

wwPDB X-ray Structure Validation Summary Report (i)

Aug 14, 2023 – 10:40 am BST

PDB ID	:	8CFF
Title	:	Crystal structure of arsenite oxidase from Alcaligenes faecalis (Af Aio) bound
		to arsenite
Authors	:	Engrola, F.; Correia, M.A.S.; Romao, M.J.; Santos-Silva, T.
Deposited on	:	2023-02-03
Resolution	:	1.57 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	:	2.35
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)	:	2.35

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 1.57 Å.

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



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703(1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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	А	823	91%	9%	_
1	С	823	90%	9%	•
1	Е	823	91%	8%	•
1	G	823	89%	11%	
2	В	134	% 90%	10%	•



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Mol	Chain	Length	Quality of chain	
2	D	134	93%	7% •
2	F	134	% 93%	5% •
2	Н	134	% 9 0%	8% •

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
11	IPA	С	906	-	-	Х	-
11	IPA	G	908	-	-	Х	-
7	GOL	С	912	-	-	Х	-
7	GOL	Е	912	-	-	Х	-
9	EDO	А	908[A]	-	-	Х	Х
9	EDO	А	908[B]	-	-	Х	Х
9	EDO	А	909	-	-	Х	-



2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 34530 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		Α	toms			ZeroOcc	AltConf	Trace			
1	Δ	823	Total	С	Ν	Ο	\mathbf{S}	0	7	0			
1	Π	025	6523	4106	1155	1220	42		1	U			
1	C	C	C	800	800	Total	С	Ν	Ο	\mathbf{S}	5	10	0
1	U	022	6555	4124	1161	1226	44	G	10	0			
1	F	822	Total	С	Ν	Ο	\mathbf{S}	0	7	0			
1		022	6526	4108	1157	1218	43	0	1	0			
1	С	822	Total	Ċ	Ν	Ō	S	1	8	0			
	G	022	6517	4101	1153	1221	42		8				

• Molecule 1 is a protein called Arsenite oxidase subunit AioA.

• Molecule 2 is a protein called Arsenite oxidase subunit AioB.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
0	D	194	Total	С	Ν	0	\mathbf{S}	0	9	0
	D	104	1018	637	170	202	9	0	0	0
0	П	194	Total	С	Ν	0	\mathbf{S}	2	2	0
	D	104	1015	635	170	201	9			0
0	Б	194	Total	С	Ν	0	S	1	2	0
	Г	104	1009	632	169	199	9	L		0
0	ц	124	Total	С	Ν	0	S	2	2	0
	п	104	1018	637	170	202	9		ن ا	U

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	0	LEU	-	expression tag	UNP Q7SIF3
D	0	LEU	-	expression tag	UNP Q7SIF3
F	0	LEU	-	expression tag	UNP Q7SIF3
Н	0	LEU	-	expression tag	UNP Q7SIF3

• Molecule 3 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		А	tom	IS			ZeroOcc	AltConf
2	Δ	1	Total	С	Ν	Ο	Р	S	0	0
0	A	1	47	20	10	13	2	2	0	0
9	Δ	1	Total	С	Ν	Ο	Р	S	0	0
0	3 A	1	47	20	10	13	2	2	0	0
2	C	1	Total	С	Ν	Ο	Р	S	0	0
0	U	1	47	20	10	13	2	2	0	0
2	С	1	Total	С	Ν	Ο	Р	S	0	0
0			47	20	10	13	2	2		0
2	F	1	Total	С	Ν	Ο	Р	S	0	0
0	Ľ	1	47	20	10	13	2	2	0	0
3	F	1	Total	С	Ν	Ο	Р	S	0	0
0	Ľ	1	47	20	10	13	2	2	0	0
3	С	1	Total	С	Ν	Ο	Р	S	0	0
0	G	1	47	20	10	13	2	2	0	0
3	G	1	Total	С	Ν	Ο	Р	S	0	0
5	G	L	47	20	10	13	2	2	U	U

• Molecule 4 is MOLYBDENUM ATOM (three-letter code: MO) (formula: Mo) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Mo 1 1	0	0
4	С	1	Total Mo 1 1	0	0
4	Е	1	Total Mo 1 1	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Mo 1 1	0	0

• Molecule 5 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe₃S₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	TotalFeS734	0	0
5	С	1	TotalFeS734	0	0
5	Ε	1	TotalFeS734	0	0
5	G	1	TotalFeS734	0	0

• Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	Total C O 20 12 8	0	1
6	G	1	Total C O 10 6 4	0	0

• Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	Ε	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
7	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 8 is ARSENITE (three-letter code: AST) (formula: AsO₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	А	1	Total As 4 1	O 3	0	0
8	С	1	Total As 4 1	O 3	0	0
8	Ε	1	Total As 4 1	O 3	0	0
8	G	1	Total As 4 1	0 3	0	0



• Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 8 & 4 & 4 \end{array}$	0	1
9	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
9	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
9	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
9	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 8 4 4 \end{array}$	0	1
9	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	С	1	$\begin{array}{c cc} \text{Total} & \text{C} & \overline{\text{O}} \\ 4 & 2 & 2 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
9	Е	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
9	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	Ε	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	G	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 8 4 4 \end{array}$	0	1
9	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
9	G	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
9	G	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0

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





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
10	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0

• Molecule 11 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



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

• Molecule 12 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	В	1	TotalFeS422	0	0
12	D	1	TotalFeS422	0	0
12	F	1	TotalFeS422	0	0
12	Н	1	Total Fe S 4 2 2	0	0

• Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	А	806	Total O 806 806	0	0
13	В	137	Total O 137 137	0	0
13	С	760	Total O 760 760	0	0
13	D	148	Total O 148 148	0	0
13	Ε	751	Total O 751 751	0	0
13	F	129	Total O 129 129	0	0
13	G	799	Total O 799 799	0	0
13	Н	153	Total O 153 153	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: Arsenite oxidase subunit AioA





• Molecule 1: Arsenite oxidase subunit AioA





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	90.31Å 108.98Å 116.89Å	Depositor
a, b, c, α , β , γ	97.50° 90.21° 96.06°	Depositor
Bosolution(A)	65.62 - 1.57	Depositor
	107.43 - 1.57	EDS
% Data completeness	$73.2\ (65.62-1.57)$	Depositor
(in resolution range)	73.2(107.43-1.57)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.87 (at 1.57 Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
P. P.	0.168 , 0.204	Depositor
n, n_{free}	0.178 , 0.213	DCC
R_{free} test set	22459 reflections $(4.96%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	12.4	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.37, 33.1	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	0.95	EDS
Total number of atoms	34530	wwPDB-VP
Average B, all atoms $(Å^2)$	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 11.54% 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: AST, MO, PEG, IPA, MGD, GOL, FES, EDO, F3S, PGE

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		
WIOI	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.86	4/6691~(0.1%)	0.97	9/9069~(0.1%)	
1	С	0.85	6/6722~(0.1%)	0.95	3/9107~(0.0%)	
1	Ε	0.86	5/6696~(0.1%)	0.97	6/9073~(0.1%)	
1	G	0.90	9/6690~(0.1%)	1.01	15/9066~(0.2%)	
2	В	0.87	1/1042~(0.1%)	0.97	1/1419~(0.1%)	
2	D	1.79	3/1036~(0.3%)	1.01	2/1412~(0.1%)	
2	F	0.93	4/1033~(0.4%)	0.95	1/1407~(0.1%)	
2	Н	0.90	1/1042~(0.1%)	1.00	2/1419~(0.1%)	
All	All	0.92	33/30952~(0.1%)	0.98	39/41972~(0.1%)	

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

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	D	5	GLN	CD-NE2	49.81	2.57	1.32
1	G	121	LYS	CE-NZ	-20.86	0.96	1.49
1	G	663	GLU	CD-OE2	8.61	1.35	1.25
2	D	5	GLN	CD-OE1	-8.59	1.05	1.24
1	А	721	GLU	CD-OE1	8.50	1.35	1.25

The worst 5 of 39 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	G	121	LYS	CD-CE-NZ	18.84	155.03	111.70
1	А	295	ARG	NE-CZ-NH1	13.25	126.93	120.30
1	А	295	ARG	NE-CZ-NH2	-12.76	113.92	120.30
1	G	295	ARG	NE-CZ-NH1	10.90	125.75	120.30
1	G	295	ARG	NE-CZ-NH2	-10.27	115.17	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Group
1	А	22	HIS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	6523	0	6319	75	0
1	С	6555	0	6342	68	1
1	Е	6526	0	6328	61	0
1	G	6517	0	6311	62	1
2	В	1018	0	999	12	0
2	D	1015	0	995	8	0
2	F	1009	0	994	6	0
2	Н	1018	0	999	9	0
3	А	94	0	44	1	0
3	С	94	0	44	3	0
3	Е	94	0	44	2	0
3	G	94	0	44	1	0
4	А	1	0	0	0	0
4	С	1	0	0	0	0
4	Е	1	0	0	1	0
4	G	1	0	0	0	0
5	А	7	0	0	0	0
5	С	7	0	0	0	0
5	Е	7	0	0	0	0
5	G	7	0	0	0	0
6	A	20	0	28	5	0
6	G	10	0	14	1	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	А	6	0	8	2	0
7	С	18	0	24	6	0
7	Е	18	0	24	8	0
7	G	12	0	16	4	0
8	А	4	0	0	0	0
8	С	4	0	0	0	0
8	Е	4	0	0	1	0
8	G	4	0	0	0	0
9	А	32	0	45	18	0
9	С	28	0	42	7	0
9	D	4	0	6	1	0
9	Е	20	0	30	0	0
9	G	28	0	41	7	0
10	А	7	0	10	3	0
10	В	7	0	10	3	0
11	А	4	0	8	3	0
11	С	4	0	8	4	0
11	Ε	4	0	8	0	0
11	G	4	0	8	7	0
12	В	4	0	0	0	0
12	D	4	0	0	0	0
12	F	4	0	0	0	0
12	Н	4	0	0	0	0
13	А	806	0	0	19	3
13	В	137	0	0	4	0
13	С	760	0	0	27	11
13	D	148	0	0	2	1
13	Е	751	0	0	14	4
13	F	129	0	0	3	0
13	G	799	0	0	29	7
13	Н	153	0	0	4	4
All	All	34530	0	29793	316	16

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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 5.

The worst 5 of 316 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
9:A:908[A]:EDO:O1	9:A:909:EDO:C1	1.91	1.19	
9:A:908[A]:EDO:O1	9:A:909:EDO:H11	1.40	1.17	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
1:G:484[A]:MET:HE3	13:G:1007:HOH:O	1.48	1.14	
9:C:910:EDO:H21	13:C:1110:HOH:O	1.44	1.12	
11:A:913:IPA:H33	13:A:1527:HOH:O	1.52	1.10	

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The worst 5 of 16 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:GLN:NE2	1:G:471[A]:GLU:OE2[1_455]	1.51	0.69
13:C:1758:HOH:O	13:G:1797:HOH:O[1_455]	1.64	0.56
13:C:1642:HOH:O	13:G:1732:HOH:O[1_455]	1.68	0.52
13:A:1806:HOH:O	13:G:1799:HOH:O[1_465]	1.69	0.51
13:A:1788:HOH:O	13:E:1744:HOH:O[1_455]	1.70	0.50

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	828/823~(101%)	796~(96%)	30 (4%)	2(0%)	47	25
1	С	831/823~(101%)	802 (96%)	29 (4%)	0	100	100
1	Ε	828/823~(101%)	797~(96%)	28 (3%)	3~(0%)	34	15
1	G	828/823~(101%)	801~(97%)	26 (3%)	1 (0%)	51	28
2	В	135/134~(101%)	130~(96%)	5 (4%)	0	100	100
2	D	134/134~(100%)	128~(96%)	6 (4%)	0	100	100
2	F	134/134~(100%)	128 (96%)	6 (4%)	0	100	100
2	Η	135/134~(101%)	126 (93%)	9 (7%)	0	100	100
All	All	3853/3828 (101%)	3708 (96%)	139 (4%)	6 (0%)	47	25

5 of 6 Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	Ε	392	ASP
1	А	392	ASP
1	G	392	ASP
1	Е	518	THR
1	А	793	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	683/676~(101%)	672~(98%)	11 (2%)	62 39
1	С	686/676~(102%)	670~(98%)	16 (2%)	50 23
1	Ε	683/676~(101%)	668~(98%)	15 (2%)	52 25
1	G	683/676~(101%)	667~(98%)	16 (2%)	50 23
2	В	115/112~(103%)	113~(98%)	2(2%)	60 36
2	D	114/112~(102%)	113~(99%)	1 (1%)	78 64
2	F	114/112~(102%)	111~(97%)	3(3%)	46 19
2	Н	115/112~(103%)	112 (97%)	3 (3%)	46 19
All	All	3193/3152~(101%)	3126 (98%)	67 (2%)	55 27

5 of 67 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	G	486	LYS
1	G	532	HIS
2	Н	104	ARG
1	С	548	ARG
1	С	532	HIS

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such side chains are listed below:

Mol	Chain	Res	Type				
1	Е	485	GLN				
Continued on next nage							



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Mol	Chain	Res	Type
1	Ε	792	ASN
2	Н	51	ASN
1	G	504	GLN
1	С	77	ASN

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 70 ligands modelled in this entry, 4 are monoatomic - leaving 66 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	l Type Chain Bes		Link	Bo	ond leng	sths	Bond angles			
	туре	Ullalli	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	С	912	-	$5,\!5,\!5$	0.38	0	$5,\!5,\!5$	0.97	0
7	GOL	G	905	-	$5,\!5,\!5$	0.49	0	$5,\!5,\!5$	0.86	0
9	EDO	G	909[A]	-	$3,\!3,\!3$	0.23	0	2,2,2	0.61	0
11	IPA	А	913	-	$3,\!3,\!3$	0.42	0	3,3,3	0.40	0
9	EDO	G	915	-	$3,\!3,\!3$	0.28	0	2,2,2	0.21	0
9	EDO	А	911	-	$3,\!3,\!3$	0.19	0	2,2,2	0.73	0
8	AST	С	905	-	0,3,3	-	-	0,3,3	-	-
9	EDO	Е	910	-	$3,\!3,\!3$	0.94	0	2,2,2	0.83	0
9	EDO	G	911	-	3,3,3	0.19	0	2,2,2	0.53	0
7	GOL	С	909	-	$5,\!5,\!5$	0.24	0	$5,\!5,\!5$	0.82	0



N T 1	T		Б	T · 1	Bond lengths		Bond angles			
IVIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	PEG	А	910	-	$6,\!6,\!6$	0.32	0	$5,\!5,\!5$	0.24	0
3	MGD	А	901	4	41,52,52	1.00	3 (7%)	40,81,81	1.49	4 (10%)
5	F3S	Е	904	1	0,9,9	-	-	-		
7	GOL	G	913	-	5, 5, 5	0.27	0	5, 5, 5	1.07	0
9	EDO	С	911[B]	-	3,3,3	0.30	0	2,2,2	0.39	0
9	EDO	G	914	-	3,3,3	0.71	0	2,2,2	0.37	0
10	PEG	В	2301	-	$6,\!6,\!6$	0.30	0	$5,\!5,\!5$	0.25	0
12	FES	В	2302	2	0,4,4	-	-	-		
9	EDO	G	912	-	3,3,3	0.76	0	2,2,2	0.44	0
12	FES	Н	201	2	$0,\!4,\!4$	-	-	-		
9	EDO	Е	908	-	3, 3, 3	0.74	0	$2,\!2,\!2$	1.13	0
9	EDO	Ε	909	-	3, 3, 3	0.78	0	$2,\!2,\!2$	0.53	0
3	MGD	G	902	4	$41,\!52,\!52$	0.98	4 (9%)	40,81,81	1.25	<mark>6 (15%)</mark>
9	EDO	А	912	-	3,3,3	0.42	0	2,2,2	0.31	0
9	EDO	А	909	-	3,3,3	0.71	0	2,2,2	0.94	0
9	EDO	Е	907	-	3,3,3	0.94	0	2,2,2	0.57	0
12	FES	F	201	2	0,4,4	-	-	-		
6	PGE	А	905[B]	-	$9,\!9,\!9$	0.19	0	8,8,8	0.25	0
9	EDO	С	907	-	3,3,3	0.70	0	2,2,2	1.19	0
11	IPA	С	906	-	3,3,3	0.98	0	$3,\!3,\!3$	0.63	0
9	EDO	С	910	-	3, 3, 3	0.57	0	$2,\!2,\!2$	0.63	0
9	EDO	А	915	-	3, 3, 3	0.69	0	$2,\!2,\!2$	0.64	0
9	EDO	А	908[B]	-	3, 3, 3	1.05	0	$2,\!2,\!2$	0.82	0
11	IPA	G	908	-	3, 3, 3	0.87	0	3, 3, 3	1.18	0
7	GOL	Е	912	-	$5,\!5,\!5$	0.14	0	$5,\!5,\!5$	0.55	0
8	AST	A	907	-	0,3,3	-	-	$0,\!3,\!3$	-	-
8	AST	G	906	-	0,3,3	-	-	$0,\!3,\!3$	-	-
7	GOL	E	913	-	$5,\!5,\!5$	0.21	0	$5,\!5,\!5$	0.62	0
11	IPA	E	905	-	3,3,3	0.46	0	3, 3, 3	0.58	0
9	EDO	A	914	-	3,3,3	0.58	0	2,2,2	0.67	0
9	EDO	G	909[B]	-	3,3,3	0.36	0	$2,\!2,\!2$	0.59	0
3	MGD	Ε	901	4	$41,\!52,\!52$	1.13	3 (7%)	40,81,81	1.24	4 (10%)
9	EDO	С	911[A]	-	3,3,3	0.37	0	$2,\!2,\!2$	0.81	0
3	MGD	А	902	4	$41,\!52,\!52$	1.00	2 (4%)	40,81,81	1.36	4 (10%)
9	EDO	D	202	-	3,3,3	0.73	0	2,2,2	0.49	0
3	MGD	Е	903	4	41,52,52	1.14	3 (7%)	40,81,81	1.27	4 (10%)
9	EDO	С	914	-	3,3,3	1.01	0	2,2,2	0.91	0
12	FES	D	201	2	0,4,4	-	-	-		·
3	MGD	С	902	4	41,52,52	0.98	2 (4%)	40,81,81	1.23	4 (10%)
5	F3S	А	904	1	0,9,9	-	-	-		
6	PGE	А	905[A]	-	$9,\!9,\!9$	0.61	0	8,8,8	0.58	0
8	AST	Е	906	-	0,3,3	-	-	0,3,3	-	-



Mal	Tuno	Chain	Dog	Link	Bo	ond leng	ths	В	ond ang	les
WIOI	Type	Ullalli	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
9	EDO	С	915	-	3,3,3	0.16	0	$2,\!2,\!2$	0.41	0
9	EDO	Е	911	-	3,3,3	0.52	0	$2,\!2,\!2$	0.51	0
9	EDO	G	910	-	3,3,3	0.15	0	2,2,2	0.36	0
5	F3S	G	904	1	0,9,9	-	-	-		
7	GOL	С	908	-	$5,\!5,\!5$	0.20	0	$5,\!5,\!5$	0.30	0
3	MGD	G	903	4	$41,\!52,\!52$	1.03	4 (9%)	40,81,81	1.01	3 (7%)
7	GOL	Е	914	-	$5,\!5,\!5$	0.20	0	$5,\!5,\!5$	0.23	0
7	GOL	А	906	-	$5,\!5,\!5$	0.47	0	$5,\!5,\!5$	0.94	0
3	MGD	С	903	4	$41,\!52,\!52$	1.12	3 (7%)	40,81,81	1.31	3 (7%)
5	F3S	С	904	1	$0,\!9,\!9$	-	-	-		
9	EDO	А	908[A]	-	3, 3, 3	0.26	0	$2,\!2,\!2$	0.40	0
9	EDO	С	913	-	3, 3, 3	0.29	0	$2,\!2,\!2$	0.37	0
9	EDO	A	916	-	3, 3, 3	1.05	0	2,2,2	0.89	0
6	PGE	G	907	-	9,9,9	0.83	0	8,8,8	0.33	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
7	GOL	С	912	-	-	4/4/4/4	-
7	GOL	G	905	-	-	4/4/4/4	-
9	EDO	G	909[A]	-	-	1/1/1/1	-
9	EDO	G	915	-	-	1/1/1/1	-
9	EDO	А	911	-	-	0/1/1/1	-
9	EDO	E	910	-	-	1/1/1/1	-
9	EDO	G	911	-	-	0/1/1/1	-
7	GOL	С	909	-	-	4/4/4/4	-
10	PEG	А	910	-	-	2/4/4/4	-
3	MGD	А	901	4	-	4/18/66/66	0/6/6/6
7	GOL	G	913	-	-	4/4/4/4	-
9	EDO	G	914	-	-	0/1/1/1	-
9	EDO	С	911[B]	-	-	1/1/1/1	-
10	PEG	В	2301	-	-	3/4/4/4	-
5	F3S	Е	904	1	-	-	0/3/3/3
12	FES	В	2302	2	-	-	0/1/1/1
9	EDO	G	912	-	-	1/1/1/1	-
12	FES	Н	201	2	-	-	0/1/1/1
9	EDO	E	908	-	-	1/1/1/1	-
9	EDO	Е	909	-	-	0/1/1/1	-



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MGD	G	902	4	-	4/18/66/66	0/6/6/6
9	EDO	A	912	-	_	0/1/1/1	-
9	EDO	А	909	-	-	1/1/1/1	-
9	EDO	Е	907	-	-	1/1/1/1	-
12	FES	F	201	2	-	-	0/1/1/1
6	PGE	А	905[B]	-	-	5/7/7/7	-
9	EDO	С	907	-	-	0/1/1/1	-
9	EDO	С	910	-	-	1/1/1/1	-
9	EDO	A	915	-	-	0/1/1/1	-
9	EDO	A	908[B]	-	-	0/1/1/1	-
7	GOL	E	912	-	-	4/4/4/4	-
7	GOL	Е	913	-	-	0/4/4/4	-
9	EDO	A	914	-	-	0/1/1/1	-
9	EDO	G	909[B]	-	-	1/1/1/1	-
3	MGD	E	901	4	-	4/18/66/66	0/6/6/6
9	EDO	С	911[A]	-	-	0/1/1/1	-
3	MGD	А	902	4	-	4/18/66/66	0/6/6/6
9	EDO	D	202	-	-	0/1/1/1	-
3	MGD	Е	903	4	-	4/18/66/66	0/6/6/6
9	EDO	С	914	-	-	1/1/1/1	-
12	FES	D	201	2	-	-	0/1/1/1
3	MGD	С	902	4	-	4/18/66/66	0/6/6/6
6	PGE	А	905[A]	-	-	3/7/7/7	-
9	EDO	С	915	-	-	0/1/1/1	-
9	EDO	Е	911	-	-	1/1/1/1	-
9	EDO	G	910	-	-	1/1/1/1	-
5	F3S	А	904	1	-	-	0/3/3/3
5	F3S	G	904	1	-	-	0/3/3/3
7	GOL	С	908	-	-	4/4/4/4	-
3	MGD	G	903	4	-	5/18/66/66	0/6/6/6
7	GOL	Е	914	-	-	0/4/4/4	-
7	GOL	А	906	-	-	2/4/4/4	-
3	MGD	С	903	4	-	5/18/66/66	0/6/6/6
5	F3S	C	904	1	-	-	0/3/3/3
9	EDO	A	908[A]	-	-	1/1/1/1	-
9	EDO	С	913	-	-	1/1/1/1	-
9	EDO	A	916	-	-	0/1/1/1	-
6	PGE	G	907	-	-	5/7/7/7	-

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The worst 5 of 24 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
3	Е	901	MGD	C23-C14	4.02	1.56	1.53
3	С	903	MGD	C23-C14	3.40	1.56	1.53
3	Е	903	MGD	C5-C6	-3.07	1.41	1.47
3	G	903	MGD	C5-C6	-2.86	1.41	1.47
3	С	902	MGD	C23-C14	-2.82	1.51	1.53

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	А	901	MGD	O11-C23-C14	6.18	113.08	108.96
3	С	903	MGD	O11-C23-C14	5.35	112.53	108.96
3	А	902	MGD	O11-C23-C14	4.19	111.76	108.96
3	Е	901	MGD	C19-N20-C21	3.66	120.04	113.43
3	А	902	MGD	C19-N20-C21	3.34	119.47	113.43

There are no chirality outliers.

5 of 93 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	901	MGD	C5'-O5'-PB-O1B
3	А	902	MGD	C5'-O5'-PB-O1B
3	А	902	MGD	C5'-O5'-PB-O3B
3	С	902	MGD	C5'-O5'-PB-O1B
3	С	902	MGD	C5'-O5'-PB-O3B

There are no ring outliers.

34 monomers are involved in 87 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	С	912	GOL	4	0
7	G	905	GOL	1	0
11	А	913	IPA	3	0
9	G	915	EDO	2	0
7	С	909	GOL	2	0
10	А	910	PEG	3	0
3	А	901	MGD	1	0
7	G	913	GOL	3	0
9	С	911[B]	EDO	1	0
9	G	914	EDO	2	0
10	В	2301	PEG	3	0
9	G	912	EDO	1	0
9	А	912	EDO	2	0



Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	А	909	EDO	8	0
9	С	907	EDO	2	0
11	С	906	IPA	4	0
9	С	910	EDO	1	0
9	А	908[B]	EDO	5	0
11	G	908	IPA	7	0
7	Е	912	GOL	7	0
9	А	914	EDO	2	0
9	G	909[B]	EDO	2	0
3	Е	901	MGD	2	0
9	С	911[A]	EDO	3	0
9	D	202	EDO	1	0
6	А	905[A]	PGE	5	0
8	Е	906	AST	1	0
3	G	903	MGD	1	0
7	Е	914	GOL	1	0
7	А	906	GOL	2	0
3	С	903	MGD	3	0
9	А	908[A]	EDO	7	0
9	А	916	EDO	1	0
6	G	907	PGE	1	0

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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 sufficient 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	$OWAB(Å^2)$	Q < 0.9
1	А	823/823~(100%)	-0.31	2 (0%) 95 94	8, 13, 22, 33	1 (0%)
1	С	822/823~(99%)	-0.37	2 (0%) 95 94	9, 13, 22, 36	3~(0%)
1	Ε	822/823~(99%)	-0.37	1 (0%) 95 95	9, 13, 22, 33	1 (0%)
1	G	822/823~(99%)	-0.31	0 100 100	9, 13, 22, 34	2 (0%)
2	В	134/134~(100%)	-0.29	2 (1%) 73 75	10, 13, 22, 35	0
2	D	134/134~(100%)	-0.32	0 100 100	10, 14, 21, 34	2(1%)
2	F	134/134~(100%)	-0.27	1 (0%) 87 88	10, 14, 22, 32	1 (0%)
2	Н	134/134~(100%)	-0.28	1 (0%) 87 88	10, 14, 23, 39	2(1%)
All	All	3825/3828~(99%)	-0.33	9 (0%) 95 94	8, 13, 22, 39	12 (0%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	3	PRO	3.4
1	С	435	ASP	2.6
1	А	528[A]	LEU	2.6
2	В	44	PRO	2.6
1	С	485	GLN	2.5

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	\mathbf{RSR}	B-factors(Å ²)	Q<0.9
6	PGE	G	907	10/10	0.58	0.21	29,32,36,36	0
11	IPA	С	906	4/4	0.61	0.18	16,16,18,21	0
9	EDO	А	908[B]	4/4	0.64	0.46	20,21,23,24	4
9	EDO	А	908[A]	4/4	0.64	0.46	24,25,26,26	4
11	IPA	G	908	4/4	0.65	0.21	15,16,19,23	0
9	EDO	G	912	4/4	0.73	0.16	34,35,35,36	0
11	IPA	А	913	4/4	0.74	0.17	23,24,24,26	0
9	EDO	С	911[A]	4/4	0.75	0.19	28,28,28,29	4
9	EDO	С	911[B]	4/4	0.75	0.19	23,24,25,25	4
9	EDO	G	911	4/4	0.77	0.16	31,32,32,33	0
9	EDO	G	915	4/4	0.80	0.16	25,25,26,26	0
7	GOL	Е	912	6/6	0.82	0.25	16,17,18,18	0
9	EDO	G	909[A]	4/4	0.82	0.12	15,16,16,17	4
9	EDO	G	909[B]	4/4	0.82	0.12	15,15,15,16	4
9	EDO	С	910	4/4	0.83	0.14	25,28,29,32	0
6	PGE	А	905[A]	10/10	0.83	0.17	16,19,22,22	10
6	PGE	А	905[B]	10/10	0.83	0.17	14,14,15,15	10
11	IPA	Е	905	4/4	0.83	0.10	27,28,28,29	0
9	EDO	Е	910	4/4	0.83	0.12	26,26,26,27	0
9	EDO	С	907	4/4	0.85	0.17	25,26,27,28	0
7	GOL	С	908	6/6	0.86	0.11	32,33,34,34	0
10	PEG	А	910	7/7	0.86	0.12	28,28,29,32	0
9	EDO	D	202	4/4	0.87	0.22	22,22,24,24	0
9	EDO	С	914	4/4	0.87	0.08	19,20,21,22	0
7	GOL	С	909	6/6	0.88	0.14	28,29,31,32	0
7	GOL	G	905	6/6	0.90	0.13	14,16,18,22	0
9	EDO	Е	907	4/4	0.90	0.11	24,27,27,28	0
9	EDO	Е	909	4/4	0.90	0.09	23,26,27,27	0
9	EDO	А	914	4/4	0.90	0.17	20,24,24,26	0
9	EDO	А	916	4/4	0.90	0.21	22,22,23,25	0
9	EDO	С	913	4/4	0.90	0.18	32,32,33,35	0
7	GOL	Е	913	6/6	0.90	0.17	23,24,25,25	0
7	GOL	А	906	6/6	0.91	0.15	13,16,19,25	0
9	EDO	А	911	4/4	0.91	0.07	30,32,33,34	0
9	EDO	А	912	4/4	0.91	0.15	26,26,28,28	0
9	EDO	Е	911	4/4	0.91	0.15	24,25,27,28	0
7	GOL	G	913	6/6	0.91	0.13	21,25,27,27	0



8CFF	
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
8	AST	А	907	4/4	0.91	0.11	13,14,14,15	1
7	GOL	Е	914	6/6	0.91	0.14	21,23,25,26	0
9	EDO	А	915	4/4	0.92	0.11	15,17,17,18	0
10	PEG	В	2301	7/7	0.93	0.18	23,24,24,25	0
9	EDO	G	910	4/4	0.94	0.05	30,30,30,31	0
7	GOL	С	912	6/6	0.95	0.16	15,18,19,23	0
9	EDO	G	914	4/4	0.95	0.07	21,22,22,24	0
9	EDO	А	909	4/4	0.95	0.12	14,15,17,17	0
9	EDO	С	915	4/4	0.96	0.07	20,20,21,21	0
9	EDO	Е	908	4/4	0.96	0.07	14,15,16,16	0
8	AST	G	906	4/4	0.96	0.09	12,12,12,13	1
8	AST	Е	906	4/4	0.97	0.12	12,13,14,14	1
8	AST	С	905	4/4	0.97	0.09	11,12,13,13	1
3	MGD	А	902	47/47	0.98	0.07	7,9,10,10	0
3	MGD	С	902	47/47	0.98	0.06	8,9,10,12	0
3	MGD	С	903	47/47	0.98	0.06	9,9,10,10	0
3	MGD	Е	901	47/47	0.98	0.06	9,9,10,10	0
3	MGD	Е	903	47/47	0.98	0.06	8,9,10,10	0
3	MGD	G	902	47/47	0.98	0.06	8,9,10,11	0
3	MGD	А	901	47/47	0.98	0.07	8,9,10,11	0
3	MGD	G	903	47/47	0.99	0.06	7,9,10,10	0
12	FES	В	2302	4/4	0.99	0.06	10,11,11,12	0
12	FES	F	201	4/4	0.99	0.06	11,12,12,12	0
12	FES	Н	201	4/4	0.99	0.06	10,11,11,11	0
5	F3S	С	904	7/7	1.00	0.07	9,9,9,9	0
5	F3S	Е	904	7/7	1.00	0.07	8,9,9,10	0
5	F3S	G	904	7/7	1.00	0.08	8,8,8,8	0
4	MO	А	903	1/1	1.00	0.05	9,9,9,9	0
4	MO	С	901	1/1	1.00	0.05	10,10,10,10	0
4	MO	Е	902	1/1	1.00	0.05	10,10,10,10	0
12	FES	D	201	4/4	1.00	0.05	11,11,11,12	0
4	MO	G	901	1/1	1.00	0.06	9,9,9,9	0
5	F3S	A	904	7/7	1.00	0.07	8,9,9,9	0

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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.

