:A:104[A]:LYS:HA	1:A:104[A]:LYS:NZ	2.32	0.44
1:A:138:THR:HG21	1:A:243[A]:ARG:HH21	1.83	0.44
2:E:334:LEU:HG	2:E:416:VAL:HG11	1.99	0.44
1:A:323[A]:CYS:SG	1:A:567:PHE:CE2	3.11	0.43
1:D:206:LEU:HD21	1:D:238[B]:ILE:HD11	2.00	0.43
2:B:334:LEU:HG	2:B:416:VAL:HG11	2.00	0.43
1:A:121:ASN:HA	1:A:374:SER:OG	2.19	0.43
1:A:351:THR:HB	1:A:352:PRO:HD3	2.01	0.42
1:D:3:LYS:HB2	1:D:3:LYS:HE2	1.70	0.42
1:D:149[B]:THR:OG1	1:D:153:ARG:HD3	2.19	0.42
2:B:334:LEU:HD11	2:B:355:LEU:HA	2.03	0.41
2:B:395[A]:SER:HB2	13:B:908:HOH:O	2.19	0.41
2:B:429[A]:VAL:HG11	1:D:145:ILE:HG23	2.02	0.41
3:C:214:ARG:HD3	13:C:1330:HOH:O	2.19	0.41
1:A:297[B]:MET:SD	1:A:554:ILE:HD12	2.61	0.41
1:A:17:MET:HB3	1:A:22[B]:MET:HE1	2.01	0.41
2:B:356[B]:LEU:HD13	2:B:357:TYR:CZ	2.56	0.41
1:D:56[A]:ARG:CZ	1:D:56[A]:ARG:HB2	2.50	0.41
1:D:121:ASN:HA	1:D:374:SER:OG	2.21	0.41
1:D:490:GL3:S	1:D:491:HIC:C	3.09	0.40
2:E:7[B]:LYS:HE3	13:E:781[B]:HOH:O	2.20	0.40
3:F:231:ASP:N	3:F:232:PRO:CD	2.84	0.40
1:A:490:GL3:S	1:A:491:HIC:C	3.10	0.40
1:D:60[A]:GLU:HG3	13:D:1520:HOH:O	2.21	0.40

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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	Percen	ntiles
1	А	614/595~(103%)	597~(97%)	15~(2%)	2(0%)	41	14
1	D	618/595~(104%)	601~(97%)	15~(2%)	2(0%)	41	14
2	В	497/467~(106%)	487 (98%)	10 (2%)	0	100	100
2	Ε	501/467~(107%)	495~(99%)	6 (1%)	0	100	100
3	С	285/266~(107%)	280~(98%)	5(2%)	0	100	100
3	F	287/266~(108%)	280~(98%)	7 (2%)	0	100	100
All	All	2802/2656~(106%)	2740~(98%)	58 (2%)	4 (0%)	51	19

All (4) Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	D	252[A]	SER
1	D	252[B]	SER
1	А	252[A]	SER
1	А	252[B]	SER

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	Percer	ntiles
1	А	499/470~(106%)	486~(97%)	13 (3%)	46	13
1	D	502/470~(107%)	496~(99%)	6 (1%)	71	39
2	В	396/364~(109%)	393~(99%)	3 (1%)	81	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percer	ntiles
2	Ε	400/364~(110%)	393~(98%)	7(2%)	59	25
3	С	258/236~(109%)	253~(98%)	5 (2%)	57	23
3	F	259/236~(110%)	253~(98%)	6 (2%)	50	16
All	All	2314/2140~(108%)	2274 (98%)	40 (2%)	67	27

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All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	42[A]	ARG
1	А	42[B]	ARG
1	А	65	ASN
1	А	72[A]	LEU
1	А	72[B]	LEU
1	А	104[A]	LYS
1	А	104[B]	LYS
1	А	243[A]	ARG
1	А	243[B]	ARG
1	А	258	ARG
1	А	323[A]	CYS
1	А	323[B]	CYS
1	А	489	TYR
2	В	216[A]	MET
2	В	216[B]	MET
2	В	223	HIS
3	С	56	ASN
3	С	70	ARG
3	С	117	ASN
3	С	156	TYR
3	С	257	ASN
1	D	3	LYS
1	D	65	ASN
1	D	258	ARG
1	D	323[A]	CYS
1	D	323[B]	CYS
1	D	489	TYR
2	Е	216[A]	MET
2	Е	216[B]	MET
2	Е	223	HIS
2	E	233[A]	LEU
2	Е	233[B]	LEU
2	Е	254[A]	ILE



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Mol	Chain	Res	Type
2	Е	254[B]	ILE
3	F	56	ASN
3	F	70[A]	ARG
3	F	70[B]	ARG
3	F	117	ASN
3	F	156	TYR
3	F	257	ASN

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)

14 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).

Mal	Tune	Chain	Dec	Tink	Bo	ond leng	ths	Bond angles			
INIOI	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
1	GL3	A	490	1	$2,\!3,\!4$	2.98	1(50%)	1,2,4	0.09	0	
1	MGN	А	445	1	6, 9, 10	0.66	0	$5,\!12,\!14$	0.42	0	
1	HIC	А	491	1	8,11,12	1.26	2(25%)	$6,\!14,\!16$	0.73	0	
1	I2M	А	377	1	6,8,9	1.16	1(16%)	$6,\!11,\!13$	0.90	0	
1	MGN	D	445	1	6, 9, 10	0.66	0	$5,\!12,\!14$	0.30	0	
1	SMC	D	354	1	$5,\!6,\!7$	0.58	0	$2,\!6,\!8$	1.11	0	
1	MHS	А	291	1	7,11,12	0.64	0	$6,\!14,\!16$	1.85	2(33%)	
1	GL3	D	490	1	$2,\!3,\!4$	<mark>3.85</mark>	1(50%)	1,2,4	0.26	0	
1	MHS	D	291	1	7,11,12	0.72	0	6,14,16	1.91	2 (33%)	
1	I2M	D	377	1	6,8,9	0.85	0	$6,\!11,\!13$	0.95	0	
1	AGM	А	305	1	10, 11, 12	0.48	0	$6,\!13,\!15$	0.52	0	
1	HIC	D	491	1	8,11,12	1.04	1 (12%)	$6,\!14,\!16$	0.72	0	



Mal	ol Tuno Chain Bog		Tink	Bo	ond leng	\mathbf{ths}	Bond angles			
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	AGM	D	305	1	10, 11, 12	0.50	0	$6,\!13,\!15$	0.58	0
1	SMC	А	354	1	$5,\!6,\!7$	0.61	0	$2,\!6,\!8$	1.14	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	GL3	А	490	1	-	0/1/1/2	-
1	MGN	А	445	1	-	0/7/9/12	-
1	HIC	А	491	1	-	1/5/6/8	0/1/1/1
1	I2M	А	377	1	-	0/8/11/13	-
1	MGN	D	445	1	-	0/7/9/12	-
1	SMC	D	354	1	-	0/3/5/7	-
1	MHS	А	291	1	-	0/5/6/8	0/1/1/1
1	GL3	D	490	1	-	0/1/1/2	-
1	MHS	D	291	1	-	0/5/6/8	0/1/1/1
1	I2M	D	377	1	-	0/8/11/13	-
1	AGM	А	305	1	-	2/10/11/13	-
1	HIC	D	491	1	-	1/5/6/8	0/1/1/1
1	AGM	D	305	1	-	2/10/11/13	-
1	SMC	А	354	1	-	0/3/5/7	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	D	490	GL3	C-S	-5.44	1.61	1.80
1	А	490	GL3	C-S	-4.21	1.66	1.80
1	А	377	I2M	CB-CA	-2.53	1.53	1.57
1	А	491	HIC	CD2-NE2	-2.30	1.34	1.38
1	А	491	HIC	CD2-CG	2.15	1.39	1.36
1	D	491	HIC	CD2-NE2	-2.04	1.35	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	D	291	MHS	NE2-CE1-ND1	-3.18	107.54	112.26
1	А	291	MHS	NE2-CE1-ND1	-3.00	107.80	112.26
1	А	291	MHS	CB-CA-C	-2.67	106.47	111.47
1	D	291	MHS	CB-CA-C	-2.61	106.57	111.47



There are no chirality outliers.

Mol	Chain	\mathbf{Res}	Type	Atoms
1	А	491	HIC	CA-CB-CG-ND1
1	D	491	HIC	CA-CB-CG-ND1
1	D	305	AGM	CE2-CD-NE1-CZ
1	А	305	AGM	CE2-CD-NE1-CZ
1	А	305	AGM	NE1-CD-CG-CB
1	D	305	AGM	NE1-CD-CG-CB

All (6) torsion outliers are listed below:

There are no ring outliers.

4 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	А	490	GL3	1	0
1	А	491	HIC	1	0
1	D	490	GL3	1	0
1	D	491	HIC	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 11 are monoatomic - leaving 14 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	Dog	Tink	Bo	ond leng	$_{\rm sths}$	Bo	nd angl	d angles RMSZ< $\# Z > 2$ 0.61 0 1.34 1 (10%) 0.36 0	
	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
5	TP7	D	1102	-	16,20,20	0.54	0	$18,\!26,\!26$	0.61	0	
12	UUT	С	305	-	$9,\!12,\!12$	0.74	0	$10,\!14,\!14$	1.34	1 (10%)	
9	TRS	Е	501[A]	-	7,7,7	0.32	0	9,9,9	0.36	0	
4	GOL	Е	505[A]	-	5, 5, 5	0.17	0	5, 5, 5	0.60	0	
12	UUT	D	1105	_	$9,\!12,\!12$	0.54	0	10,14,14	1.12	1 (10%)	





Mal	Tune	Chain	Dog	Tink	Bo	ond leng	\mathbf{ths}	Bond angles			
	туре	Cham	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
4	GOL	А	601	-	5, 5, 5	0.16	0	5, 5, 5	0.24	0	
9	TRS	В	503[A]	-	7,7,7	0.28	0	9,9,9	0.48	0	
10	USN	D	1101	11	47,73,73	2.74	9 (19%)	$51,\!123,\!123$	1.19	<mark>5 (9%)</mark>	
11	COM	С	302	10	6,6,6	0.79	0	7,8,8	0.77	0	
4	GOL	Е	502	-	5, 5, 5	0.27	0	5, 5, 5	0.57	0	
4	GOL	D	1103	-	5, 5, 5	0.09	0	5, 5, 5	0.32	0	
5	TP7	А	602	-	16,20,20	0.64	0	18,26,26	0.65	0	
10	USN	С	301	11	47,73,73	2.67	8 (17%)	$51,\!123,\!123$	1.09	6 (11%)	
11	COM	F	401	10	6,6,6	0.92	0	7,8,8	0.74	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	TP7	D	1102	-	-	0/20/24/24	-
12	UUT	С	305	-	-	2/12/12/12	-
5	TP7	А	602	-	-	0/20/24/24	-
9	TRS	Е	501[A]	-	-	1/9/9/9	-
4	GOL	Е	505[A]	-	-	$\frac{4}{4/4}$	-
12	UUT	D	1105	-	-	2/12/12/12	-
4	GOL	А	601	-	-	4/4/4/4	-
9	TRS	В	503[A]	-	-	4/9/9/9	-
10	USN	D	1101	11	1/1/31/33	0/18/193/193	-
11	COM	С	302	10	-	0/4/4/4	-
4	GOL	D	1103	-	-	3/4/4/4	-
4	GOL	Е	502	-	-	0/4/4/4	-
10	USN	С	301	11	1/1/31/33	0/18/193/193	-
11	COM	F	401	10	-	0/4/4/4	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(\text{\AA})$	Ideal(Å)
10	С	301	USN	NI-NA	11.68	2.14	1.89
10	D	1101	USN	NI-NA	11.14	2.13	1.89
10	D	1101	USN	NI-NB	10.60	2.12	1.89
10	С	301	USN	NI-NB	9.40	2.09	1.89
10	D	1101	USN	NI-ND	7.82	2.06	1.89
10	С	301	USN	NI-ND	7.52	2.05	1.89



Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
10	D	1101	USN	CHC-C4B	2.48	1.46	1.39
10	С	301	USN	C5D-C2D	-2.41	1.50	1.54
10	D	1101	USN	C9A-C2A	2.31	1.58	1.54
10	С	301	USN	C8B-C2B	-2.26	1.50	1.54
10	С	301	USN	C4C-NC	2.25	1.38	1.35
10	С	301	USN	C3A-C4A	2.24	1.57	1.53
10	D	1101	USN	C8B-C2B	-2.19	1.51	1.54
10	D	1101	USN	C2-C2D	2.08	1.58	1.54
10	D	1101	USN	C5D-C2D	-2.07	1.51	1.54
10	Ċ	301	USN	CHC-C4B	2.05	1.45	1.39
10	D	1101	USN	CHC-C1C	-2.04	1.32	1.36

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All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
10	С	301	USN	C2B-C1B-NB	3.56	107.17	101.84
12	С	305	UUT	C3-O1-C1	3.26	119.88	115.02
10	D	1101	USN	C2B-C1B-NB	3.03	106.37	101.84
10	С	301	USN	CAA-CBA-CCA	-2.80	107.57	113.59
10	D	1101	USN	C9A-C2A-C3A	2.78	117.09	112.98
12	D	1105	UUT	C6-O2-C4	-2.43	111.40	115.02
10	С	301	USN	C4B-CHC-C1C	2.24	129.50	125.84
10	D	1101	USN	C4B-CHC-C1C	2.14	129.34	125.84
10	D	1101	USN	CAA-CBA-CCA	-2.09	109.10	113.59
10	С	301	USN	C8C-C9C-CAC	-2.07	109.14	113.59
10	С	301	USN	C3D-C4D-ND	2.06	105.43	102.30
10	D	1101	USN	C2D-C1D-ND	2.04	114.33	111.11
10	С	301	USN	C9A-C2A-C3A	2.02	115.96	112.98

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom	
10	С	301	USN	NC	
10	D	1101	USN	NC	

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Е	505[A]	GOL	O1-C1-C2-C3
4	Е	505[A]	GOL	C1-C2-C3-O3
9	В	503[A]	TRS	N-C-C1-O1
9	В	503[A]	TRS	C1-C-C2-O2



$7\mathrm{B}$	1S
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Mol	Chain	Res	Type	Atoms
9	В	503[A]	TRS	C3-C-C2-O2
9	В	503[A]	TRS	N-C-C2-O2
12	С	305	UUT	O-C-C1-O1
12	D	1105	UUT	C2-C1-O1-C3
4	А	601	GOL	O1-C1-C2-C3
4	D	1103	GOL	O1-C1-C2-C3
4	Е	505[A]	GOL	O1-C1-C2-O2
4	Е	505[A]	GOL	O2-C2-C3-O3
12	D	1105	UUT	C4-C3-O1-C1
4	А	601	GOL	O2-C2-C3-O3
4	D	1103	GOL	O2-C2-C3-O3
12	С	305	UUT	O-C-C1-C2
4	А	601	GOL	O1-C1-C2-O2
4	А	601	GOL	C1-C2-C3-O3
4	D	1103	GOL	O1-C1-C2-O2
9	Е	501[A]	TRS	C3-C-C1-O1

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There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Ε	502	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.























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	$\mathbf{OWAB}(\mathbf{\AA}^2)$	$Q{<}0.9$
1	А	584/595~(98%)	-0.19	2 (0%) 94 88	4, 7, 14, 31	0
1	D	586/595~(98%)	-0.18	4 (0%) 87 82	4,6,14,35	0
2	В	466/467~(99%)	-0.16	7 (1%) 73 65	4,8,17,32	0
2	Е	466/467~(99%)	-0.18	0 100 100	4, 7, 15, 24	0
3	С	265/266~(99%)	-0.01	8 (3%) 50 41	6,11,21,30	0
3	F	265/266~(99%)	-0.02	9 (3%) 45 36	4, 9, 19, 28	0
All	All	2632/2656~(99%)	-0.14	30 (1%) 80 74	4,8,17,35	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	2	VAL	7.9
1	А	5	PRO	6.3
3	С	2	VAL	5.5
1	D	3	LYS	4.5
1	D	337	ASP	3.9
3	С	179[A]	ILE	3.7
3	С	197[A]	ASP	3.7
3	С	182	GLY	3.4
2	В	88	TYR	3.3
3	F	71[A]	GLU	3.2
2	В	84	PRO	3.2
3	С	178[A]	CYS	3.0
2	В	85	GLY	3.0
3	F	69[A]	ILE	3.0
1	D	42[A]	ARG	3.0
1	D	4	TYR	2.8
3	С	195	PRO	2.7
1	A	42[A]	ARG	2.6
3	F	62	ILE	2.6



Mol	Chain	Res	Type	RSRZ
2	В	122	ASP	2.6
3	F	197[A]	ASP	2.6
3	F	179[A]	ILE	2.5
3	F	180[A]	MET	2.4
2	В	87	LYS	2.2
3	F	195	PRO	2.2
2	В	2	ALA	2.2
3	С	180[A]	MET	2.1
3	F	182	GLY	2.1
2	В	86	GLY	2.0
3	С	199	PRO	2.0

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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	B-factors(Å ²)	Q<0.9
1	MHS	А	291	11/12	0.99	0.06	4,5,6,6	0
1	MHS	D	291	11/12	0.99	0.06	5, 5, 6, 7	0
1	AGM	А	305	12/13	0.99	0.07	4,5,5,6	0
1	AGM	D	305	12/13	0.99	0.06	4,5,5,6	0
1	I2M	А	377	9/10	0.99	0.06	5, 5, 8, 9	0
1	I2M	D	377	9/10	0.99	0.08	4,4,7,9	0
1	MGN	А	445	10/11	0.99	0.06	5, 6, 6, 6	0
1	MGN	D	445	10/11	0.99	0.07	4,4,4,5	0
1	HIC	А	491	11/12	0.99	0.07	4,5,5,5	0
1	HIC	D	491	11/12	0.99	0.07	3,4,4,4	0
1	GL3	А	490	4/5	1.00	0.07	4,5,5,5	0
1	GL3	D	490	4/5	1.00	0.07	3, 3, 4, 4	0
1	SMC	А	354	7/8	1.00	0.06	$4,5,\!6,\!8$	0
1	SMC	D	354	7/8	1.00	0.06	4,4,5,7	0

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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
4	GOL	Е	502	6/6	0.62	0.23	$35,\!36,\!36,\!36$	0
4	GOL	Е	505[A]	6/6	0.62	0.34	$14,\!17,\!18,\!19$	6
4	GOL	D	1103	6/6	0.64	0.26	$39,\!40,\!40,\!40$	0
4	GOL	А	601	6/6	0.71	0.16	$38,\!39,\!39,\!39$	0
9	TRS	Е	501[A]	8/8	0.83	0.22	$10,\!15,\!16,\!18$	8
12	UUT	С	305	13/13	0.91	0.14	14,22,28,29	0
9	TRS	В	503[A]	8/8	0.93	0.10	12,13,14,14	8
12	UUT	D	1105	13/13	0.95	0.14	11,20,28,29	0
7	K	А	605[A]	1/1	0.97	0.09	14,14,14,14	1
7	K	А	604	1/1	0.98	0.10	19,19,19,19	0
8	CL	F	402	1/1	0.98	0.08	$31,\!31,\!31,\!31$	0
5	TP7	D	1102	21/21	0.99	0.06	4,5,6,7	0
8	CL	С	303	1/1	0.99	0.09	$31,\!31,\!31,\!31$	0
10	USN	С	301	64/64	0.99	0.06	4,5,8,9	0
10	USN	D	1101	64/64	0.99	0.07	$3,\!4,\!6,\!7$	0
8	CL	Е	504	1/1	0.99	0.05	8,8,8,8	1
5	TP7	А	602	21/21	0.99	0.06	$5,\!6,\!7,\!7$	0
8	CL	В	501	1/1	1.00	0.04	$11,\!11,\!11,\!11$	0
8	CL	В	502	1/1	1.00	0.05	8,8,8,8	1
6	MN	А	603	1/1	1.00	0.04	8,8,8,8	0
8	CL	Е	503	1/1	1.00	0.04	$10,\!10,\!10,\!10$	0
11	COM	С	302	7/7	1.00	0.05	5,6,6,7	0
11	COM	F	401	7/7	1.00	0.06	4,4,6,6	0
7	K	С	304	1/1	1.00	0.09	$15,\!15,\!15,\!15$	0
7	K	D	1104[A]	1/1	1.00	0.04	12,12,12,12	1

6.5 Other polymers (i)

There are no such residues in this entry.

