

wwPDB X-ray Structure Validation Summary Report (i)

Nov 29, 2023 – 09:59 pm GMT

PDB ID	:	7NPA
Title	:	Crystal structure of the Coenzyme F420-dependent sulfite reductase from
		Methanothermococcus thermolithotrophicus at 1.55-A resolution
Authors	:	Jespersen, M.; Wagner, T.
Deposited on	:	2021-02-26
Resolution	:	1.55 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 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

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 1.55 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.



Matria	Whole archive	Similar resolution		
Metric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
R_{free}	130704	1483 (1.56-1.56)		
Clashscore	141614	1529 (1.56-1.56)		
Ramachandran outliers	138981	1498 (1.56-1.56)		
Sidechain outliers	138945	1495 (1.56-1.56)		
RSRZ outliers	127900	1465 (1.56-1.56)		

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	٨	619		
1	A	018	95%	5%
1	В	618	94%	6%
1	С	618	96%	.
		010	2%	-
1	D	618	92%	8%
	-		3%	
1	E	618	91%	9%



Mol	Chain	Length	Quality of chain	
1	F	618	93%	6%
1	G	618	2% 	6%
1	Н	618	94%	6%
1	Ι	618	94%	6%
1	J	618	93%	6%
1	K	618	94%	5%
1	L	618	94%	6%
1	М	618	95%	•
1	Ν	618	82%	17%
1	Ο	618	93%	6%
1	Р	618	93%	6%

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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
2	SF4	N	1006[A]	-	-	Х	-
2	SF4	N	1007[A]	-	-	Х	-
5	SRM	A	1109	X	-	-	-
5	SRM	В	4210	X	-	-	-
5	SRM	С	3910	X	-	-	-
5	SRM	D	4610	X	-	-	-
5	SRM	Е	1109	Х	-	-	-
5	SRM	F	1109	X	-	-	-
5	SRM	G	1109	Х	-	-	-
5	SRM	Н	4410	X	-	-	-
5	SRM	Ι	1109	Х	-	-	-
5	SRM	J	1109	Х	-	-	-
5	SRM	K	1109	Х	-	-	-
5	SRM	L	1109	Х	-	-	-
5	SRM	М	1109	Х	-	-	-
5	SRM	N	1012	Х	-	-	-
5	SRM	0	1109	Х	-	-	-
5	SRM	Р	1109	Х	-	-	-



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2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 93689 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.

Mol	Chain	Residues		At	toms			ZeroOcc	AltConf	Trace
1	А	618	Total 4869	C 3083	N 820	0 925	S 41	0	4	0
1	В	618	Total 4863	C 3081	N 821	O 920	S 41	0	3	0
1	С	618	Total 4862	C 3079	N 820	O 922	S 41	0	3	0
1	D	617	Total 4838	C 3064	N 816	O 918	S 40	0	1	0
1	Е	617	Total 4845	C 3068	N 817	O 920	S 40	0	2	0
1	F	618	Total 4877	C 3090	N 823	O 923	S 41	0	5	0
1	G	618	Total 4858	C 3077	N 819	O 920	S 42	0	3	0
1	Н	617	Total 4843	C 3067	N 817	O 918	S 41	0	2	0
1	Ι	618	Total 4863	C 3081	N 821	O 920	S 41	0	3	0
1	J	618	Total 4855	C 3075	N 819	O 920	S 41	0	2	0
1	K	617	Total 4845	C 3068	N 817	O 920	S 40	0	2	0
1	L	617	Total 4847	C 3070	N 819	O 918	S 40	0	2	0
1	М	617	Total 4837	C 3064	N 816	O 917	S 40	0	1	0
1	N	616	Total 6587	C 4178	N 1095	O 1263	S 51	0	266	0
1	О	617	Total 4837	C 3064	N 816	0 917	S 40	0	1	0
1	Р	617	Total 4837	C 3064	N 816	0 917	\overline{S} 40	0	1	0

• Molecule 1 is a protein called Coenzyme F420-dependent sulfite reductase.



• Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	TotalFeS844	0	0
2	А	1	TotalFeS844	0	0
2	А	1	TotalFeS844	0	0
2	А	1	TotalFeS844	0	0
2	А	1	TotalFeS844	0	0
2	А	1	TotalFeS844	0	0
2	В	1	TotalFeS844	0	0
2	В	1	TotalFeS844	0	0
2	В	1	TotalFeS844	0	0
2	В	1	TotalFeS844	0	0
2	В	1	TotalFeS844	0	0
2	В	1	TotalFeS844	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	С	1	TotalFeS844	0	0
2	С	1	Total Fe S 8 4 4	0	0
2	С	1	TotalFeS844	0	0
2	С	1	TotalFeS844	0	0
2	С	1	TotalFeS844	0	0
2	С	1	TotalFeS844	0	0
2	D	1	TotalFeS844	0	0
2	D	1	TotalFeS844	0	0
2	D	1	TotalFeS844	0	0
2	D	1	TotalFeS844	0	0
2	D	1	TotalFeS844	0	0
2	D	1	TotalFeS844	0	0
2	Е	1	TotalFeS844	0	0
2	Е	1	TotalFeS844	0	0
2	Е	1	TotalFeS844	0	0
2	Е	1	TotalFeS844	0	0
2	Е	1	TotalFeS844	0	0
2	Е	1	TotalFeS844	0	0
2	F	1	TotalFeS844	0	0
2	F	1	TotalFeS844	0	0
2	F	1	TotalFeS844	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total Fe S 8 4 4	0	0
2	F	1	Total Fe S 8 4 4	0	0
2	F	1	Total Fe S 8 4 4	0	0
2	G	1	Total Fe S 8 4 4	0	0
2	G	1	TotalFeS844	0	0
2	G	1	TotalFeS844	0	0
2	G	1	TotalFeS844	0	0
2	G	1	TotalFeS844	0	0
2	G	1	TotalFeS844	0	0
2	Н	1	TotalFeS844	0	0
2	Н	1	TotalFeS844	0	0
2	Н	1	Total Fe S 8 4 4	0	0
2	Н	1	Total Fe S 8 4 4	0	0
2	Н	1	TotalFeS844	0	0
2	Н	1	Total Fe S 8 4 4	0	0
2	Ι	1	Total Fe S 8 4 4	0	0
2	Ι	1	Total Fe S 8 4 4	0	0
2	Ι	1	TotalFeS844	0	0
2	Ι	1	TotalFeS844	0	0
2	Ι	1	TotalFeS844	0	0
2	Ι	1	TotalFeS844	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	J	1	Total Fe S 8 4 4	0	0
2	J	1	Total Fe S 8 4 4	0	0
2	J	1	Total Fe S 8 4 4	0	0
2	J	1	Total Fe S 8 4 4	0	0
2	J	1	TotalFeS844	0	0
2	J	1	Total Fe S 8 4 4	0	0
2	K	1	TotalFeS844	0	0
2	К	1	Total Fe S 8 4 4	0	0
2	К	1	TotalFeS844	0	0
2	К	1	TotalFeS844	0	0
2	К	1	TotalFeS844	0	0
2	K	1	TotalFeS844	0	0
2	L	1	TotalFeS844	0	0
2	L	1	TotalFeS844	0	0
2	L	1	TotalFeS844	0	0
2	L	1	TotalFeS844	0	0
2	L	1	TotalFeS844	0	0
2	L	1	TotalFeS844	0	0
2	М	1	TotalFeS844	0	0
2	М	1	TotalFeS844	0	0
2	М	1	TotalFeS844	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	М	1	Total Fe S 8 4 4	0	0
2	М	1	Total Fe S 8 4 4	0	0
2	М	1	Total Fe S 8 4 4	0	0
2	N	1	Total Fe S 8 4 4	0	0
2	Ν	1	Total Fe S 8 4 4	0	0
2	Ν	1	Total Fe S 8 4 4	0	0
2	Ν	1	Total Fe S 8 4 4	0	0
2	Ν	1	Total Fe S 16 8 8	0	1
2	N	1	Total Fe S 8 4 4	0	1
2	N	1	Total Fe S 8 4 4	0	1
2	0	1	Total Fe S 8 4 4	0	0
2	0	1	Total Fe S 8 4 4	0	0
2	0	1	Total Fe S 8 4 4	0	0
2	О	1	Total Fe S 8 4 4	0	0
2	О	1	Total Fe S 8 4 4	0	0
2	0	1	Total Fe S 8 4 4	0	0
2	Р	1	TotalFeS844	0	0
2	Р	1	TotalFeS844	0	0
2	Р	1	TotalFeS844	0	0
2	Р	1	TotalFeS844	0	0
2	Р	1	TotalFeS844	0	0



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Mol	Chain	Residues	Ate	\mathbf{oms}		ZeroOcc	AltConf
2	Р	1	Total 8	Fe 4	$\frac{S}{4}$	0	0

• Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf		
3	Λ	1	Total	С	Ν	Ο	Р	0	0		
0	Л	1	53	27	9	15	2	0	0		
3	В	1	Total	С	Ν	Ο	Р	0	0		
0	D	1	53	27	9	15	2	0	0		
3	С	1	Total	С	Ν	Ο	Р	0	0		
0	U	1	53	27	9	15	2	0	0		
3	Л	1	Total	С	Ν	Ο	Р	0	0		
0	D	T	53	27	9	15	2		0		
3	Е	\mathbf{E}	E	1	Total	\mathbf{C}	Ν	Ο	Р	0	0
0		I	53	27	9	15	2				
3	F	F	1	Total	\mathbf{C}	Ν	Ο	Р	0	0	
0		1	53	27	9	15	2	0	0		
3	G	3 G	1	Total	С	Ν	Ο	Р	0	0	
0	<u>u</u>	1	53	27	9	15	2	0	0		
3	н	1	Total	С	Ν	Ο	Р	0	0		
0	11	I	53	27	9	15	2	0	0		
3	T	1	Total	\mathbf{C}	Ν	Ο	Р	0	0		
J	L	1	53	27	9	15	2	0	0		
3	I	1	Total	\mathbf{C}	Ν	Ο	Р	0	0		
3	J	1	53	27	9	15	2	U			



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	V	1	Total C N O P	0	0
3	Λ	1	53 27 9 15 2	0	0
2	L	1	Total C N O P	0	0
່ <u>ບ</u>		1	53 27 9 15 2	0	0
2	3 M	1	Total C N O P	0	0
5		1	53 27 9 15 2	0	0
3	N	1	Total C N O P	0	1
J			53 27 9 15 2	0	1
3	Ν	1	Total C N O P	0	1
5	11	T	53 27 9 15 2	0	L
3	0	O 1	Total C N O P	0	0
5			53 27 9 15 2	0	0
3	Р	1	Total C N O P	0	0
0	L	L	53 27 9 15 2	0	

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• Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{c cc} \hline \text{Total} & \text{C} & \text{O} \\ \hline 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	1
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	1
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	1
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	Е	1	$\begin{array}{c c} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	Е	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	F	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	F	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	1
4	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	1
4	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	G	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	G	1	$\begin{array}{c c} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	Н	1	$\begin{array}{c ccc} \hline \text{Total} & \text{C} & \text{O} \\ \hline 4 & 2 & 2 \end{array}$	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	Н	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	Ι	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	Ι	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	Ι	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	Ι	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	Ι	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	Ι	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	Ι	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	Ι	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	J	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	J	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	J	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	J	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	J	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	J	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	J	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	К	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	K	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	К	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	K	1	$\begin{array}{c cc} \hline \text{Total} & \text{C} & \text{O} \\ \hline 4 & 2 & 2 \end{array}$	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	К	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	К	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	K	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	L	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	L	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	L	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	L	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	М	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	М	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	М	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	М	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	М	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	М	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	М	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	М	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	М	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	М	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	М	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	М	1	$\begin{array}{c c} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	М	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	Ν	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	N	1	Total C O	0	0
			4 2 2 Total C O		
4	Ο	1	$\begin{array}{cccc} 10tal & 0 \\ 4 & 2 & 2 \end{array}$	0	0
4	0	1	Total C O	0	0
		_	4 2 2		0
4	0	1	$\begin{array}{c cc} Total & C & O \\ 4 & 2 & 2 \end{array}$	0	0
1	0	1	Total C O	0	0
		T	4 2 2	0	
4	0	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	0	1	Total C O	0	0
			4 2 2		
4	0	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	0	1	Total C O	0	0
	Ŭ	-	4 2 2	Ŭ	Ŭ
4	Ο	1	Total C O 4 2 2	0	0
			$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		
4	Р	1	4 2 2	0	0

Total

Total

Total

С

С

С

Ο

 $\mathbf{2}$

 α tio d fa

Р

Р

Р

• Molecule 5 is SIROHEME (three-letter code: SRM) (formula: $C_{42}H_{44}FeN_4O_{16}$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		At	oms			ZeroOcc	AltConf		
F	٨	1	Total	С	Fe	Ν	0	0	0		
6	А	1	63	42	1	4	16	0	0		
-	р	1	Total	С	Fe	Ν	0	0	0		
5	D	1	63	42	1	4	16	0	0		
5	C	1	Total	С	Fe	Ν	0	0	0		
0	U	1	63	42	1	4	16	0	0		
F	л	1	Total	С	Fe	Ν	0	0	0		
0	D	1	63	42	1	4	16	0	0		
5	Б	1	Total	С	Fe	Ν	0	0	0		
0	Ľ	1	63	42	1	4	16	0	0		
5	Б	1	Total	С	Fe	Ν	0	0	0		
0	Г	L	63	42	1	4	16	0			
5	5 G	1	Total	С	Fe	Ν	0	0	0		
0		1	63	42	1	4	16	0	0		
5	Ц	н	н	1	Total	С	Fe	Ν	0	0	0
0	11	1	63	42	1	4	16	0	0		
5	т	T	1	Total	С	Fe	Ν	0	0	0	
0	1	1	63	42	1	4	16	0	0		
5	т	1	Total	С	Fe	Ν	0	0	0		
0	1	1	63	42	1	4	16	0	0		
5	K	1	Total	С	Fe	Ν	0	0	0		
0	Γ	1	63	42	1	4	16	0	0		
5	т	1	Total	С	Fe	Ν	0	0	0		
0		1	63	42	1	4	16	0	0		
5	5 M	1	Total	С	Fe	Ν	0	0	0		
5		1	63	42	1	4	16		U		
5	N	1	Total	С	Fe	Ν	0	0	0		
5	IN	N	1	63	42	1	4	16	0	U	



$\alpha \cdot \cdot \cdot$	C		
Continued	trom	previous	page
	5	1	1 0

Mol	Chain	Residues		At	\mathbf{oms}			ZeroOcc	AltConf	
5	0	1	Total	С	Fe	Ν	0	0	0	
	Ŭ	-	63	42	1	4	16	Ŭ	U U	
F	D	1	Total	С	Fe	Ν	0	0	0	
5	I.		63	42	1	4	16	0	0	



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	Δ	1	Total O S	0	0
0	Π	T	5 4 1	0	
6	В	1	Total O S	0	0
0	D	1	5 4 1	0	0
6	В	1	Total O S	0	0
0		1	5 4 1		0
6	С	1	Total O S	0	0
0	0	1	5 4 1		0
6	D	1	Total O S	0	0
	D	Ĩ	5 4 1		Ŭ
6	D	1	Total O S	0	0
	D	Ĩ	5 4 1		Ŭ
6	D	1	Total O S	0	0
	D	I.	5 4 1		
6	E	1	Total O S	0	0
		1	5 4 1		
6	F	1	Total O S	0	0
	1	*	5 4 1		



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
C	F	1	Total O S	0	0
6	F	1	5 4 1	0	0
-			Total O S	0	0
6	F,	1	5 4 1	0	0
			Total O S		
6	F,	1	5 4 1	0	0
	~		Total O S		
6	G	1	5 4 1	0	0
			Total O S		
6	Н	1	5 4 1	0	0
			Total O S		
6	Н	1	5 4 1	0	0
			Total O S		
6	Ι	1	5 4 1	0	0
			5 + 1 Total O S		
6	J	1	5 4 1	0	0
			Total O S		
6	J	1	$\begin{bmatrix} 10tal & 0 & 5 \\ 5 & 4 & 1 \end{bmatrix}$	0	0
6	Κ	1	Total O S	0	0
			5 4 1		
6	Κ	1	Total O S	0	0
			5 4 1		
6	L	1	Total O S	0	0
			5 4 1		
6	L	1	Total O S	0	0
	-	-	5 4 1	Ŭ	
6	L	1	Total O S	0	0
		T	5 4 1	0	0
6	М	1	Total O S	0	0
0	111	I	5 4 1	0	0
6	М	1	Total O S	0	0
0	111	1	$5 \ 4 \ 1$	0	0
6	М	1	Total O S	0	0
0	111	1	$5 \ 4 \ 1$	0	0
G	N	1	Total O S	0	0
0	1N		5 4 1		
C	0	1	Total O S	0	0
0	U	1	5 4 1		U
6	0	- 1	Total O S	0	6
6	U		5 4 1	0	0
			Total O S		
6	Р		5 4 1	0	0



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Mol	Chain	Residues	Atom	\mathbf{s}	ZeroOcc	AltConf
6	Р	1	Total C 5 4	${ m S}$	0	0

• Molecule 7 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H₂S) (labeled as "Ligand of Interest" by depositor).

H2S	
H ₂ S	S

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	1	Total S 1 1	0	0
7	В	1	Total S 1 1	0	0
7	С	1	Total S 1 1	0	0
7	D	1	Total S 1 1	0	0
7	Е	1	Total S 1 1	0	0
7	F	1	Total S 1 1	0	0
7	G	1	Total S 1 1	0	0
7	Н	1	Total S 1 1	0	0
7	Ι	1	Total S 1 1	0	0
7	J	1	Total S 1 1	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	K	1	Total S 1 1	0	0
7	L	1	Total S 1 1	0	0
7	М	1	Total S 1 1	0	0
7	Ν	1	Total S 1 1	0	0
7	О	1	Total S 1 1	0	0
7	Р	1	Total S 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	2	Total Cl 2 2	0	1
8	В	2	Total Cl 2 2	0	1
8	С	2	Total Cl 2 2	0	1
8	D	2	Total Cl 2 2	0	1
8	Е	2	Total Cl 2 2	0	1
8	F	1	Total Cl 1 1	0	1
8	G	2	Total Cl 2 2	0	1
8	Н	2	Total Cl 2 2	0	1
8	Ι	2	Total Cl 2 2	0	1
8	J	2	Total Cl 2 2	0	1
8	K	2	Total Cl 2 2	0	1
8	L	1	Total Cl 1 1	0	1
8	М	2	Total Cl 2 2	0	1



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	Ν	1	Total Cl 1 1	0	1
8	О	2	Total Cl 2 2	0	1
8	Р	2	Total Cl 2 2	0	1

• Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	В	1	Total C O	0	1
9	В	1	Total C O	0	1
		-	$\begin{array}{ccc} 6 & 3 & 3 \\ \hline \text{Total} & C & O \end{array}$	Ŭ	-
9	В	1	6 3 3	0	0
9	С	1	Total C O	0	0
9	С	1	Total C O	0	0
0	E	1	$\begin{array}{ccc} 6 & 3 & 3 \\ \hline \text{Total} & \text{C} & \text{O} \end{array}$	0	0
9	E	1	6 3 3	0	0
9	F	1	$\begin{bmatrix} Total & C & O \\ 6 & 3 & 3 \end{bmatrix}$	0	0
9	G	1	Total C O	0	1
			0 3 3		



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	Ι	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
9	Ι	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
9	J	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
9	J	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	1
9	К	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
9	М	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
9	Ν	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
9	Ν	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
9	О	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
9	Р	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
9	Р	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 10 is LITHIUM ION (three-letter code: LI) (formula: Li).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	С	1	Total Li 1 1	0	0
10	F	1	Total Li 1 1	0	0
10	L	1	Total Li 1 1	0	0
10	Р	1	Total Li 1 1	0	0

• Molecule 11 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $\rm C_4H_{10}O_3).$





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
11	K	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
11	М	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
11	М	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
11	Ν	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0

• Molecule 12 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
12	Н	1	Total C N O 8 4 1 3	0	0
12	Ι	1	Total C N O 8 4 1 3	0	0

• Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	А	800	Total O 800 800	0	6
13	В	744	Total O 744 744	0	4
13	С	762	Total O 762 762	0	0
13	D	713	Total O 713 713	0	5
13	Е	645	Total O 645 645	0	0
13	F	605	Total O 605 605	0	0
13	G	748	Total O 748 748	0	3
13	Н	685	Total O 685 685	0	0
13	Ι	704	Total O 704 704	0	7
13	J	567	Total O 567 567	0	1



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	К	766	Total O 766 766	0	1
13	L	681	Total O 681 681	0	3
13	М	690	Total O 690 690	0	2
13	Ν	465	Total O 465 465	0	12
13	Ο	665	Total O 665 665	0	2
13	Р	532	Total O 532 532	0	0



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: Coenzyme F420-dependent sulfite reductase











K553 MI 4565 K565 V23 K565 V23 K569 E53 G594 S59 E609 K61 K71 55 K71 55 K71 1 E616 94 M27 N131 125 N239 125 N25

• Molecule 1: Coenzyme F420-dependent sulfite reductase



• Molecule 1: Coenzyme F420-dependent sulfite reductase



• Molecule 1: Coenzyme F420-dependent sulfite reductase





• Molecule 1: Coenzyme F420-dependent sulfite reductase







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	113.15Å 124.16Å 241.06Å	Deperitor
a, b, c, α , β , γ	102.28° 95.71° 90.25°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	77.29 - 1.55	Depositor
Resolution (A)	$121.27 \ - \ 1.55$	EDS
% Data completeness	75.5 (77.29-1.55)	Depositor
(in resolution range)	$75.5\ (121.27-1.55)$	EDS
R _{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.74 (at 1.55 Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
P.P.	0.159 , 0.171	Depositor
n, n_{free}	0.164 , 0.175	DCC
R_{free} test set	69216 reflections $(4.96%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	13.8	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.35 , 47.4	EDS
L-test for twinning ²	$< L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	0.010 for -h,k,-k-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	93689	wwPDB-VP
Average B, all atoms $(Å^2)$	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 14.18% 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.



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: LI, CL, SF4, SRM, TRS, FAD, PEG, SO4, GOL, EDO, H2S

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	Chain	Bond lengths		Bond angles	
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.42	0/4946	0.60	0/6639
1	В	0.44	0/4940	0.60	0/6628
1	С	0.42	0/4939	0.58	0/6628
1	D	0.43	0/4915	0.59	0/6596
1	Е	0.44	0/4922	0.59	0/6607
1	F	0.42	0/4954	0.58	0/6648
1	G	0.45	0/4935	0.60	0/6624
1	Н	0.42	0/4920	0.57	0/6604
1	Ι	0.42	0/4940	0.59	0/6628
1	J	0.41	0/4932	0.57	0/6617
1	Κ	0.42	0/4922	0.60	0/6607
1	L	0.41	0/4925	0.58	0/6612
1	М	0.44	0/4914	0.60	0/6596
1	Ν	0.46	0/6693	0.57	0/8982
1	0	0.42	0/4914	0.58	0/6596
1	Р	0.45	0/4914	0.58	0/6596
All	All	0.43	0/80625	0.59	0/108208

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.



1 T A T T T T

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	4869	0	4909	25	0
1	В	4863	0	4917	35	0
1	С	4862	0	4908	19	0
1	D	4838	0	4881	35	0
1	Е	4845	0	4884	36	0
1	F	4877	0	4931	27	0
1	G	4858	0	4906	31	0
1	Н	4843	0	4885	29	0
1	Ι	4863	0	4917	28	0
1	J	4855	0	4905	34	0
1	Κ	4845	0	4884	24	0
1	L	4847	0	4888	25	0
1	М	4837	0	4881	21	0
1	Ν	6587	0	6651	104	0
1	0	4837	0	4881	30	0
1	Р	4837	0	4881	31	0
2	А	48	0	0	2	0
2	В	48	0	0	2	0
2	С	48	0	0	0	0
2	D	48	0	0	1	0
2	Е	48	0	0	1	0
2	F	48	0	0	0	0
2	G	48	0	0	2	0
2	Н	48	0	0	1	0
2	Ι	48	0	0	0	0
2	J	48	0	0	1	0
2	K	48	0	0	0	0
2	L	48	0	0	0	0
2	М	48	0	0	2	0
2	N	64	0	0	5	0
2	0	48	0	0	1	0
2	Р	48	0	0	1	0
3	А	53	0	31	0	0
3	B	53	0	31	0	0
3	С	53	0	31	0	0
3	D	53	0	31	1	0
3	Е	53	0	31	1	0
3	F	53	0	31	0	0
3	G	53	0	31	0	0
3	H	53	0	31	0	0
3	I	53	0	31	1	0
3	J	53	0	31	0	0
3	K	53	0	31	1	0



7	Ν	F)/	1
•	τ,	T.	4	r

	Chain	Non-H	$\frac{page}{\mathbf{H}(\mathbf{modol})}$	H(addod)	Clashos	Symm_Clashos
2	T	52				Symm-Clashes
0 9		50	0	01 91	0	0
3 2	N	106	0	62	0	0
່ <u>ບ</u>		52	0	21	0	0
0 9	D	50	0	01 91	0	0
3	Г		0	51 60	2	0
4	A	40	0	00	2	0
4	B	0Z	0	18	2	0
4		32	0	48	1	0
4		30	0	34	1	0
4	E	32	0	48	1	0
4	F C	20	0	30	2	0
4	G	48	0	72	4	0
4	H	16	0	24	4	0
4	l	32	0	48	1	0
4	J	28	0	42	4	0
4	K	28	0	42	1	0
4	L	16	0	24	0	0
4	М	52	0	78	0	0
4	N	8	0	12	0	0
4	0	36	0	54	0	0
4	Р	16	0	24	0	0
5	A	63	0	34	0	0
5	В	63	0	34	0	0
5	С	63	0	34	0	0
5	D	63	0	34	0	0
5	E	63	0	34	1	0
5	F	63	0	34	1	0
5	G	63	0	34	0	0
5	Н	63	0	34	0	0
5	Ι	63	0	34	0	0
5	J	63	0	34	0	0
5	K	63	0	34	0	0
5	L	63	0	34	0	0
5	М	63	0	34	1	0
5	Ν	63	0	34	1	0
5	0	63	0	34	1	0
5	Р	63	0	34	0	0
6	А	5	0	0	0	0
6	В	10	0	0	1	0
6	С	5	0	0	0	0
6	D	15	0	0	0	0
6	Е	5	0	0	0	0

Continued from previous page...



MoiChamNon-HH(model)H(added)ClashesSymm-Clashes6F2000106G500006H1000006J1000006K1000006L1500006M1500006M500006N500006P1000006P1000007A100007B100007F100007F100007F100007H100007H100007H100007H100007H100007H100007H100007H100007			i previous	puye	TT (11 1)		
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	6	F	20	0	0	1	0
6 H 10 0 0 0 0 6 J 10 0 0 0 0 6 J 10 0 0 0 0 6 K 10 0 0 0 0 6 L 15 0 0 0 0 6 M 15 0 0 0 0 6 N 5 0 0 0 0 6 N 5 0 0 0 0 6 N 10 0 0 0 0 7 B 1 0 0 0 0 7 D 1 0 0 0 0 7 D 1 0 0 0 0 7 D 1 0 0 0 0 7 D 0	6	G	5	0	0	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	6	H	10	0	0	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	6	I	5	0	0	0	0
6 K 10 1 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 1 1 1 1 1 1 1 1	6	J	10	0	0	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	6	K	10	0	0	0	0
	6	L	15	0	0	0	0
6 N 5 0 0 0 0 0 6 P 10 0 0 0 0 0 7 A 1 0 0 0 0 0 7 B 1 0 0 0 0 0 7 B 1 0 0 0 0 0 7 D 1 0 0 0 0 0 7 D 1 0 0 0 0 0 7 F 1 0 0 0 0 7 F 1 0 0 0 0 7 H 1 0 0 0 0 7 H 1 0 0 0 0 7 K 1 0 0 0 0 7 N <t< td=""><td>6</td><td>М</td><td>15</td><td>0</td><td>0</td><td>0</td><td>0</td></t<>	6	М	15	0	0	0	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	6	N	5	0	0	0	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	6	0	10	0	0	0	0
7 A 1 0 0 0 0 0 7 B 1 0 0 0 0 0 7 C 1 0 0 0 0 0 7 D 1 0 0 0 0 0 7 E 1 0 0 0 0 0 7 F 1 0 0 0 0 0 7 G 1 0 0 0 0 0 7 H 1 0 0 0 0 0 7 H 1 0 0 0 0 0 7 K 1 0 0 0 0 0 7 N 1 0 0 0 0 0 7 N 1 0 0 0 0 </td <td>6</td> <td>Р</td> <td>10</td> <td>0</td> <td>0</td> <td>0</td> <td>0</td>	6	Р	10	0	0	0	0
7 B 1 0 0 0 0 7 C 1 0 0 0 0 0 7 D 1 0 0 0 0 0 7 E 1 0 0 0 0 0 7 F 1 0 0 0 0 0 7 G 1 0 0 0 0 0 7 H 1 0 0 0 0 0 7 I 1 0 0 0 0 0 7 J 1 0 0 0 0 0 7 K 1 0 0 0 0 0 7 M 1 0 0 0 0 0 7 N 1 0 0 0 0 0	7	А	1	0	0	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	В	1	0	0	0	0
7 D 1 0 0 0 0 7 E 1 0 0 0 0 7 F 1 0 0 0 0 7 G 1 0 0 0 0 7 H 1 0 0 0 0 7 H 1 0 0 0 0 7 J 1 0 0 0 0 7 K 1 0 0 0 0 7 K 1 0 0 0 0 7 M 1 0 0 0 0 7 N 1 0 0 0 0 7 P 1 0 0 0 0 7 P 1 0 0 0 0 8 <td< td=""><td>7</td><td>С</td><td>1</td><td>0</td><td>0</td><td>0</td><td>0</td></td<>	7	С	1	0	0	0	0
7 E 1 0 0 0 0 0 7 F 1 0 0 0 0 0 7 G 1 0 0 0 0 0 7 H 1 0 0 0 0 0 7 H 1 0 0 0 0 0 7 J 1 0 0 0 0 0 7 J 1 0 0 0 0 0 7 K 1 0 0 0 0 0 7 M 1 0 0 0 0 0 7 N 1 0 0 0 0 0 7 P 1 0 0 0 0 0 8 A 2 0 0 0 0 0	7	D	1	0	0	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	Е	1	0	0	0	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	F	1	0	0	0	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	G	1	0	0	0	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	Н	1	0	0	0	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	Ι	1	0	0	0	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	J	1	0	0	0	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	K	1	0	0	0	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	L	1	0	0	0	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	М	1	0	0	0	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	Ν	1	0	0	0	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	7	0	1	0	0	0	0
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	7	Р	1	0	0	0	0
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	8	А	2	0	0	0	0
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	8	В	2	0	0	0	0
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	8	С	2	0	0	0	0
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	8	D	2	0	0	0	0
8 F 1 0	8	Е	2	0	0	0	0
8 G 2 0	8	F	1	0	0	0	0
8 H 2 0	8	G	2	0	0	0	0
8 I 2 0	8	Н	2	0	0	0	0
8 J 2 0 0 0 0 8 K 2 0 0 0 0 0 8 L 1 0 0 0 0 0	8	Ι	2	0	0	0	0
8 K 2 0 0 0 0 8 L 1 0 0 0 0 0	8	J	2	0	0	0	0
8 L 1 0 0 0 0	8	K	2	0	0	0	0
	8	L	1	0	0	0	0
8 M 2 0 0 0 0	8	М	2	0	0	0	0
8 N 1 0 0 0 0	8	N	1	0	0	0	0
8 O 2 O 0 O 0	8	0	2	0	0	0	0

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	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	1000-11				
0	I P	2 19	0	0	0	0
9	D C	10	0	16	2	0
9	E E	6	0	10	0	0
9	E F	6	0	8	0	0
9	r C	6	0	8	0	0
9	G I	10	0	0	0	0
9	I	12	0	10	4	0
9	J K	6	0	8	0	0
9	M	6	0	8	1	0
9	N	12	0	16	1	0
9	<u>N</u>	6	0	8	0	0
9	P	12	0	16	0	0
10	I C	12	0	10	0	0
10	E E	1	0	0	0	0
10	I	1	0	0	0	0
10	P	1	0	0	0	0
10	D	7	0	10	0	0
11	K K	7	0	10	1	0
11	M	14	0	20	2	0
11	N	7	0	10	0	0
12	Н	8	0	12	0	0
12	Ι	8	0	12	0	0
13	A	800	0	0	5	0
13	В	744	0	0	7	0
13	С	762	0	0	1	0
13	D	713	0	0	2	0
13	Е	645	0	0	2	0
13	F	605	0	0	4	0
13	G	748	0	0	3	0
13	Н	685	0	0	1	0
13	Ι	704	0	0	3	0
13	J	567	0	0	7	0
13	K	766	0	0	3	0
13	L	681	0	0	5	0
13	М	690	0	0	2	0
13	Ν	465	0	0	2	0
13	0	665	0	0	3	0
13	Р	532	0	0	4	0
All	All	93689	0	82144	518	0

d fa ntin C

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 3.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
1:B:274:VAL:HG21	1:B:311:LEU:CD1	2.03	0.87	
1:N:263[B]:ASP:OD2	1:N:312[B]:ARG:NE	2.16	0.78	
1:B:274:VAL:HG21	1:B:311:LEU:HD12	1.70	0.71	
1:J:252:LEU:HD23	1:J:252:LEU:H	1.55	0.69	
1:J:252:LEU:H	1:J:252:LEU:CD2	2.05	0.68	

The worst 5 of 518 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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	Favoured Allowed		Outliers Percent	
1	А	620/618~(100%)	605~(98%)	15~(2%)	0	100	100
1	В	619/618~(100%)	604~(98%)	15~(2%)	0	100	100
1	С	619/618~(100%)	603~(97%)	16 (3%)	0	100	100
1	D	616/618~(100%)	601~(98%)	15~(2%)	0	100	100
1	Е	617/618~(100%)	604~(98%)	13~(2%)	0	100	100
1	F	621/618~(100%)	606~(98%)	15~(2%)	0	100	100
1	G	619/618~(100%)	606~(98%)	13~(2%)	0	100	100
1	Н	617/618~(100%)	605~(98%)	12 (2%)	0	100	100
1	Ι	619/618~(100%)	604~(98%)	15~(2%)	0	100	100
1	J	618/618~(100%)	603~(98%)	15~(2%)	0	100	100
1	К	617/618~(100%)	602~(98%)	15 (2%)	0	100	100
1	L	617/618~(100%)	603~(98%)	14 (2%)	0	100	100
1	М	616/618~(100%)	602~(98%)	14 (2%)	0	100	100
1	Ν	836/618~(135%)	800 (96%)	34 (4%)	2(0%)	47	23



001000	continuou fronte processas pagon										
Mol	Chain	Analysed	Analysed Favoured Allowed Ou		Outliers	Percentiles					
1	Ο	616/618~(100%)	602~(98%)	14 (2%)	0	100	100				
1	Р	616/618~(100%)	600~(97%)	16 (3%)	0	100	100				
All	All	10103/9888 (102%)	9850~(98%)	251 (2%)	2 (0%)	100	100				

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Ν	243[A]	HIS
1	N	243[B]	HIS

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	528/524~(101%)	526 (100%)	2 (0%)	91	82	
1	В	527/524~(101%)	524 (99%)	3~(1%)	86	73	
1	С	527/524~(101%)	525 (100%)	2 (0%)	91	82	
1	D	524/524~(100%)	520~(99%)	4 (1%)	81	66	
1	Е	525/524~(100%)	520 (99%)	5 (1%)	76	57	
1	F	529/524~(101%)	525~(99%)	4 (1%)	81	66	
1	G	527/524~(101%)	525 (100%)	2(0%)	91	82	
1	Н	525/524~(100%)	521 (99%)	4 (1%)	81	66	
1	Ι	527/524~(101%)	525 (100%)	2(0%)	91	82	
1	J	526/524~(100%)	525 (100%)	1 (0%)	93	86	
1	К	525/524~(100%)	523 (100%)	2(0%)	91	82	
1	L	525/524~(100%)	522~(99%)	3 (1%)	86	73	
1	М	524/524~(100%)	522 (100%)	2(0%)	91	82	
1	Ν	718/524~(137%)	710 (99%)	8 (1%)	73	53	
1	Ο	524/524~(100%)	521 (99%)	3 (1%)	86	73	
1	Р	524/524~(100%)	520 (99%)	4 (1%)	81	66	



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
All	All	8605/8384~(103%)	8554 (99%)	51 (1%)	86 73		

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	554	THR
1	М	554	THR
1	Р	459	TYR
1	Κ	252	LEU
1	L	459	TYR

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 360 ligands modelled in this entry, 16 are modelled with single atom and 33 are monoatomic - leaving 311 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).



	т		Б	T • 1	B	ond leng	gths	Bo	ond ang	les
NIOI	Type	Chain	Res	Link	Counts	RMSZ	$\left \# Z > 2 \right $	Counts	RMSZ	# Z > 2
2	SF4	А	1101	1	0,12,12	-	-	_		
9	GOL	J	1114	-	$5,\!5,\!5$	0.09	0	5,5,5	0.30	0
2	SF4	Р	1107	1	0,12,12	-	-	-		
4	EDO	Ι	1112	-	3,3,3	0.06	0	2,2,2	0.26	0
2	SF4	L	1104	1	0,12,12	-	-	-		
6	SO4	L	1113	-	4,4,4	0.12	0	6,6,6	0.17	0
4	EDO	В	4201	-	3,3,3	0.10	0	2,2,2	0.04	0
2	SF4	N	1002	1	$0,\!12,\!12$	-	-	-		
6	SO4	М	1125	-	4,4,4	0.17	0	6,6,6	0.15	0
2	SF4	K	1107	1	$0,\!12,\!12$	-	-	-		
4	EDO	F	1108	-	3, 3, 3	0.41	0	2,2,2	0.55	0
4	EDO	0	1108	-	3,3,3	0.51	0	2,2,2	0.50	0
6	SO4	N	1016	-	4,4,4	0.15	0	6,6,6	0.27	0
6	SO4	L	1114	-	4,4,4	0.15	0	6,6,6	0.18	0
4	EDO	A	1118	-	3,3,3	0.13	0	2,2,2	0.13	0
6	SO4	I	1120	-	4,4,4	0.13	0	6,6,6	0.28	0
2	SF4	J	1104	1	0,12,12	-	_	_		
2	SF4	I	1103	1	0,12,12	-	_	_		
2	SF4	J	1103	1	$0,\!12,\!12$	-	-	-		
2	SF4	K	1102	1	0,12,12	-	_	_		
4	EDO	0	1114	-	3,3,3	0.07	0	2,2,2	0.28	0
2	SF4	Н	4402	1	0,12,12	-	-	-		
2	SF4	I	1102	1	0,12,12	-	_	_		
11	PEG	N	1014	-	6,6,6	0.12	0	5,5,5	0.08	0
5	SRM	K	1109	1	68,70,70	2.49	20 (29%)	81,112,112	1.61	18 (22%)
2	SF4	N	1003	1	0,12,12	-	-	-		
2	SF4	Е	1102	1	0,12,12	-	-	-		
5	SRM	Е	1109	1	68,70,70	2.52	18 (26%)	81,112,112	1.63	20 (24%)
2	SF4	L	1102	1	0,12,12	-	-	-		
5	SRM	А	1109	1	68,70,70	2.47	20 (29%)	81,112,112	1.64	17 (20%)
2	SF4	G	1103	1	0,12,12	-	-	_		
9	GOL	N	1011	-	5,5,5	0.11	0	5,5,5	0.32	0
2	SF4	Ι	1101	1	0,12,12	-	-	-		1
9	GOL	М	1114	-	5,5,5	0.12	0	5,5,5	0.32	0
2	SF4	Ι	1105	1	0,12,12	-	-	-		1
4	EDO	G	1112	-	3,3,3	0.09	0	2,2,2	0.20	0
4	EDO	М	1108	-	3,3,3	0.44	0	2,2,2	0.35	0
4	EDO	F	1112[A]	-	3,3,3	0.14	0	2,2,2	0.35	0
2	SF4	С	3903	1	0,12,12	-	-	-		
2	SF4	G	1102	1	0,12,12	-	-	-		
4	EDO	А	1111	-	3,3,3	0.11	0	2,2,2	0.31	0
4	EDO	М	1110	-	3,3,3	0.41	0	2,2,2	0.71	0



N /L = 1	— ———————————————————————————————————		D	T	В	ond leng	gths	Bo	ond ang	les
	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	GOL	С	3913	-	$5,\!5,\!5$	0.10	0	5,5,5	0.33	0
4	EDO	J	1110	-	3,3,3	0.05	0	2,2,2	0.16	0
4	EDO	J	1116	-	3,3,3	0.06	0	2,2,2	0.24	0
6	SO4	F	1116	-	4,4,4	0.45	0	6,6,6	0.06	0
3	FAD	С	3907	-	$53,\!58,\!58$	1.29	8 (15%)	68,89,89	1.15	7 (10%)
4	EDO	С	3918	-	3,3,3	0.10	0	2,2,2	0.06	0
4	EDO	G	1117	-	3,3,3	0.10	0	2,2,2	0.28	0
5	SRM	Р	1109	1	68,70,70	2.42	18 (26%)	81,112,112	1.56	15 (18%)
2	SF4	С	3906	1	0,12,12	-	-	-		
4	EDO	J	1115	-	3,3,3	0.12	0	2,2,2	0.09	0
6	SO4	F	1117	-	4,4,4	0.43	0	6,6,6	0.06	0
9	GOL	В	4218[B]	-	$5,\!5,\!5$	0.13	0	5,5,5	0.37	0
2	SF4	K	1103	1	0,12,12	-	-	-		-
3	FAD	Ν	1009[B]	-	$53,\!58,\!58$	0.61	0	68,89,89	0.68	1 (1%)
2	SF4	D	4604	1	0,12,12	-	-	-		
6	SO4	Н	4415	-	4,4,4	0.14	0	6,6,6	0.16	0
2	SF4	F	1103	1	0,12,12	-	-	-		
4	EDO	G	1121	-	3,3,3	0.06	0	2,2,2	0.10	0
4	EDO	D	4609	-	3,3,3	0.40	0	2,2,2	0.56	0
6	SO4	В	4226	-	$4,\!4,\!4$	0.14	0	6,6,6	0.22	0
4	EDO	Н	4413	-	3,3,3	0.05	0	2,2,2	0.19	0
4	EDO	A	1117	-	3,3,3	0.04	0	2,2,2	0.12	0
4	EDO	I	1114	-	3,3,3	0.06	0	2,2,2	0.21	0
2	SF4	Ι	1107	1	0,12,12	-	-	-		
3	FAD	D	4607	-	53,58,58	1.34	7 (13%)	68,89,89	1.26	13 (19%)
2	SF4	G	1105	1	$0,\!12,\!12$	-	-	-		
4	EDO	Ι	1115	-	3,3,3	0.05	0	2,2,2	0.19	0
4	EDO	0	1115	-	3, 3, 3	0.07	0	2,2,2	0.18	0
2	SF4	J	1105	1	$0,\!12,\!12$	-	-	-		-
4	EDO	L	1112	-	3,3,3	0.06	0	2,2,2	0.18	0
2	SF4	K	1104	1	0,12,12	-	-	-		
11	PEG	K	1115	-	6,6,6	0.12	0	5,5,5	0.08	0
6	SO4	P	1116	-	4,4,4	0.43	0	6,6,6	0.08	0
2	SF4	H	4405	1	0,12,12	-	-	-		
4	EDO	C	3916	-	3,3,3	0.06	0	2,2,2	0.14	0
2	SF4	A	1103	1	0,12,12	-	-	-	0.10	0
4	EDO	M	1112	-	3,3,3	0.04	0	2,2,2	0.18	0
2	SF4	N	1005		0,12,12	-	-	-		
	SF4		3905		0,12,12	-	-	-		
2	SF4		1103		0,12,12	-	-	-	0.10	0
4	EDO	A	1112	-	3,3,3	0.08	0	2,2,2	0.19	0
4	EDO	М	1116	-	3,3,3	0.05	0	2,2,2	0.18	0



	т	<u> </u>	Ъ	T • 1	B	ond leng	gths	Bo	ond ang	les
IVI01	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	GOL	Е	1114	-	5,5,5	0.12	0	5,5,5	0.36	0
4	EDO	А	1108	-	3,3,3	0.45	0	2,2,2	0.39	0
4	EDO	G	1118	-	3,3,3	0.06	0	2,2,2	0.19	0
4	EDO	В	4220[B]	-	3,3,3	0.07	0	2,2,2	0.18	0
4	EDO	G	1113	-	3,3,3	0.08	0	2,2,2	0.28	0
6	SO4	F	1118	-	4,4,4	0.37	0	6,6,6	0.05	0
4	EDO	0	1117	-	3,3,3	0.05	0	2,2,2	0.19	0
4	EDO	E	1110	-	3,3,3	0.10	0	2,2,2	0.28	0
4	EDO	G	1114	-	3,3,3	0.11	0	2,2,2	0.03	0
4	EDO	Н	4409	-	3,3,3	0.53	0	2,2,2	0.14	0
4	EDO	M	1117	-	3,3,3	0.05	0	2,2,2	0.19	0
4	EDO	A	1110	-	3,3,3	0.47	0	2,2,2	0.28	0
6	SO4	0	1120	-	4,4,4	0.43	0	6,6,6	0.05	0
4	EDO	M	1118	-	3,3,3	0.06	0	2,2,2	0.10	0
6	SO4	D	4619	-	4,4,4	0.14	0	6,6,6	0.15	0
2	SF4	L	1103	1	0,12,12	-	-	-		
3	FAD	В	4207	-	$53,\!58,\!58$	1.28	6 (11%)	68,89,89	1.17	6 (8%)
2	SF4	D	4603	1	0,12,12	-	-	-		
2	SF4	F	1104	1	0,12,12	-	-	-		
4	EDO	0	1112	-	3,3,3	0.09	0	2,2,2	0.25	0
4	EDO	В	4213	-	3,3,3	0.05	0	2,2,2	0.18	0
4	EDO	Ι	1116	-	3,3,3	0.06	0	2,2,2	0.10	0
4	EDO	N	1010	-	3,3,3	0.11	0	2,2,2	0.38	0
2	SF4	М	1102	1	0,12,12	-	-	-		
5	SRM	М	1109	1	68,70,70	2.75	22 (32%)	81,112,112	1.88	25 (30%)
3	FAD	Ν	1001[A]	-	53,58,58	0.61	0	68,89,89	0.71	2 (2%)
6	SO4	Р	1115	-	4,4,4	0.14	0	6,6,6	0.15	0
4	EDO	С	3914	-	3,3,3	0.14	0	2,2,2	0.30	0
4	EDO	D	4615	-	3,3,3	0.10	0	2,2,2	0.07	0
9	GOL	В	4217[A]	-	5,5,5	0.11	0	5,5,5	0.35	0
5	SRM	G	1109	1	68,70,70	2.48	19 (27%)	81,112,112	1.65	16 (19%)
2	SF4	М	1101	1	0,12,12	-	-	-		
9	GOL	Р	1111	-	$5,\!5,\!5$	0.10	0	5,5,5	0.32	0
4	EDO	0	1113	-	3,3,3	0.05	0	2,2,2	0.19	0
4	EDO	А	1115	-	3,3,3	0.11	0	2,2,2	0.17	0
5	SRM	J	1109	1	68,70,70	2.43	19 (27%)	81,112,112	1.54	13 (16%)
2	SF4	Ι	1104	1	0,12,12	-	-	-		
2	SF4	М	1105	1	0,12,12	-	-	-		
2	SF4	В	4202	1	0,12,12	-	-	-		
4	EDO	L	1108	-	3,3,3	0.46	0	2,2,2	0.39	0
4	EDO	С	3909	-	3,3,3	0.50	0	2,2,2	0.14	0
4	$ED\overline{O}$	D	4611	-	3,3,3	0.10	0	$2,2,\overline{2}$	$0.2\overline{9}$	0



N T 1	T		Ъ	T · 1	B	ond leng	gths	Bo	ond ang	les
NIOI	Type	Chain	Res	LINK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	PEG	М	1120	-	6,6,6	0.13	0	5,5,5	0.09	0
5	SRM	Н	4410	1	68,70,70	2.87	23 (33%)	81,112,112	1.97	27 (33%)
6	SO4	0	1119	-	4,4,4	0.15	0	6,6,6	0.26	0
2	SF4	В	4205	1	0,12,12	-	-	-		I
5	SRM	Ν	1012	1	68,70,70	2.55	21 (30%)	81,112,112	1.64	18 (22%)
3	FAD	J	1106	-	53,58,58	1.28	6 (11%)	68,89,89	1.22	9 (13%)
4	EDO	K	1110	-	3,3,3	0.58	0	2,2,2	0.05	0
6	SO4	В	4225	-	4,4,4	0.54	0	6,6,6	0.09	0
2	SF4	L	1101	1	0,12,12	_	_	_		I
4	EDO	Н	4411	-	3,3,3	0.08	0	2,2,2	0.36	0
4	EDO	М	1113	-	3,3,3	0.06	0	2,2,2	0.19	0
4	EDO	Ν	1013	-	3,3,3	0.05	0	2,2,2	0.16	0
2	SF4	D	4608	1	0,12,12	-	-	-		-
3	FAD	М	1106	-	53,58,58	1.29	<mark>6 (11%)</mark>	68,89,89	1.19	7 (10%)
4	EDO	Е	1116	-	3,3,3	0.06	0	2,2,2	0.19	0
4	EDO	Е	1108	-	3,3,3	0.48	0	2,2,2	0.54	0
9	GOL	N	1015	-	$5,\!5,\!5$	0.11	0	5,5,5	0.32	0
4	EDO	Р	1108	-	3,3,3	0.41	0	2,2,2	0.55	0
2	SF4	Н	4404	1	0,12,12	-	-	-		
12	TRS	Ι	1119	-	7,7,7	0.17	0	9,9,9	0.20	0
4	EDO	В	4222[A]	-	3,3,3	0.07	0	2,2,2	0.33	0
4	EDO	Р	1114	-	3,3,3	0.09	0	2,2,2	0.15	0
4	EDO	D	4616	-	3,3,3	0.09	0	2,2,2	0.26	0
4	EDO	Е	1113	-	3,3,3	0.13	0	2,2,2	0.20	0
2	SF4	L	1105	1	0,12,12	-	_	_		
2	SF4	М	1107	1	0,12,12	-	-	_		
2	SF4	0	1107	1	0,12,12	-	-	-		
4	EDO	I	1118	-	3,3,3	0.05	0	2,2,2	0.18	0
4	EDO	М	1119	-	3,3,3	0.06	0	2,2,2	0.18	0
3	FAD	Е	1106	-	53,58,58	1.33	7 (13%)	68,89,89	1.17	7 (10%)
3	FAD	Ι	1106	-	53,58,58	0.70	0	$68,\!89,\!89$	0.69	1 (1%)
4	EDO	С	3911	-	3,3,3	0.55	0	2,2,2	0.35	0
4	EDO	С	3912	-	3,3,3	0.11	0	2,2,2	0.33	0
4	EDO	Н	4412	-	3,3,3	0.06	0	2,2,2	0.27	0
2	SF4	М	1104	1	0,12,12	-	-	-		
4	EDO	I	1110	-	3,3,3	0.05	0	2,2,2	0.18	0
4	EDO	C	3915	_	3,3,3	0.06	0	2,2,2	0.19	0
4	$ED\overline{O}$	J	1111	_	3,3,3	$0.0\overline{7}$	0	$2,2,\overline{2}$	0.18	0
6	SO4	J	1118	_	4,4,4	0.14	0	6,6,6	0.12	0
4	EDO	В	4216		3,3,3	0.05	0	2,2,2	0.18	0
4	EDO	K	1111	-	3,3,3	0.09	0	2,2,2	0.28	0
2	SF4	G	1101	1	0,12,12	-				



Ъ / [_]	— ———————————————————————————————————		D	T	B	ond leng	gths	Bo	ond ang	es
IVI01	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
4	EDO	В	4219[A]	-	3,3,3	0.06	0	2,2,2	0.18	0
6	SO4	G	1122	-	4,4,4	0.18	0	6,6,6	0.24	0
4	EDO	G	1110	-	3,3,3	0.10	0	2,2,2	0.31	0
4	EDO	М	1122	-	3,3,3	0.05	0	2,2,2	0.24	0
6	SO4	K	1119	-	4,4,4	0.42	0	6,6,6	0.05	0
4	EDO	В	4211	-	3,3,3	0.06	0	2,2,2	0.19	0
2	SF4	E	1103	1	0,12,12	-	-	-		
4	EDO	A	1114	-	3,3,3	0.11	0	2,2,2	0.19	0
2	SF4	N	1004	1	0,12,12	-	-	-		
4	EDO	D	4612	-	3,3,3	0.05	0	2,2,2	0.18	0
6	SO4	М	1127	-	4,4,4	0.43	0	6,6,6	0.05	0
5	SRM	I	1109	1	68,70,70	2.55	20 (29%)	81,112,112	1.61	13 (16%)
4	EDO	G	1120	-	3,3,3	0.05	0	2,2,2	0.19	0
2	SF4	0	1104	1	0,12,12	-	-	-		
11	PEG	М	1115	-	6,6,6	0.14	0	5,5,5	0.08	0
4	EDO	D	4617	-	3,3,3	0.05	0	2,2,2	0.18	0
2	SF4	F	1101	1	0,12,12	-	-	-		
2	SF4	D	4605	1	0,12,12	-	-	-		
2	SF4	L	1107	1	0,12,12	-	-	-		
9	GOL	0	1116	-	5,5,5	0.11	0	5,5,5	0.40	0
4	EDO	E	1111	-	3,3,3	0.09	0	2,2,2	0.16	0
3	FAD	G	1106	-	$53,\!58,\!58$	0.70	0	$68,\!89,\!89$	0.66	1 (1%)
4	EDO	G	1116	-	3,3,3	0.05	0	2,2,2	0.18	0
4	EDO	J	1108	-	3,3,3	0.50	0	2,2,2	0.49	0
4	EDO	В	4212	-	3,3,3	0.10	0	2,2,2	0.19	0
4	EDO	E	1112	-	3,3,3	0.06	0	2,2,2	0.19	0
2	SF4	Н	4408	1	0,12,12	-	-	-		
6	SO4	D	4620	-	4,4,4	0.38	0	6,6,6	0.05	0
2	SF4	D	4606	1	0,12,12	-	-	-		
4	EDO	0	1118	-	3,3,3	0.12	0	2,2,2	0.12	0
2	SF4	A	1102	1	0,12,12	-	-	-		
2	SF4		1103		0,12,12	-	-	-	0.01	0
9	GOL		1112	-	5,5,5	0.10	0	5,5,5	0.31	0
2	SF4	B	4208		0,12,12	-	-	-	0.10	0
4	EDO CD4		1115	-	3,3,3	0.06	0	2,2,2	0.19	U
2	SF4		1102		0,12,12	-	-	-	0.00	0
4	EDO		1113	-	3,3,3	0.10		2,2,2	0.09	0
4	EDO	Λ V	1108	-	3,3,3	0.42	0	2,2,2	0.41	0
$\frac{4}{2}$	EDU SE4	n F	1114	- 1	0,3,3 0,10,10	0.00	U	2,2,2	0.19	U
	Sr4 FDO		1104		0,12,12		-	-	0.49	Ο
4 9			1121	-	0,0,0 50 50 50	1.00	(1907)	<i>4,2,2</i>	0.42	$\frac{11}{(1607)}$
5	FAD	Н	4407	-	53,58,58	1.20	7 (13%)	08,89,89	1.29	11 (16%)



	m		Ъ	T • 1	B	ond leng	gths	Bo	ond ang	les
MOI	Type	Chain	Res	Link	Counts	RMSZ	$\tilde{ } \# Z > 2$	Counts	RMSZ	# Z >2
3	FAD	F	1106	-	53,58,58	1.25	<mark>6 (11%)</mark>	68,89,89	1.29	11 (16%)
2	SF4	С	3908	1	0,12,12	-	-	-		
4	EDO	Ι	1108	-	3,3,3	0.49	0	2,2,2	0.38	0
4	EDO	Р	1113	-	3,3,3	0.08	0	2,2,2	0.22	0
2	SF4	0	1102	1	0,12,12	-	-	-		
2	SF4	Р	1104	1	0,12,12	-	-	-		
2	SF4	F	1107	1	0,12,12	-	-	-		
3	FAD	А	1106	-	53,58,58	1.21	6 (11%)	68,89,89	1.20	7 (10%)
2	SF4	N	1006[A]	1	0,12,12	_	_	-		
5	SRM	D	4610	1	68,70,70	2.39	19 (27%)	81,112,112	1.70	17 (20%)
4	EDO	В	4221	-	3,3,3	0.07	0	2,2,2	0.05	0
4	EDO	D	4618	-	3,3,3	0.13	0	2,2,2	0.18	0
2	SF4	Р	1101	1	0,12,12	-	-	-		1
4	EDO	Е	1117	-	3,3,3	0.11	0	2,2,2	0.28	0
2	SF4	0	1101	1	0,12,12	-	-	-		
4	EDO	D	4613	-	3,3,3	0.05	0	2,2,2	0.22	0
2	SF4	D	4602	1	0,12,12	-	-	-		
9	GOL	В	4224	-	$5,\!5,\!5$	0.11	0	5,5,5	0.32	0
4	EDO	А	1113	-	3,3,3	0.08	0	2,2,2	0.14	0
2	SF4	Н	4406	1	0,12,12	-	-	-		
4	EDO	G	1111	-	3,3,3	0.06	0	2,2,2	0.18	0
2	SF4	A	1105	1	0,12,12	-	-	-		
5	SRM	С	3910	1	68,70,70	2.48	19 (27%)	81,112,112	1.62	16 (19%)
4	EDO	М	1123	-	3,3,3	0.10	0	2,2,2	0.20	0
4	EDO	В	4215	-	3,3,3	0.07	0	2,2,2	0.15	0
6	SO4	А	1119	-	4,4,4	0.19	0	6,6,6	0.21	0
2	SF4	N	1007[A]	1	0,12,12	-	-	-		
4	EDO	С	3917	-	3,3,3	0.09	0	2,2,2	0.19	0
4	EDO	A	1116	-	3,3,3	0.08	0	2,2,2	0.16	0
9	GOL	F	1114	-	5,5,5	0.11	0	5,5,5	0.31	0
2	SF4	С	3904	1	0,12,12	-	-	-		
3	FAD	Ο	1106	-	53,58,58	1.30	6 (11%)	68,89,89	1.19	6 (8%)
2	SF4	F	1102	1	0,12,12	-	-	-		
5	SRM	F	1109	1	68,70,70	2.48	20 (29%)	81,112,112	1.73	16 (19%)
2	SF4	G	1107	1	0,12,12	-	-	-		
2	SF4	P	1105	1	0,12,12	-	-	-		
9	GOL	С	3901	-	$5,\!5,\!5$	0.09	0	5,5,5	0.32	0
2	SF4	K	1105	1	0,12,12	_	-	-		
6	SO4	D	4621	_	4,4,4	0.41	0	6,6,6	0.05	0
2	SF4	В	4206	1	0,12,12		-	-		
2	SF4	М	1103	1	0,12,12	-	-	-		
2	SF4	F	1105	1	0,12,12	-	-	-		



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Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SF4	0	1105	1	0,12,12	-	-	_		
4	EDO	В	4209	-	3,3,3	0.40	0	2,2,2	0.64	0
4	EDO	М	1124	-	3,3,3	0.08	0	2,2,2	0.19	0
2	SF4	J	1107	1	0,12,12	-	-	-		·
4	EDO	K	1112	-	3,3,3	0.08	0	2,2,2	0.17	0
9	GOL	J	1117[A]	-	$5,\!5,\!5$	0.09	0	$5,\!5,\!5$	0.36	0
4	EDO	0	1111	-	3,3,3	0.05	0	2,2,2	0.18	0
4	EDO	K	1116	-	3,3,3	0.10	0	2,2,2	0.10	0
4	EDO	J	1112	-	3,3,3	0.05	0	2,2,2	0.18	0
5	SRM	L	1109	1	68,70,70	2.57	20 (29%)	81,112,112	1.61	16 (19%)
2	SF4	J	1102	1	0,12,12	-	-	-		
5	SRM	0	1109	1	68,70,70	3.62	25 (36%)	81,112,112	2.39	33 (40%)
9	GOL	Ι	1117	-	5,5,5	0.10	0	5,5,5	0.32	0
2	SF4	В	4203	1	0,12,12	-	-	-		
4	EDO	0	1110	-	3,3,3	0.42	0	2,2,2	0.55	0
3	FAD	L	1106	-	53,58,58	1.29	6 (11%)	68,89,89	1.16	8 (11%)
6	SO4	Н	4414	-	4,4,4	0.48	0	6,6,6	0.07	0
2	SF4	J	1101	1	0,12,12	-	-	-		1
2	SF4	Ν	1008[B]	1	0,12,12	-	-	-		
4	EDO	D	4614	-	3,3,3	0.06	0	2,2,2	0.19	0
12	TRS	Н	4401	-	7,7,7	0.16	0	9,9,9	0.29	0
4	EDO	G	1108	-	3,3,3	0.59	0	2,2,2	0.31	0
9	GOL	G	1119[A]	-	$5,\!5,\!5$	0.10	0	$5,\!5,\!5$	0.35	0
2	SF4	С	3902	1	0,12,12	-	-	-		-
4	EDO	F	1111	-	3,3,3	0.05	0	2,2,2	0.18	0
2	SF4	Н	4403	1	0,12,12	-	-	-		
6	SO4	С	3919	-	4,4,4	0.46	0	6,6,6	0.07	0
2	SF4	В	4204	1	0,12,12	-	-	-		
2	SF4	E	1107	1	0,12,12	-	-	-		1
9	GOL	K	1117	-	5,5,5	0.09	0	5,5,5	0.35	0
4	EDO	J	1113	-	3,3,3	0.17	0	2,2,2	0.17	0
4	EDO	G	1115	-	3,3,3	0.06	0	2,2,2	0.18	0
2	SF4	K	1101	1	0,12,12	-	-	-	0.10	0
4	EDO	K	1113	-	3,3,3	0.05	0	2,2,2	0.18	0
6	SO4	M	1126	-	4,4,4	0.38	0	6,6,6	0.05	0
2	SF4		1006[B]	1	0,12,12	-	-	-		
		G T	1104		0,12,12	-	-	-	0.20	0
9	GOL FDO	T I	1111	-	0,0,0	0.11	0	0,0,0	0.52	
4	FDO	D D	4999	-	0,0,0 2,2,0	0.42	0		0.01	0
4	EDO	D I	4220	-	0,0,0 2,2,2	0.07	0	2,2,2	0.19	0
4 9	SE4	E I	1110	- 1	0,0,0	0.00	U		0.19	0
	5Г4		1101		0,12,12	-	-	-		



Mal	Tuno	Chain	Pog	Link	B	ond leng	gths	Bond angles		
	туре	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FAD	K	1106	-	53,58,58	1.21	5 (9%)	68,89,89	1.17	7 (10%)
6	SO4	K	1118	-	4,4,4	0.47	0	6,6,6	0.05	0
3	FAD	Р	1106	-	53,58,58	1.20	6 (11%)	68,89,89	1.31	10 (14%)
4	EDO	В	4214	-	3,3,3	0.06	0	2,2,2	0.15	0
4	EDO	Р	1110	-	3,3,3	0.08	0	2,2,2	0.28	0
6	SO4	J	1119	-	4,4,4	0.42	0	6,6,6	0.07	0
6	SO4	L	1115	-	4,4,4	0.44	0	6,6,6	0.06	0
6	SO4	E	1118	-	4,4,4	0.17	0	6,6,6	0.24	0
2	SF4	А	1107	1	0,12,12	-	-	-		
4	EDO	F	1110[B]	-	3,3,3	0.24	0	2,2,2	0.18	0
6	SO4	F	1115	-	4,4,4	0.13	0	6,6,6	0.27	0
4	EDO	М	1111	-	3,3,3	0.09	0	2,2,2	0.27	0
4	EDO	L	1111	-	3,3,3	0.09	0	2,2,2	0.27	0
5	SRM	В	4210	1	68,70,70	2.61	20 (29%)	81,112,112	1.62	17 (20%)
2	SF4	A	1104	1	0,12,12	-	-	-		
11	PEG	D	4601	-	6,6,6	0.14	0	5,5,5	0.08	0
2	SF4	E	1105	1	0,12,12	-	-	-		

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	EDO	В	4215	-	-	1/1/1/1	-
2	SF4	А	1101	1	-	-	0/6/5/5
3	FAD	Ι	1106	-	-	1/30/50/50	0/6/6/6
4	EDO	С	3911	-	-	1/1/1/1	-
4	EDO	С	3912	-	-	0/1/1/1	-
4	EDO	Ι	1115	-	-	1/1/1/1	-
4	EDO	0	1115	-	_	0/1/1/1	-
9	GOL	J	1114	-	-	4/4/4/4	-
2	SF4	Р	1107	1	-	-	0/6/5/5
4	EDO	Ι	1112	-	-	1/1/1/1	-
2	SF4	J	1105	1	-	-	0/6/5/5
4	EDO	С	3917	-	-	1/1/1/1	-
2	SF4	Ν	1007[A]	1	-	-	0/6/5/5
4	EDO	L	1112	-	_	1/1/1/1	-
11	PEG	K	1115	-	-	3/4/4/4	-
2	SF4	K	1104	1	-	-	0/6/5/5
4	EDO	А	1116	-	-	0/1/1/1	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	Н	4412	_	_	1/1/1/1	-
4	EDO	Ι	1110	-	_	1/1/1/1	_
2	SF4	М	1104	1	-	_	0/6/5/5
9	GOL	F	1114	_	-	1/4/4/4	_
2	SF4	С	3904	1	-	-	0/6/5/5
3	FAD	Ο	1106	-	-	2/30/50/50	0/6/6/6
2	SF4	Н	4405	1	-	-	0/6/5/5
2	SF4	L	1104	1	-	-	0/6/5/5
2	SF4	F	1102	1	-	-	0/6/5/5
5	SRM	F	1109	1	1/1/19/23	11/38/126/126	-
4	EDO	С	3916	-	-	1/1/1/1	-
4	EDO	С	3915	-	-	1/1/1/1	-
4	EDO	М	1112	_	-	1/1/1/1	-
2	SF4	А	1103	1	-	-	0/6/5/5
2	SF4	G	1107	1	-	-	0/6/5/5
2	SF4	N	1005	1	-	-	0/6/5/5
2	SF4	Р	1105	1	_	-	0/6/5/5
9	GOL	С	3901	-	-	2/4/4/4	-
4	EDO	В	4201	-	-	0/1/1/1	-
4	EDO	J	1111	-	-	1/1/1/1	-
2	SF4	N	1002	1	-	-	0/6/5/5
2	SF4	С	3905	1	_	-	0/6/5/5
2	SF4	Κ	1107	1	-	-	0/6/5/5
4	EDO	А	1112	-	_	0/1/1/1	-
2	SF4	0	1103	1	_	_	0/6/5/5
2	SF4	K	1105	1	-	-	0/6/5/5
4	EDO	М	1116	-	-	0/1/1/1	-
9	GOL	Ε	1114	_	-	4/4/4/4	-
4	EDO	В	4216	-	_	0/1/1/1	-
4	EDO	F	1108	-	-	0/1/1/1	-
4	EDO	K	1111	-	-	0/1/1/1	-
4	EDO	0	1108	-	-	0/1/1/1	-
2	SF4	G	1101	1	-	-	0/6/5/5
4	EDO	А	1108	-	_	0/1/1/1	-
4	EDO	G	1118	-	-	0/1/1/1	-
4	EDO	В	4219[A]	-	-	0/1/1/1	-
2	SF4	В	4206	1	-	-	0/6/5/5
4	EDO	В	4220[B]	-	-	0/1/1/1	-
4	EDO	G	1113	-	-	1/1/1/1	-
4	EDO	A	1118	-	-	1/1/1/1	-
2	SF4	М	1103	1	-	-	0/6/5/5



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	0	1117	-	-	1/1/1/1	-
4	EDO	В	4209	-	-	0/1/1/1	-
4	EDO	Е	1110	-	-	0/1/1/1	-
4	EDO	G	1110	-	-	0/1/1/1	-
4	EDO	G	1114	-	-	0/1/1/1	-
4	EDO	Н	4409	-	-	0/1/1/1	-
4	EDO	М	1117	-	-	1/1/1/1	-
4	EDO	М	1122	-	-	1/1/1/1	-
2	SF4	F	1105	1	-	-	0/6/5/5
2	SF4	0	1105	1	-	-	0/6/5/5
4	EDO	А	1110	-	-	1/1/1/1	-
4	EDO	В	4211	-	_	0/1/1/1	-
4	EDO	М	1124	-	-	0/1/1/1	-
2	SF4	Е	1103	1	-	-	0/6/5/5
4	EDO	А	1114	-	-	0/1/1/1	-
2	SF4	Ν	1004	1	-	-	0/6/5/5
2	SF4	J	1104	1	_	-	0/6/5/5
2	SF4	J	1107	1	-	-	0/6/5/5
4	EDO	K	1112	-	_	0/1/1/1	-
4	EDO	D	4612	-	-	1/1/1/1	-
2	SF4	Ι	1103	1	-	-	0/6/5/5
2	SF4	J	1103	1	-	-	0/6/5/5
9	GOL	J	1117[A]	-	-	2/4/4/4	-
2	SF4	K	1102	1	-	-	0/6/5/5
4	EDO	0	1111	-	-	0/1/1/1	-
4	EDO	М	1118	-	-	1/1/1/1	-
2	SF4	L	1103	1	-	-	0/6/5/5
3	FAD	В	4207	-	_	1/30/50/50	0/6/6/6
5	SRM	Ι	1109	1	1/1/19/23	11/38/126/126	-
4	EDO	K	1116	-	-	1/1/1/1	-
4	EDO	G	1120	-	-	1/1/1/1	-
4	EDO	J	1112	-	-	1/1/1/1	-
5	SRM	L	1109	1	1/1/19/23	12/38/126/126	-
2	SF4	D	4603	1	-	-	0/6/5/5
2	SF4	0	1104	1	_	-	0/6/5/5
2	SF4	F	1104	1	-	-	0/6/5/5
4	EDO	0	1114	-	-	1/1/1/1	-
11	PEG	М	1115	-	-	4/4/4/4	-
2	SF4	Н	4402	1	-	-	0/6/5/5
4	EDO	D	4617	-	-	1/1/1/1	-
2	SF4	Ι	1102	1	-		0/6/5/5



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	F	1101	1	-	-	0/6/5/
2	SF4	J	1102	1	-	-	0/6/5/
5	SRM	Ο	1109	1	1/1/19/23	13/38/126/126	-
4	EDO	0	1112	-	-	1/1/1/1	-
9	GOL	Ι	1117	-	-	4/4/4/4	-
2	SF4	D	4605	1	-	-	0/6/5/
11	PEG	N	1014	_	-	3/4/4/4	_
2	SF4	L	1107	1	-		0/6/5/
2	SF4	В	4203	1	-	_	0/6/5/
4	EDO	В	4213	-	-	1/1/1/1	-
5	SRM	K	1109	1	1/1/19/23	11/38/126/126	-
4	EDO	0	1110	_	_	1/1/1/1	_
3	FAD	L	1106	_	-	1/30/50/50	0/6/6/
4	EDO	Ι	1116	_	-	0/1/1/1	
4	EDO	N	1010	-	-	0/1/1/1	-
9	GOL	0	1116	_	-	$\frac{4}{4}/\frac{4}{4}$	-
2	SF4	М	1102	1	_	_	0/6/5/
5	SRM	М	1109	1	1/1/19/23	11/38/126/126	
3	FAD	N	1001[A]	_	_	9/30/50/50	0/6/6
4	EDO	Е	1111	_	_	0/1/1/1	
3	FAD	G	1106	_	_	$\frac{372}{1/30/50/50}$	0/6/6
2	SF4	J	1101	1	-		0/6/5
4	EDO	G	1116	_	-	1/1/1/1	-
2	SF4	N	1008[B]	1	-	_	0/6/5/
2	SF4	N	1003	1	-	-	0/6/5
4	EDO	С	3914	-	-	0/1/1/1	-
4	EDO	D	4615	-	-	1/1/1/1	-
4	EDO	J	1108	-	-	0/1/1/1	-
4	EDO	В	4212	-	_	0/1/1/1	-
9	GOL	В	4217[A]	-	-	2/4/4/4	-
5	SRM	Е	1109	1	1/1/19/23	12/38/126/126	-
4	EDO	D	4614	-	-	1/1/1/1	-
5	SRM	G	1109	1	1/1/19/23	11/38/126/126	-
4	EDO	Е	1112	_	-	1/1/1/1	-
2	SF4	Е	1102	1	-	_	0/6/5
2	SF4	L	1102	1	-	-	0/6/5
2	SF4	М	1101	1	-	-	0/6/5
9	GOL	Р	1111	-	-	1/4/4/4	-
4	EDO	0	1113	-	-	1/1/1/1	-
5	SRM	A	1109	1	1/1/19/23	12/38/126/126	-
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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings		
2	SF4	G	1105	1	-	-	0/6/5/5		
4	EDO	А	1115	-	_	1/1/1/1	_		
2	SF4	G	1103	1	_	-	0/6/5/5		
2	SF4	Н	4408	1	-	-	0/6/5/5		
12	TRS	Η	4401	-	-	6/9/9/9	-		
9	GOL	Ν	1011	-	-	2/4/4/4	-		
2	SF4	Ι	1101	1	-	-	0/6/5/5		
5	SRM	J	1109	1	1/1/19/23	11/38/126/126	-		
9	GOL	М	1114	-	-	1/4/4/4	-		
2	SF4	Ι	1104	1	-	-	0/6/5/5		
4	EDO	G	1108	-	-	0/1/1/1	-		
9	GOL	G	1119[A]	-	-	0/4/4/4	-		
2	SF4	Ι	1105	1	-	-	0/6/5/5		
4	EDO	G	1112	-	-	1/1/1/1	-		
4	EDO	0	1118	-	-	0/1/1/1	-		
2	SF4	D	4606	1	-	-	0/6/5/5		
2	SF4	М	1105	1	-	-	0/6/5/5		
4	EDO	М	1108	-	-	0/1/1/1	-		
2	SF4	А	1102	1	-	-	0/6/5/5		
2	SF4	С	3902	1	-	-	0/6/5/5		
4	EDO	F	1111	-	-	1/1/1/1	-		
4	EDO	F	1112[A]	-	-	0/1/1/1	-		
2	SF4	Н	4403	1	-	-	0/6/5/5		
4	EDO	А	1111	-	-	0/1/1/1	-		
9	GOL	\mathbf{C}	3913	-	-	4/4/4/4	-		
2	SF4	С	3903	1	-	-	0/6/5/5		
4	EDO	М	1110	-	-	1/1/1/1	-		
2	SF4	G	1102	1	-	-	0/6/5/5		
2	SF4	В	4202	1	-	-	0/6/5/5		
4	EDO	L	1108	-	-	0/1/1/1	-		
4	EDO	J	1110	-	-	1/1/1/1	-		
4	EDO	С	3909	-	-	0/1/1/1	-		
4	EDO	J	1116	-	-	0/1/1/1	-		
2	SF4	В	4204	1	-	-	0/6/5/5		
4	EDO	D	4611	-	-	0/1/1/1	-		
11	PEG	М	1120	-	-	1/4/4/4	-		
2	SF4	Р	1103	1			0/6/5/5		
9	GOL	Р	1112	-		0/4/4/4	-		
3	FAD	С	3907	-	-	3/30/50/50	0/6/6/6		
2	SF4	Ε	1107	1	-	-	0/6/5/5		
9	GOL	К	1117	_	_	3/4/4/4	_		



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	В	4208	1	-	-	0/6/5/5
4	EDO	С	3918	-	-	1/1/1/1	-
5	SRM	Р	1109	1	1/1/19/23	12/38/126/126	-
4	EDO	G	1117	-	-	0/1/1/1	-
2	SF4	С	3906	1	_	_	0/6/5/5
5	SRM	Н	4410	1	1/1/19/23	11/38/126/126	-
4	EDO	Е	1115	-	-	1/1/1/1	-
4	EDO	G	1115	-	-	1/1/1/1	-
4	EDO	J	1113	-	-	1/1/1/1	-
2	SF4	К	1101	1	-	-	0/6/5/5
2	SF4	В	4205	1	-	-	0/6/5/5
5	SRM	Ν	1012	1	1/1/19/23	14/38/126/126	-
3	FAD	J	1106	-	-	2/30/50/50	0/6/6/6
4	EDO	J	1115	-	-	0/1/1/1	-
4	EDO	K	1113	-	-	1/1/1/1	-
4	EDO	K	1110	-	-	0/1/1/1	-
2	SF4	Р	1102	1	-	-	0/6/5/5
2	SF4	N	1006[B]	1	-	-	0/6/5/5
4	EDO	F	1113	-	-	0/1/1/1	-
9	GOL	В	4218[B]	-	-	2/4/4/4	-
2	SF4	L	1101	1	-	-	0/6/5/5
4	EDO	K	1108	-	-	0/1/1/1	-
4	EDO	K	1114	-	-	1/1/1/1	-
4	EDO	Н	4411	-	-	0/1/1/1	-
2	SF4	Е	1104	1	-	-	0/6/5/5
2	SF4	G	1104	1	-	-	0/6/5/5
4	EDO	М	1113	-	-	1/1/1/1	-
9	GOL	Ι	1111	-	-	1/4/4/4	-
4	EDO	L	1110	-	-	0/1/1/1	-
4	EDO	В	4223	-	-	1/1/1/1	-
4	EDO	М	1121	-	-	1/1/1/1	-
4	EDO	N	1013	-	-	0/1/1/1	-
4	EDO	Ι	1113	-	-	0/1/1/1	-
2	SF4	Е	1101	1	-	-	0/6/5/5
3	FAD	K	1106	-	_	$1/30/\overline{50/50}$	0/6/6/6
3	FAD	Р	1106	-	-	2/30/50/50	0/6/6/6
4	EDO	В	4214	-	-	1/1/1/1	-
2	SF4	Κ	1103	1	-	_	0/6/5/5
2	SF4	D	4608	1		-	0/6/5/5
3	FAD	Н	4407	-	-	2/30/50/50	0/6/6/6



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	F	1106	-	-	3/30/50/50	0/6/6/6
3	FAD	N	1009[B]	-	-	2/30/50/50	0/6/6/6
4	EDO	М	1119	-	-	0/1/1/1	-
2	SF4	С	3908	1	-	-	0/6/5/5
4	EDO	Ι	1108	-	-	0/1/1/1	-
4	EDO	Р	1113	-	-	1/1/1/1	-
2	SF4	D	4604	1	-	-	0/6/5/5
2	SF4	0	1102	1	-	-	0/6/5/5
2	SF4	Р	1104	1	_	-	0/6/5/5
3	FAD	М	1106	-	-	2/30/50/50	0/6/6/6
2	SF4	F	1107	1	-	-	0/6/5/5
4	EDO	Р	1110	-	-	0/1/1/1	-
4	EDO	Е	1116	-	-	1/1/1/1	-
4	EDO	Е	1108	-	-	0/1/1/1	-
9	GOL	Ν	1015	-	-	1/4/4/4	-
3	FAD	А	1106	-	-	1/30/50/50	0/6/6/6
4	EDO	Р	1108	-	-	0/1/1/1	-
2	SF4	Ν	1006[A]	1	-	-	0/6/5/5
5	SRM	D	4610	1	1/1/19/23	11/38/126/126	-
2	SF4	F	1103	1	-	-	0/6/5/5
4	EDO	В	4221	-	-	1/1/1/1	-
2	SF4	Н	4404	1	-	-	0/6/5/5
4	EDO	G	1121	-	-	0/1/1/1	-
4	EDO	D	4618	-	-	0/1/1/1	-
12	TRS	Ι	1119	-	-	6/9/9/9	-
2	SF4	А	1107	1	-	-	0/6/5/5
4	EDO	F	1110[B]	-	-	1/1/1/1	-
2	SF4	Р	1101	1	-	-	0/6/5/5
4	EDO	Е	1117	-	-	1/1/1/1	-
4	EDO	D	4609	-	_	0/1/1/1	-
4	EDO	В	4222[A]	-	_	1/1/1/1	-
4	EDO	Р	1114	-	-	1/1/1/1	-
2	SF4	0	1101	1	_	-	0/6/5/5
4	EDO	М	1111	-	-	0/1/1/1	-
4	EDO	D	4616	-	-	0/1/1/1	-
4	EDO	L	1111	-	-	0/1/1/1	-
3	FAD	E	1106	-	-	1/30/50/50	0/6/6/6
4	EDO	E	1113	-	-	1/1/1/1	-
5	SRM	В	4210	1	1/1/19/23	12/38/126/126	-
4	EDO	D	4613	-	-	1/1/1/1	-
4	EDO	Н	4413	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	D	4602	1	-	-	0/6/5/5
9	GOL	В	4224	-	-	3/4/4/4	-
4	EDO	А	1113	-	-	1/1/1/1	-
2	SF4	Н	4406	1	-	-	0/6/5/5
2	SF4	L	1105	1	-	-	0/6/5/5
4	EDO	А	1117	-	-	1/1/1/1	-
5	SRM	С	3910	1	1/1/19/23	12/38/126/126	-
4	EDO	G	1111	-	-	0/1/1/1	-
2	SF4	А	1104	1	-	-	0/6/5/5
4	EDO	Ι	1114	-	-	1/1/1/1	-
2	SF4	А	1105	1	-	-	0/6/5/5
2	SF4	М	1107	1	-	-	0/6/5/5
2	SF4	0	1107	1	-	-	0/6/5/5
4	EDO	Ι	1118	-	_	1/1/1/1	-
4	EDO	М	1123	-	-	1/1/1/1	-
2	SF4	Ι	1107	1	_	_	0/6/5/5
11	PEG	D	4601	-	-	3/4/4/4	-
2	SF4	Е	1105	1	-	-	0/6/5/5
3	FAD	D	4607	-	_	2/30/50/50	$0\overline{6/6/6}$

The worst 5 of 405 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
5	0	1109	SRM	C4A-NA	-20.04	1.21	1.35
5	М	1109	SRM	C4A-NA	-15.21	1.24	1.35
5	Н	4410	SRM	C4A-NA	-15.08	1.24	1.35
5	В	4210	SRM	C4A-NA	-13.42	1.25	1.35
5	L	1109	SRM	C4A-NA	-13.40	1.25	1.35

The worst 5 of 411 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	0	1109	SRM	C3D-CDD-CED	7.20	122.82	114.21
5	0	1109	SRM	C1A-NA-C4A	6.87	113.01	105.23
5	0	1109	SRM	C4C-NC-C1C	6.76	111.97	105.35
5	F	1109	SRM	C2A-C1A-CHA	-5.75	118.29	123.54
5	0	1109	SRM	C2A-C1A-CHA	-5.36	118.65	123.54

5 of 16 chirality outliers are listed below:



Mol	Chain	Res	Type	Atom
5	А	1109	SRM	NC
5	В	4210	SRM	NC
5	С	3910	SRM	NC
5	D	4610	SRM	NC
5	Е	1109	SRM	NC

5 of 353 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Ν	1001[A]	FAD	C2'-C3'-C4'-C5'
3	Ν	1001[A]	FAD	O3'-C3'-C4'-C5'
3	Ν	1001[A]	FAD	C5'-O5'-P-O3P
4	J	1110	EDO	O1-C1-C2-O2
5	Ν	1012	SRM	C2C-C3C-CAC-CBC

There are no ring outliers.

57 monomers are involved in 72 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	1101	SF4	1	0
2	J	1104	SF4	1	0
5	Е	1109	SRM	1	0
9	Ν	1011	GOL	1	0
9	М	1114	GOL	1	0
4	J	1110	EDO	2	0
6	F	1117	SO4	1	0
3	Ν	1009[B]	FAD	1	0
6	В	4226	SO4	1	0
4	Н	4413	EDO	1	0
3	D	4607	FAD	1	0
4	Ι	1115	EDO	1	0
11	Κ	1115	PEG	1	0
2	Н	4405	SF4	1	0
4	G	1118	EDO	2	0
6	F	1118	SO4	1	0
5	М	1109	SRM	1	0
3	Ν	1001[A]	FAD	2	0
4	D	4615	EDO	1	0
9	В	4217[A]	GOL	1	0
9	Р	1111	GOL	2	0
2	В	4202	SF4	1	0
2	В	4205	SF4	1	0
5	Ν	1012	SRM	1	0



Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Е	1106	FAD	1	0
3	Ι	1106	FAD	1	0
4	Н	4412	EDO	3	0
2	М	1104	SF4	1	0
4	В	4216	EDO	1	0
2	G	1101	SF4	1	0
4	В	4211	EDO	1	0
4	G	1120	EDO	1	0
11	М	1115	PEG	2	0
2	D	4605	SF4	1	0
4	G	1116	EDO	1	0
4	Е	1112	EDO	1	0
4	F	1113	EDO	1	0
2	Е	1104	SF4	1	0
2	Р	1104	SF4	1	0
2	N	1006[A]	SF4	2	0
2	N	1007[A]	SF4	3	0
4	А	1116	EDO	2	0
9	F	1114	GOL	1	0
5	F	1109	SRM	1	0
9	С	3901	GOL	3	0
2	М	1103	SF4	1	0
2	0	1105	SF4	1	0
4	K	1116	EDO	1	0
4	J	1112	EDO	2	0
5	0	1109	SRM	1	0
9	Ι	1117	GOL	2	0
2	G	1104	SF4	1	0
9	Ι	1111	GOL	2	0
3	K	1106	FAD	1	0
3	Р	1106	FAD	2	0
4	F	1110[B]	EDO	1	0
2	А	1104	SF4	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.








































































Rings

Torsions














































































































































































































































































































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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	618/618~(100%)	-0.44	2 (0%) 94 95	9, 16, 38, 83	0
1	В	618/618~(100%)	-0.42	1 (0%) 95 95	9, 18, 42, 83	0
1	С	618/618~(100%)	-0.44	1 (0%) 95 95	9, 17, 40, 77	0
1	D	617/618~(99%)	-0.28	12 (1%) 66 73	9, 20, 53, 94	0
1	Е	617/618~(99%)	-0.22	20 (3%) 47 55	10, 22, 59, 88	0
1	F	618/618~(100%)	-0.18	6 (0%) 82 86	10, 25, 54, 79	0
1	G	618/618~(100%)	-0.33	10 (1%) 72 77	9, 17, 46, 94	0
1	Η	617/618~(99%)	-0.27	19 (3%) 49 57	9, 21, 55, 86	0
1	Ι	618/618~(100%)	-0.45	1 (0%) 95 95	13, 20, 42, 78	0
1	J	618/618~(100%)	-0.29	7 (1%) 80 84	11, 24, 54, 79	0
1	Κ	617/618~(99%)	-0.46	1 (0%) 95 95	11, 17, 37, 61	0
1	L	617/618~(99%)	-0.43	0 100 100	10, 20, 45, 61	0
1	М	617/618~(99%)	-0.38	4 (0%) 89 92	11, 22, 45, 66	0
1	Ν	616/618~(99%)	0.51	96~(15%) 2 1	12, 30, 52, 71	16 (2%)
1	Ο	617/618~(99%)	-0.42	1 (0%) 95 95	11, 21, 44, 65	0
1	Р	$61\overline{7/618}~(99\%)$	0.08	45 (7%) 15 17	9, 30, 74, 102	0
All	All	9878/9888 ($99%$)	-0.28	226 (2%) 60 66	9, 21, 50, 102	16 (0%)

The worst 5 of 226 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Р	219	ILE	8.4
1	Е	215	ALA	8.1
1	N	305[A]	LEU	7.6
1	G	231	LYS	7.6
1	Ν	232[A]	GLY	6.7



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	Res	Atoms	RSCC	RSR	$\mathbf{B} extsf{-}\mathbf{factors}(\mathbf{A}^2)$	Q<0.9
9	GOL	В	4218[B]	6/6	0.24	0.26	42,50,52,52	6
9	GOL	J	1114	6/6	0.28	0.34	70,71,72,72	0
11	PEG	N	1014	7/7	0.45	0.21	$59,\!63,\!65,\!65$	0
4	EDO	L	1112	4/4	0.55	0.30	63,63,64,65	0
9	GOL	В	4217[A]	6/6	0.57	0.21	55,57,57,58	6
9	GOL	Р	1112	6/6	0.60	0.19	69,69,71,71	0
12	TRS	Ι	1119	8/8	0.60	0.23	52,54,56,58	0
4	EDO	В	4221	4/4	0.61	0.14	58,59,59,60	0
4	EDO	Ι	1113	4/4	0.68	0.18	41,41,42,43	0
9	GOL	Е	1114	6/6	0.69	0.15	56,59,60,60	0
9	GOL	F	1114	6/6	0.69	0.17	$56,\!56,\!57,\!58$	0
4	EDO	М	1113	4/4	0.70	0.19	47,47,48,49	0
4	EDO	D	4618	4/4	0.72	0.17	60,60,61,62	0
10	LI	L	1118	1/1	0.72	0.27	11,11,11,11	0
4	EDO	А	1114	4/4	0.72	0.13	57,57,57,58	0
4	EDO	D	4617	4/4	0.72	0.18	53,53,54,54	0
4	EDO	G	1120	4/4	0.73	0.12	37,38,39,40	0
4	EDO	В	4211	4/4	0.73	0.22	40,42,43,47	0
11	PEG	K	1115	7/7	0.73	0.14	41,45,50,50	0
4	EDO	М	1117	4/4	0.73	0.14	$51,\!51,\!52,\!52$	0
4	EDO	K	1113	4/4	0.73	0.14	37,39,40,40	0
4	EDO	J	1111	4/4	0.74	0.23	$51,\!53,\!55,\!56$	0
4	EDO	Е	1116	4/4	0.74	0.17	39,40,43,45	0
4	EDO	J	1110	4/4	0.74	0.17	$53,\!54,\!54,\!55$	0
9	GOL	K	1117	6/6	0.75	0.15	38,41,43,46	0
9	GOL	В	4224	6/6	0.75	0.15	$52,\!55,\!57,\!57$	0
4	EDO	М	1124	4/4	0.75	0.21	$51,\!51,\!51,\!51$	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors($Å^2$)	Q<0.9
4	EDO	Ι	1112	4/4	0.76	0.11	48,48,49,50	0
4	EDO	N	1013	4/4	0.76	0.16	49,50,51,53	0
4	EDO	Ι	1118	4/4	0.76	0.19	52,52,54,54	0
9	GOL	М	1114	6/6	0.76	0.14	53,54,54,56	0
9	GOL	N	1015	6/6	0.76	0.13	56,56,57,59	0
6	SO4	J	1119	5/5	0.77	0.28	86,87,87,87	0
4	EDO	F	1111	4/4	0.77	0.14	35,37,37,37	0
4	EDO	М	1122	4/4	0.77	0.12	$57,\!58,\!58,\!59$	0
4	EDO	D	4615	4/4	0.77	0.17	50,50,50,51	0
4	EDO	Ι	1116	4/4	0.77	0.15	45,46,47,48	0
9	GOL	0	1116	6/6	0.78	0.16	59,60,61,61	0
4	EDO	А	1117	4/4	0.78	0.15	64,64,64,65	0
4	EDO	Е	1112	4/4	0.78	0.14	46,47,47,47	0
4	EDO	G	1111	4/4	0.79	0.13	44,45,46,47	0
9	GOL	Ι	1117	6/6	0.79	0.14	60,61,62,63	0
4	EDO	Н	4412	4/4	0.79	0.26	46,46,46,46	0
4	EDO	G	1112	4/4	0.80	0.12	45,46,47,48	0
9	GOL	С	3913	6/6	0.80	0.13	43,45,47,49	0
4	EDO	G	1115	4/4	0.80	0.11	45,45,45,47	0
4	EDO	С	3917	4/4	0.80	0.25	59,60,61,63	0
4	EDO	А	1118	4/4	0.80	0.13	47,48,49,49	0
9	GOL	J	1117[A]	6/6	0.81	0.10	43,49,49,50	0
4	EDO	K	1116	4/4	0.81	0.12	42,42,44,44	0
4	EDO	Ι	1114	4/4	0.81	0.17	50,50,50,51	0
11	PEG	М	1115	7/7	0.81	0.17	36,39,42,45	0
4	EDO	J	1116	4/4	0.81	0.17	58,60,60,60	0
4	EDO	В	4222[A]	4/4	0.81	0.16	25,28,29,31	4
4	EDO	G	1118	4/4	0.82	0.17	53,54,54,54	0
4	EDO	J	1112	4/4	0.82	0.15	38,39,39,39	0
4	EDO	J	1113	4/4	0.82	0.17	52,52,52,53	0
4	EDO	0	1117	4/4	0.82	0.13	49,50,50,51	0
6	SO4	F	1118	5/5	0.82	0.31	101,102,102,102	0
4	EDO	D	4613	4/4	0.83	0.16	51,53,53,54	0
4	EDO	K	1114	4/4	0.83	0.23	$50,\!51,\!53,\!53$	0
4	EDO	0	1118	4/4	0.83	0.11	40,40,41,42	0
4	EDO	Р	1114	4/4	0.83	0.17	58, 58, 58, 59	0
10	LI	F	1121	1/1	0.83	0.32	$18,\!18,\!18,\!18$	0
4	EDO	F	1113	4/4	0.84	0.15	$47, \overline{47, 48, 48}$	0
6	SO4	H	4414	5/5	0.84	0.15	75,75,76,77	0
4	EDO	М	1118	4/4	0.84	0.14	51,52,53,53	0
12	TRS	Η	4401	8/8	0.84	0.15	34,46,50,51	0
6	SO4	Р	1116	5/5	0.84	0.29	91,91,92,92	0



7	Ν	F	2	ł

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors($Å^2$)	Q<0.9
9	GOL	Р	1111	6/6	0.85	0.26	53,54,55,57	0
4	EDO	В	4216	4/4	0.85	0.18	38,38,40,40	0
4	EDO	С	3916	4/4	0.85	0.13	51,51,52,53	0
4	EDO	М	1112	4/4	0.85	0.15	46,46,46,46	0
4	EDO	Н	4413	4/4	0.85	0.12	45,45,45,45	0
4	EDO	М	1116	4/4	0.85	0.20	45,45,45,46	0
4	EDO	Р	1113	4/4	0.85	0.15	46,47,47,48	0
4	EDO	G	1117	4/4	0.85	0.17	63,63,64,64	0
4	EDO	В	4215	4/4	0.85	0.14	49,50,52,53	0
9	GOL	С	3901	6/6	0.86	0.12	57,59,61,62	0
4	EDO	G	1114	4/4	0.86	0.10	48,48,49,49	0
11	PEG	D	4601	7/7	0.86	0.14	40,45,48,49	0
4	EDO	D	4612	4/4	0.86	0.12	46,47,47,47	0
6	SO4	F	1117	5/5	0.86	0.18	88,88,89,89	0
11	PEG	М	1120	7/7	0.86	0.14	$56,\!58,\!59,\!59$	0
9	GOL	Ι	1111	6/6	0.86	0.23	40,45,46,47	0
4	EDO	М	1119	4/4	0.86	0.14	47,47,48,48	0
4	EDO	Е	1111	4/4	0.86	0.13	43,43,45,46	0
4	EDO	Е	1115	4/4	0.87	0.10	31,35,35,36	0
10	LI	Р	1120	1/1	0.87	0.24	11,11,11,11	0
6	SO4	М	1127	5/5	0.87	0.15	93,93,94,94	0
4	EDO	0	1111	4/4	0.87	0.13	19,21,24,25	0
8	CL	N	1018[A]	1/1	0.87	0.09	40,40,40,40	1
9	GOL	G	1119[A]	6/6	0.87	0.10	37,43,45,45	0
4	EDO	0	1113	4/4	0.87	0.13	52,53,54,55	0
4	EDO	В	4213	4/4	0.87	0.12	36,37,38,38	0
4	EDO	G	1116	4/4	0.87	0.16	67,67,67,67	0
4	EDO	С	3915	4/4	0.88	0.11	43,43,45,46	0
4	EDO	А	1116	4/4	0.88	0.12	46,47,48,50	0
4	EDO	Ι	1110	4/4	0.88	0.12	40,41,42,42	0
4	EDO	В	4220[B]	4/4	0.88	0.16	$47,\!47,\!48,\!49$	4
4	EDO	Ν	1010	4/4	0.88	0.14	24,24,27,28	0
4	EDO	D	4616	4/4	0.88	0.11	$52,\!52,\!53,\!53$	0
4	EDO	С	3918	4/4	0.88	0.20	$51,\!52,\!52,\!52$	0
9	GOL	Ν	1011	6/6	0.88	0.20	$31,\!33,\!37,\!39$	0
4	EDO	G	1121	4/4	0.88	0.18	39,39,41,42	0
6	SO4	K	1119	5/5	0.88	0.19	$67, \overline{68}, \overline{70}, \overline{71}$	0
6	$SO\overline{4}$	L	1115	5/5	0.88	0.21	86,86,87,87	0
4	EDO	J	1115	4/4	0.89	0.18	$56,\!56,\!56,\!57$	0
4	EDO	В	4223	4/4	0.89	0.09	$52,\!52,\!52,\!53$	0
6	$SO\overline{4}$	M	1126	5/5	0.89	0.21	70,71,72,73	0
4	EDO	K	1110	4/4	0.89	0.16	$28,\!29,\!31,\!31$	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	D	4614	4/4	0.89	0.11	49,49,49,50	0
4	EDO	М	1123	4/4	0.89	0.13	47,47,48,49	0
4	EDO	В	4214	4/4	0.89	0.10	29,30,30,32	0
4	EDO	А	1110	4/4	0.90	0.13	47,48,48,48	0
4	EDO	0	1115	4/4	0.90	0.11	44,46,48,50	0
4	EDO	В	4219[A]	4/4	0.90	0.09	45,45,46,46	4
4	EDO	L	1110	4/4	0.90	0.09	31,32,32,35	0
4	EDO	С	3914	4/4	0.90	0.10	40,41,42,43	0
4	EDO	Ι	1115	4/4	0.91	0.35	64,64,64,65	0
4	EDO	М	1111	4/4	0.91	0.12	20,21,23,24	0
4	EDO	Е	1117	4/4	0.91	0.14	29,31,31,32	0
4	EDO	А	1115	4/4	0.91	0.07	49,49,50,51	0
6	SO4	F	1116	5/5	0.91	0.35	88,88,88,89	0
4	EDO	G	1113	4/4	0.91	0.10	38,38,39,40	0
4	EDO	А	1113	4/4	0.91	0.10	30,31,32,33	0
4	EDO	0	1112	4/4	0.91	0.11	42,42,42,43	0
4	EDO	G	1110	4/4	0.91	0.13	$17,\!19,\!23,\!24$	0
4	EDO	0	1114	4/4	0.91	0.10	28,32,32,33	0
4	EDO	Н	4411	4/4	0.91	0.14	18,24,24,26	0
4	EDO	А	1111	4/4	0.92	0.12	17,20,23,24	0
4	EDO	В	4201	4/4	0.92	0.12	45,46,46,48	0
4	EDO	Р	1110	4/4	0.92	0.11	21,22,24,24	0
4	EDO	М	1110	4/4	0.92	0.10	35,37,39,40	0
4	EDO	E	1113	4/4	0.92	0.12	54,54,55,55	0
8	CL	В	4229[B]	1/1	0.92	0.09	28,28,28,28	1
4	EDO	А	1112	4/4	0.93	0.11	33,33,34,35	0
4	EDO	F	1112[A]	4/4	0.93	0.12	12,18,18,19	4
6	SO4	D	4621	5/5	0.93	0.24	93,93,94,94	0
4	EDO	F	1110[B]	4/4	0.93	0.14	12,14,14,14	4
3	FAD	F	1106	53/53	0.94	0.07	21,25,28,30	0
4	EDO	E	1108	4/4	0.94	0.07	27,27,28,29	0
4	EDO	0	1110	4/4	0.94	0.12	36,38,38,40	0
6	SO4	D	4620	5/5	0.94	0.30	79,79,80,80	0
8	CL	M	1130[B]	1/1	0.94	0.10	32,32,32,32	1
4	EDO	K	1111	4/4	0.94	0.11	20,21,24,24	0
4	EDO	K	1112	4/4	0.94	0.07	29,29,31,32	0
2	SF4	N	1006[A]	8/8	0.95	0.09	23,26,27,27	8
4	EDO	B	4212	4/4	0.95	0.10	18,18,21,22	0
10		C	3923		0.95	0.18	18,18,18,18	0
4	EDO	0	1108	4/4	0.95	0.07	34,34,34,35	0
3	FAD	P	1106	53/53	0.95	0.08	27,31,35,38	0
4	EDO	C	3911	4/4	0.95	0.08	$28,\!29,\!29,\!30$	0



7	Ν	F	2	ł

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors($Å^2$)	Q<0.9
6	SO4	F	1115	5/5	0.95	0.11	42,42,43,46	0
4	EDO	С	3912	4/4	0.95	0.12	17,20,21,22	0
4	EDO	L	1111	4/4	0.95	0.09	18,20,22,23	0
4	EDO	М	1121	4/4	0.95	0.10	32,33,33,34	0
2	SF4	N	1006[B]	8/8	0.95	0.09	30,33,33,35	8
4	EDO	F	1108	4/4	0.95	0.11	35,35,35,36	0
4	EDO	Е	1110	4/4	0.95	0.09	17,20,21,22	0
8	CL	F	1120[B]	1/1	0.96	0.07	29,29,29,29	1
6	SO4	J	1118	5/5	0.96	0.16	52,53,54,57	0
4	EDO	G	1108	4/4	0.96	0.06	22,23,23,24	0
4	EDO	Р	1108	4/4	0.96	0.07	37,37,37,37	0
6	SO4	L	1113	5/5	0.96	0.17	42,44,46,47	0
4	EDO	Ι	1108	4/4	0.96	0.06	26,27,29,30	0
3	FAD	N	1001[A]	53/53	0.96	0.10	16,20,26,27	53
4	EDO	J	1108	4/4	0.96	0.05	26,26,27,27	0
6	SO4	N	1016	5/5	0.96	0.17	49,51,53,54	0
4	EDO	L	1108	4/4	0.96	0.06	28,29,29,31	0
6	SO4	Н	4415	5/5	0.96	0.16	45,46,46,49	0
6	SO4	0	1119	5/5	0.97	0.13	47,47,49,49	0
6	SO4	0	1120	5/5	0.97	0.13	47,48,49,49	0
4	EDO	Κ	1108	4/4	0.97	0.07	21,21,22,23	0
3	FAD	J	1106	53/53	0.97	0.06	22,26,29,32	0
4	EDO	В	4209	4/4	0.97	0.07	24,24,25,26	0
8	CL	K	1122[B]	1/1	0.97	0.07	26,26,26,26	1
3	FAD	D	4607	53/53	0.97	0.06	20,22,25,27	0
3	FAD	N	1009[B]	53/53	0.97	0.10	15,21,24,28	53
4	EDO	D	4609	4/4	0.97	0.07	$30,\!31,\!32,\!33$	0
4	EDO	Н	4409	4/4	0.97	0.07	24,25,25,26	0
4	EDO	D	4611	4/4	0.97	0.08	$17,\!19,\!21,\!21$	0
3	FAD	Е	1106	53/53	0.97	0.06	20,22,26,29	0
4	EDO	С	3909	4/4	0.97	0.08	22,22,24,24	0
4	EDO	А	1108	4/4	0.97	0.06	$22,\!25,\!26,\!26$	0
6	SO4	L	1114	5/5	0.97	0.15	$53,\!54,\!55,\!56$	0
2	SF4	Ν	1008[B]	8/8	0.97	0.07	$29,\!31,\!33,\!34$	8
6	SO4	А	1119	5/5	0.97	0.15	$40,\!40,\!41,\!43$	0
6	SO4	С	3919	5/5	0.97	0.15	46,47,48,51	0
3	FAD	H	4407	53/53	$0.9\overline{7}$	0.06	17,20,24,26	0
3	FAD	A	1106	53/53	0.98	0.06	10,13,17,21	0
8	CL	H	4418[A]	1/1	0.98	0.07	31,31,31,31	1
8	CL	Ι	1123[B]	1/1	0.98	0.08	36,36,36,36	1
8	CL	J	$1122\overline{[A]}$	1/1	0.98	0.05	40,40,40,40	0
6	SO4	В	4225	5/5	0.98	0.14	43,43,46,46	0



7NPA	7	Ν	F	2	ł
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	CL	L	1117[B]	1/1	0.98	0.05	33,33,33,33	1
3	FAD	G	1106	53/53	0.98	0.06	11,14,17,21	0
6	SO4	D	4619	5/5	0.98	0.15	48,48,50,52	0
3	FAD	В	4207	53/53	0.98	0.06	14,17,21,27	0
3	FAD	Ι	1106	53/53	0.98	0.06	12,18,19,21	0
6	SO4	Е	1118	5/5	0.98	0.16	40,41,44,44	0
3	FAD	С	3907	53/53	0.98	0.06	12,16,18,21	0
3	FAD	K	1106	53/53	0.98	0.06	11,14,18,23	0
3	FAD	L	1106	53/53	0.98	0.06	14,19,22,26	0
3	FAD	М	1106	53/53	0.98	0.06	17,21,24,27	0
6	SO4	G	1122	5/5	0.98	0.13	34,35,37,37	0
4	EDO	М	1108	4/4	0.98	0.05	23,26,27,27	0
2	SF4	N	1007[A]	8/8	0.98	0.07	17,18,19,22	8
6	SO4	Ι	1120	5/5	0.98	0.17	47,49,51,52	0
2	SF4	N	1002	8/8	0.98	0.06	25,26,28,28	0
3	FAD	0	1106	53/53	0.98	0.06	13,18,22,28	0
5	SRM	D	4610	63/63	0.98	0.07	6,10,13,14	0
5	SRM	Е	1109	63/63	0.98	0.07	8,11,14,16	0
5	SRM	G	1109	63/63	0.98	0.07	5,9,13,16	0
5	SRM	Н	4410	63/63	0.98	0.07	9,11,15,18	0
6	SO4	М	1125	5/5	0.98	0.15	48,50,50,51	0
5	SRM	Ι	1109	63/63	0.98	0.07	$9,\!13,\!17,\!20$	0
5	SRM	J	1109	63/63	0.98	0.07	$11,\!14,\!18,\!22$	0
5	SRM	K	1109	63/63	0.98	0.07	$8,\!11,\!15,\!17$	0
5	SRM	L	1109	63/63	0.98	0.07	$8,\!11,\!15,\!17$	0
5	SRM	М	1109	63/63	0.98	0.07	$9,\!13,\!16,\!19$	0
6	SO4	Р	1115	5/5	0.98	0.14	$46,\!46,\!47,\!48$	0
5	SRM	Ν	1012	63/63	0.98	0.07	$11,\!15,\!18,\!20$	0
7	H2S	J	1120	1/1	0.98	0.04	$22,\!22,\!22,\!22$	0
7	H2S	М	1128	1/1	0.98	0.06	$19,\!19,\!19,\!19$	0
8	CL	A	1122[B]	1/1	0.98	0.09	$27,\!27,\!27,\!27$	1
5	SRM	0	1109	63/63	0.98	0.07	$8,\!11,\!14,\!17$	0
8	CL	E	1121[B]	1/1	0.98	0.06	$27,\!27,\!27,\!27$	1
2	SF4	G	1102	8/8	0.99	0.08	11,12,13,13	0
6	SO4	В	4226	5/5	0.99	0.11	40,40,41,41	0
2	SF4	G	1103	8/8	0.99	0.09	13,14,14,14	0
2	SF4	G	1104	8/8	0.99	0.08	11,11,12,12	0
2	SF4	G	1105	8/8	0.99	0.07	15,16,16,17	0
2	SF4	G	1107	8/8	0.99	0.09	10,12,12,12	0
2	SF4	Н	4402	8/8	0.99	0.07	17,18,18,18	0
2	SF4	Н	4403	8/8	0.99	0.07	17,18,18,19	0
2	SF4	Н	4404	8/8	0.99	0.09	10,10,11,11	0



7NPA	
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Mol	Type	Chain	Kes	Atoms	RSCC	KSR	$\frac{\text{B-factors}(\mathbf{A}^2)}{15.151010}$	Q<0.9
2	SF4	H	4408	8/8	0.99	0.07	15,17,18,18	0
2	SF4	l	1101	8/8	0.99	0.08	15,16,16,16	0
2	SF4	l	1103	8/8	0.99	0.08	14,14,15,15	0
2	SF4	I	1105	8/8	0.99	0.08	15,15,16,16	0
2	SF4	I	1107	8/8	0.99	0.07	15,16,17,18	0
2	SF4	J	1101	8/8	0.99	0.06	19,21,21,22	0
2	SF4	J	1102	8/8	0.99	0.07	17,17,17,18	0
2	SF4	J	1103	8/8	0.99	0.08	$13,\!13,\!13,\!13$	0
6	SO4	K	1118	5/5	0.99	0.11	41,42,44,45	0
2	SF4	J	1105	8/8	0.99	0.08	$12,\!13,\!13,\!14$	0
2	SF4	J	1107	8/8	0.99	0.07	$18,\!18,\!19,\!19$	0
2	SF4	Κ	1102	8/8	0.99	0.08	$12,\!12,\!13,\!13$	0
2	SF4	Κ	1103	8/8	0.99	0.08	$13,\!13,\!14,\!15$	0
2	SF4	Κ	1105	8/8	0.99	0.07	$14,\!16,\!16,\!17$	0
2	SF4	Κ	1107	8/8	0.99	0.08	12,12,13,14	0
2	SF4	L	1101	8/8	0.99	0.07	17,17,17,18	0
2	SF4	L	1102	8/8	0.99	0.07	16,17,18,18	0
2	SF4	L	1105	8/8	0.99	0.08	12,13,14,14	0
2	SF4	L	1107	8/8	0.99	0.07	15,16,16,16	0
2	SF4	М	1101	8/8	0.99	0.07	16,17,17,18	0
2	SF4	М	1103	8/8	0.99	0.07	15,16,17,17	0
7	H2S	В	4227	1/1	0.99	0.05	18,18,18,18	0
7	H2S	С	3920	1/1	0.99	0.06	16,16,16,16	0
7	H2S	D	4622	1/1	0.99	0.05	16,16,16,16	0
7	H2S	Е	1119	1/1	0.99	0.07	17,17,17,17	0
2	SF4	М	1104	8/8	0.99	0.08	14,14,14,15	0
7	H2S	K	1120	1/1	0.99	0.05	16,16,16,16	0
7	H2S	L	1116	1/1	0.99	0.06	18,18,18,18	0
2	SF4	М	1105	8/8	0.99	0.07	19,20,21,21	0
7	H2S	N	1017	1/1	0.99	0.05	20,20,20,20	0
2	SF4	М	1107	8/8	0.99	0.08	14,14,15,15	0
8	CL	В	4228	1/1	0.99	0.07	21,21,21,21	0
2	SF4	А	1101	8/8	0.99	0.08	10,11,12,12	0
8	CL	С	3922[B]	1/1	0.99	0.10	32,32,32,32	1
8	CL	D	4623	1/1	0.99	0.05	21,21,21,21	0
2	SF4	N	1003	8/8	0.99	0.08	12,13,14,14	0
2	SF4	N	1004	8/8	0.99	0.08	12,13,14,15	0
8	CL	G	1124	1/1	0.99	0.06	21,21,21,21	0
8	CL	G	1125[A]	1/1	0.99	0.07	31,31,31.31	1
2	SF4	N	1005	8/8	0.99	0.08	12.13.14.14	0
$\frac{1}{2}$	SF4	A	1102	8/8	0.99	0.08	12,12,13,13	0
8	CL	J	1121	1/1	0.99	0.04	27,27,27,27	0



7	Ν	F	P	ł

	Tueu jro	Chain	ls page	Atoma	DECC	DCD	D footong (λ^2)	0 < 0.0
IVI01		Chain	1105	Atoms	RSCC	RSR	$\frac{\text{B-factors}(A^{-})}{10,10,10,10}$	Q<0.9
2	SF4	A	1105	8/8	0.99	0.08	12,12,13,13	0
8	CL CD4	K	1121	1/1	0.99	0.05	19,19,19,19	0
2	SF4	A	1107	8/8	0.99	0.08	11,11,12,13	0
2	SF4	В	4202	8/8	0.99	0.07	14,15,15,15	0
2	SF4	0	1102	8/8	0.99	0.08	12,13,14,14	0
2	SF4	0	1103	8/8	0.99	0.07	19,20,20,20	0
8	CL	0	1123[B]	1/1	0.99	0.06	24,24,24,24	1
8	CL	Р	1118[B]	1/1	0.99	0.05	35,35,35,35	1
8	CL	P	1119	1/1	0.99	0.07	34,34,34,34	0
2	SF4	0	1105	8/8	0.99	0.06	23,26,27,27	0
2	SF4	0	1107	8/8	0.99	0.08	13,14,14,14	0
2	SF4	Р	1101	8/8	0.99	0.05	$30,\!31,\!32,\!32$	0
2	SF4	Р	1102	8/8	0.99	0.06	$27,\!29,\!30,\!30$	0
2	SF4	Р	1107	8/8	0.99	0.06	$29,\!31,\!32,\!33$	0
2	SF4	В	4203	8/8	0.99	0.08	$12,\!12,\!13,\!14$	0
2	SF4	В	4206	8/8	0.99	0.09	$12,\!12,\!13,\!14$	0
2	SF4	С	3903	8/8	0.99	0.08	$12,\!13,\!13,\!13$	0
2	SF4	С	3904	8/8	0.99	0.09	$11,\!12,\!12,\!12$	0
2	SF4	С	3905	8/8	0.99	0.08	10,11,11,11	0
2	SF4	С	3906	8/8	0.99	0.08	12,13,14,14	0
2	SF4	С	3908	8/8	0.99	0.08	12,13,13,14	0
2	SF4	D	4603	8/8	0.99	0.08	$14,\!15,\!15,\!15$	0
5	SRM	А	1109	63/63	0.99	0.07	6, 9, 13, 16	0
5	SRM	В	4210	63/63	0.99	0.07	$5,\!10,\!12,\!16$	0
5	SRM	С	3910	63/63	0.99	0.07	$6,\!10,\!14,\!17$	0
2	SF4	D	4606	8/8	0.99	0.09	11,11,12,12	0
2	SF4	Е	1101	8/8	0.99	0.06	$17,\!17,\!19,\!19$	0
5	SRM	F	1109	63/63	0.99	0.06	$8,\!12,\!15,\!16$	0
2	SF4	Е	1102	8/8	0.99	0.07	$13,\!13,\!14,\!14$	0
2	SF4	Ε	1103	8/8	0.99	0.08	$13,\!14,\!15,\!15$	0
2	SF4	Ε	1104	8/8	0.99	0.08	$12,\!12,\!13,\!13$	0
2	SF4	Ε	1105	8/8	0.99	0.07	$18,\!19,\!20,\!21$	0
2	SF4	Е	1107	8/8	0.99	0.07	$14,\!15,\!16,\!16$	0
2	SF4	F	1101	8/8	0.99	0.06	19,22,22,23	0
2	SF4	F	1102	8/8	0.99	0.07	20,22,23,23	0
2	SF4	F	1104	8/8	0.99	0.09	9,11,12,12	0
2	SF4	F	1107	8/8	0.99	0.06	20,22,22,23	0
5	SRM	Р	1109	63/63	0.99	0.07	11,13,19,20	0
2	SF4	G	1101	8/8	0.99	0.08	12,13,13,13	0
2	SF4	0	1104	8/8	1.00	0.08	$14,\!15,\!16,\!17$	0
2	SF4	А	1104	8/8	1.00	0.09	$10,\!10,\!11,\!12$	0
2	SF4	F	1105	8/8	1.00	0.08	12,12,12,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SF4	L	1103	8/8	1.00	0.08	12,12,13,13	0
2	SF4	L	1104	8/8	1.00	0.09	11,12,12,12	0
8	CL	М	1129	1/1	1.00	0.09	24,24,24,24	0
2	SF4	Р	1103	8/8	1.00	0.09	11,12,12,13	0
2	SF4	Р	1104	8/8	1.00	0.09	10,10,11,12	0
8	CL	0	1122	1/1	1.00	0.07	20,20,20,20	0
7	H2S	А	1120	1/1	1.00	0.06	$15,\!15,\!15,\!15$	0
2	SF4	Р	1105	8/8	1.00	0.08	12,12,12,13	0
2	SF4	Ι	1102	8/8	1.00	0.07	$15,\!15,\!17,\!17$	0
2	SF4	D	4608	8/8	1.00	0.07	$14,\!15,\!16,\!16$	0
2	SF4	Ι	1104	8/8	1.00	0.08	14,15,15,16	0
7	H2S	F	1119	1/1	1.00	0.06	20,20,20,20	0
7	H2S	G	1123	1/1	1.00	0.06	$15,\!15,\!15,\!15$	0
7	H2S	Н	4416	1/1	1.00	0.07	17,17,17,17	0
7	H2S	Ι	1121	1/1	1.00	0.04	20,20,20,20	0
2	SF4	М	1102	8/8	1.00	0.08	14,14,14,15	0
2	SF4	В	4204	8/8	1.00	0.09	10,11,11,12	0
2	SF4	В	4205	8/8	1.00	0.09	9,10,11,11	0
2	SF4	А	1103	8/8	1.00	0.08	10,11,11,12	0
2	SF4	В	4208	8/8	1.00	0.08	12,13,14,14	0
7	H2S	0	1121	1/1	1.00	0.06	17,17,17,17	0
7	H2S	Р	1117	1/1	1.00	0.07	21,21,21,21	0
8	CL	А	1121	1/1	1.00	0.06	18,18,18,18	0
2	SF4	D	4602	8/8	1.00	0.07	16,17,17,17	0
2	SF4	J	1104	8/8	1.00	0.08	12,13,14,14	0
2	SF4	С	3902	8/8	1.00	0.08	13,14,14,15	0
8	CL	С	3921	1/1	1.00	0.06	19,19,19,19	0
2	SF4	D	4604	8/8	1.00	0.09	10,11,12,12	0
2	SF4	K	1101	8/8	1.00	0.08	12,13,14,14	0
8	CL	D	4624[B]	1/1	1.00	0.08	29,29,29,29	1
8	CL	Е	1120	1/1	1.00	0.04	$25,\!25,\!25,\!25$	0
2	SF4	D	4605	8/8	1.00	0.08	9,10,10,11	0
2	SF4	F	1103	8/8	1.00	0.08	11,11,12,12	0
2	SF4	K	1104	8/8	1.00	0.08	12,12,13,13	0
2	SF4	0	1101	8/8	1.00	0.07	$13,\!14,\!15,\!15$	0
8	CL	Н	4417	1/1	1.00	0.05	24,24,24,24	0
2	SF4	Н	4405	8/8	1.00	0.09	$9,\!10,\!10,\!10$	0
8	CL	Ι	1122	1/1	1.00	0.06	23,23,23,23	0
2	SF4	Н	4406	8/8	1.00	0.08	$10,\!11,\!11,\!12$	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different



orientation to approximate a three-dimensional view.







































































































































































































































































































































































































































































































































































































6.5 Other polymers (i)

There are no such residues in this entry.

