

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	1MOW
Title	:	E-DreI
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Deposited on	:	2002-09-10
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

:	4.02b-467
:	1.8.5 (274361), CSD as541be (2020)
:	1.13
:	2.36
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	5.8.0158
:	7.0.044 (Gargrove)
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	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 2.40 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.



Motria	Whole archive	Similar resolution
wietric	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 c	chain
1	В	23	65%	35%
1	Е	23	61%	39%
1	Н	23	65%	35%
1	K	23	35%	65%
2	С	23	48%	52%



Mol	Chain	Length	Quality of chain	l
2	F	23	48%	52%
2	Ι	23	4% 52%	48%
2	L	23	57%	43%
3	А	260	73%	19% • 5%
3	D	260	72%	21% • 5%
3	G	260	6% 82%	8% 10%
3	J	260	4% 86%	• 10%

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
4	GOL	А	765	-	Х	-	-
4	GOL	А	767	-	Х	-	-
4	GOL	А	768	-	Х	-	-
4	GOL	А	769	-	Х	-	-
4	GOL	А	770	-	Х	-	-
4	GOL	А	772	-	Х	-	-
4	GOL	А	773	-	Х	-	-
4	GOL	В	762	-	Х	-	-
4	GOL	В	775	-	Х	-	-
4	GOL	D	761	-	Х	-	-
4	GOL	D	763	-	Х	-	-
4	GOL	D	764	-	Х	-	-
4	GOL	D	766	-	Х	-	-
4	GOL	D	776	-	Х	-	-
4	GOL	D	777	-	Х	-	-
4	GOL	D	778	-	Х	-	-
4	GOL	Е	771	-	Х	-	-
4	GOL	F	774	-	Х	-	-



1MOW

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 10717 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a DNA chain called 5'-D(*CP*CP*AP*AP*AP*CP*TP*GP*TP*CP*TP*CP *AP*AP*GP*TP*TP*CP*CP*GP*GP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	В	23	Total	С	Ν	Ο	Р	0	0	0
1	D	20	464	222	84	136	22	0	0	
1	F	93	Total	С	Ν	Ο	Р	0	0	0
1	Ľ	23	464	222	84	136	22	0		0
1	Ц	02	Total	С	Ν	0	Р	0	0	0
1	11	23	463	221	84	136	22	0	0	0
1	1 V	22	Total	С	Ν	0	Р	0	0	0
I K	23	464	222	84	136	22	0	0	0	

• Molecule 2 is a DNA chain called 5'-D(*CP*GP*CP*CP*GP*GP*AP*AP*CP*TP*TP*G P*AP*GP*AP*CP*AP*GP*TP*TP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
0	C	02	Total	С	Ν	0	Р	0	0	0
		23	473	225	90	136	22	0	0	0
0	Б	02	Total	С	Ν	0	Р	0	0	0
	Г	20	473	225	90	136	22	0	0	
0	т	23	Total	С	Ν	0	Р	0	0	0
	1		473	225	90	136	22	0	0	0
2 L	22	Total	С	Ν	0	Р	0	0	0	
	L	23	473	225	90	136	22	U	0	0

• Molecule 3 is a protein called chimera of homing endonuclease I-DmoI and DNA endonuclease I-CreI.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	Λ	248	Total C N O S	0	0	0
0	A	240	2022 1304 347 368 3	0	0	0
2	Л	248	Total C N O S	0	0 0	
0	D	240	2019 1303 347 366 3	0		0
2	С	233	Total C N O	0	0	0
o G	G		1153 687 233 233	0	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	J	234	Total C N O 1158 690 234 234	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	19	TRP	ILE	SEE REMARK 999	UNP p21505
А	51	PHE	HIS	SEE REMARK 999	UNP p21505
А	14	LEU	ARG	SEE REMARK 999	UNP p21505
А	103	GLY	-	linker	UNP p21505
А	104	ASN	-	linker	UNP p21505
А	105	ARG	-	linker	UNP p21505
А	108	ALA	LEU	SEE REMARK 999	UNP p05725
А	113	ILE	PHE	SEE REMARK 999	UNP p05725
А	139	THR	ALA	SEE REMARK 999	UNP p05725
А	147	GLU	GLN	SEE REMARK 999	UNP p05725
А	193	ASN	LYS	SEE REMARK 999	UNP p05725
А	194	PHE	LEU	SEE REMARK 999	UNP p05725
А	207	GLU	TRP	SEE REMARK 999	UNP p05725
А	208	GLN	ARG	SEE REMARK 999	UNP p05725
D	519	TRP	ILE	SEE REMARK 999	UNP p21505
D	551	PHE	HIS	SEE REMARK 999	UNP p21505
D	514	LEU	ARG	SEE REMARK 999	UNP p21505
D	603	GLY	-	linker	UNP p21505
D	604	ASN	-	linker	UNP p21505
D	605	ARG	-	linker	UNP p21505
D	608	ALA	LEU	SEE REMARK 999	UNP p05725
D	613	ILE	PHE	SEE REMARK 999	UNP p05725
D	639	THR	ALA	SEE REMARK 999	UNP p05725
D	647	GLU	GLN	SEE REMARK 999	UNP p05725
D	693	ASN	LYS	SEE REMARK 999	UNP p05725
D	694	PHE	LEU	SEE REMARK 999	UNP p05725
D	707	GLU	TRP	SEE REMARK 999	UNP p05725
D	708	GLN	ARG	SEE REMARK 999	UNP p05725
G	1019	TRP	ILE	SEE REMARK 999	UNP p21505
G	1051	PHE	HIS	SEE REMARK 999	UNP p21505
G	1014	LEU	ARG	SEE REMARK 999	UNP p21505
G	1103	GLY	-	linker	UNP p21505
G	1104	ASN	-	linker	UNP p21505
G	1105	ARG	-	linker	UNP p21505
G	1108	ALA	LEU	SEE REMARK 999	UNP p05725
G	1113	ILE	PHE	SEE REMARK 999	UNP p05725



Chain	Residue	Modelled	Actual	Comment	Reference
G	1139	THR	ALA	SEE REMARK 999	UNP p05725
G	1147	GLU	GLN	SEE REMARK 999	UNP p05725
G	1193	ASN	LYS	SEE REMARK 999	UNP p05725
G	1194	PHE	LEU	SEE REMARK 999	UNP p05725
G	1207	GLU	TRP	SEE REMARK 999	UNP p05725
G	1208	GLN	ARG	SEE REMARK 999	UNP $p05725$
J	1519	TRP	ILE	SEE REMARK 999	UNP p21505
J	1551	PHE	HIS	SEE REMARK 999	UNP p21505
J	1514	LEU	ARG	SEE REMARK 999	UNP p21505
J	1603	GLY	-	linker	UNP p21505
J	1604	ASN	-	linker	UNP p21505
J	1605	ARG	-	linker	UNP p21505
J	1608	ALA	LEU	SEE REMARK 999	UNP p05725
J	1613	ILE	PHE	SEE REMARK 999	UNP p05725
J	1639	THR	ALA	SEE REMARK 999	UNP $p05725$
J	1647	GLU	GLN	SEE REMARK 999	UNP p05725
J	1693	ASN	LYS	SEE REMARK 999	UNP $p05725$
J	1694	PHE	LEU	SEE REMARK 999	UNP $p05725$
J	1707	GLU	TRP	SEE REMARK 999	UNP $p05725$
J	1708	GLN	ARG	SEE REMARK 999	UNP $p05725$

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



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
4	В	1	Total 6	C 3	O 3	0	0



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

• Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Е	1	Total Mg 1 1	0	0
5	А	3	Total Mg 3 3	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	2	Total Mg 2 2	0	0



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



• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	В	41	Total O 41 41	0	0
7	С	39	Total O 39 39	0	0
7	Ε	61	Total O 61 61	0	0
7	F	37	$\begin{array}{cc} \text{Total} & \text{O} \\ 37 & 37 \end{array}$	0	0
7	А	137	Total O 137 137	0	0
7	D	139	Total O 139 139	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: 5'-D(*CP*CP*AP*AP*AP*CP*TP*GP*TP*CP*TP*CP*AP*AP*GP*TP*TP*C P*CP*GP*GP*CP*G)-3'

Chain D.			_
Cham D:	65%	35%	
C301 C302 A303 A304 A304 C315 C318 C318 C318 C322 C322 C322 C322			
• Molecule 1: 5'-F)(*CP*CP*AP*AP*AP*CP	*ТР*СР*ТР*СР*ТР*СР*	ΔΡ*ΔΡ* <u></u>
P*CP*GP*GP*CI	2*G)-3'		
Chain E:	61%	39%	
C801 C802 A803 A803 A814 A814 A814 C815 C818 C818 C819 C819 C813 C820 C823 C823			
• Molecule 1: 5'-D P*CP*GP*GP*CI	9(*CP*CP*AP*AP*AP*CP P*G)-3'	*TP*GP*TP*CP*TP*CP*.	AP*AP*GP*TP*TP*
Chain H:	65%	35%	-
C1301 C1302 C1302 A1313 A1313 A1313 A1313 C1303 C1322 C1322 C1322			
• Molecule 1: 5'-D P*CP*GP*GP*CI	P(*CP*CP*AP*AP*AP*CP P*G)-3'	*TP*GP*TP*CP*TP*CP*	AP*AP*GP*TP*TP*
Chain K:	35%	65%	-
C1801 C1802 C1803 A1803 A1805 A1805 C1806 C1806 C1806 C1806 C1808 C1815 C1815 C1815	01820 01821 01822 01823 01823		
• Molecule 2: 5'-D P*TP*TP*TP*GI	-(*CP*GP*CP*CP*GP*GP P*G)-3'	*AP*AP*CP*TP*TP*GP*A	AP*GP*AP*CP*AP*

Chain C:	48%	52%	





• Molecule 2: 5'-D(*CP*GP*CP*CP*GP*GP*AP*AP*CP*TP*TP*GP*AP*GP*AP*CP*AP*GP*AP*GP*AP*GP*AP*GP*3'

Chain F:	48%	52%	
C901 C902 C903 C903 C906 C906 C906 C906 C906 C906 C906 C906 C906 C906 C906 C906 C906 C906 C906 C906 C906 C907 C907 C907 C907 C907 C907 C907 C906 C912 C906 C912 C906 C912			
• Molecule 2: 5'-D(*CI P*TP*TP*TP*GP*G)	P*GP*CP*CP*GP*GP*AP*AP -3'	P*CP*TP*TP*GP*AP*GP*AP*CP*AP*G	r
Chain I:	52%	48%	
G1401 C1404 C1405 C1413 G1413 G1414 G1415 G1416 G1416 G1415 G1416 G1412 G1413 G1423 G1423 G1423			
• Molecule 2: 5'-D(*CI P*TP*TP*TP*GP*G)	P*GP*CP*CP*GP*GP*AP*AP -3'	P*CP*TP*TP*GP*AP*GP*AP*CP*AP*C	ŗ

Chain L:	57%	43%
C1901 C1902 C1903 C1904 C1905 C1915 C1916 C1916 C1916 C1922 C1922 C1923		

• Molecule 3: chimera of homing endonuclease I-DmoI and DNA endonuclease I-CreI



• Molecule 3: chimera of homing endonuclease I-DmoI and DNA endonuclease I-CreI



• Molecule 3: chimera of homing endonuclease I-DmoI and DNA endonuclease I-CreI





• Molecule 3: chimera of homing endonuclease I-DmoI and DNA endonuclease I-CreI





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants	131.76Å 131.76Å 120.91Å	Denesiter
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	19.86 - 2.40	Depositor
Resolution (A)	19.86 - 2.40	EDS
% Data completeness	99.8 (19.86-2.40)	Depositor
(in resolution range)	99.9 (19.86-2.40)	EDS
R _{merge}	0.08	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.76 (at 2.41Å)	
Refinement program	ogram CNS 1.0	
B B.	0.231 , 0.257	Depositor
It, Itfree	0.215 , 0.245	DCC
R_{free} test set	4592 reflections $(5.01%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	41.0	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.28 , 54.5	EDS
L-test for $twinning^2$	$< L >=0.47, < L^2>=0.30$	Xtriage
	0.015 for -h,-k,l	
Estimated twinning fraction	0.418 for h,-h-k,-l	Xtriage
	0.017 for -k,-h,-l	
F_o, F_c correlation	0.94	EDS
Total number of atoms	10717	wwPDB-VP
Average B, all atoms $(Å^2)$	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 33.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.7017e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GOL, SO4

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
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	В	0.39	0/519	0.76	0/798
1	Ε	0.41	0/519	0.77	0/798
1	Н	0.20	0/516	0.64	0/790
1	Κ	0.18	0/519	0.62	0/798
2	С	0.44	0/531	0.80	0/819
2	F	0.43	0/531	0.81	0/819
2	Ι	0.20	0/531	0.62	0/819
2	L	0.19	0/531	0.61	0/819
3	А	0.38	0/2059	0.63	0/2774
3	D	0.38	0/2056	0.64	0/2770
3	G	0.23	0/1146	0.50	0/1586
3	J	0.21	0/1149	0.49	0/1587
All	All	0.33	0/10607	0.64	0/15177

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	В	0	1
1	Ε	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	В	318	DC	Sidechain
1	Ε	818	DC	Sidechain

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	В	464	0	260	8	0
1	Е	464	0	260	7	0
1	Н	463	0	258	7	0
1	Κ	464	0	260	14	0
2	С	473	0	260	14	0
2	F	473	0	260	13	0
2	Ι	473	0	260	13	0
2	L	473	0	260	9	0
3	А	2022	0	2083	47	0
3	D	2019	0	2075	41	0
3	G	1153	0	498	10	0
3	J	1158	0	498	6	0
4	А	42	0	28	3	0
4	В	12	0	8	1	0
4	D	42	0	28	1	0
4	Ε	6	0	4	0	0
4	F	6	0	4	0	0
5	А	3	0	0	0	0
5	D	2	0	0	0	0
5	Ε	1	0	0	0	0
6	А	30	0	0	2	0
6	D	20	0	0	0	0
7	А	137	0	0	2	0
7	В	41	0	0	0	0
7	С	39	0	0	2	0
7	D	139	0	0	3	0
7	Е	61	0	0	1	0
7	F	37	0	0	5	0
All	All	10717	0	7304	169	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.



A + 1	A + D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:H:1313:DA:C4	1:H:1313:DA:C6	2.38	1.09
2:I:1404:DC:H2"	2:I:1405:DG:H5'	1.43	1.00
2:L:1904:DC:H2"	2:L:1905:DG:H5'	1.45	0.98
2:I:1423:DG:H5'	1:K:1823:DG:H5'	1.50	0.94
2:F:912:DG:H5'	3:D:645:LYS:HD3	1.55	0.87
2:C:404:DC:H2"	2:C:405:DG:H5'	1.57	0.84
3:A:221:GLU:O	3:A:224:THR:HB	1.85	0.76
2:F:904:DC:H2"	2:F:905:DG:H5'	1.67	0.75
3:D:721:GLU:O	3:D:724:THR:HB	1.87	0.75
1:H:1313:DA:C6	1:H:1313:DA:N7	2.56	0.74
3:A:69:ILE:HB	4:A:772:GOL:H12	1.69	0.74
3:A:15:LEU:HD11	3:A:95:LEU:HD13	1.68	0.74
3:A:210:PRO:HG2	7:A:2046:HOH:O	1.92	0.70
3:D:710:PRO:HG2	7:D:2052:HOH:O	1.92	0.68
3:D:505:GLU:OE2	3:D:555:ARG:NH1	2.27	0.68
2:C:412:DG:H5'	3:A:145:LYS:HD3	1.75	0.67
2:F:904:DC:H2"	2:F:905:DG:C5'	2.23	0.67
1:H:1302:DC:H2"	1:H:1303:DA:C8	2.30	0.66
3:A:177:GLU:HB3	3:A:180:PRO:HD2	1.78	0.66
3:D:602:ASN:C	3:D:602:ASN:HD22	2.00	0.65
2:C:423:DG:H2"	2:F:903:DC:H1'	1.79	0.64
3:A:161:VAL:HG12	3:A:162:GLY:H	1.61	0.64
2:C:404:DC:H2"	2:C:405:DG:C5'	2.26	0.64
2:I:1415:DA:H2"	2:I:1416:DC:O5'	1.98	0.64
3:D:723:CYS:O	3:D:726:VAL:HG13	1.97	0.64
2:C:423:DG:H5'	1:E:823:DG:H5'	1.80	0.63
3:D:679:LYS:HB3	3:D:680:PRO:HD3	1.80	0.63
3:A:65:VAL:HA	6:A:275:SO4:O1	1.99	0.63
3:D:516:GLY:CA	3:D:613:ILE:HD12	2.29	0.62
3:D:723:CYS:HA	3:D:726:VAL:CG1	2.31	0.61
3:D:602:ASN:C	3:D:602:ASN:ND2	2.54	0.61
3:A:5:GLU:OE1	4:A:767:GOL:H11	2.01	0.61
3:A:16:GLY:HA2	3:A:113:ILE:HD12	1.82	0.61
3:A:16:GLY:CA	3:A:113:ILE:HD12	2.31	0.60
3:D:515:LEU:HD11	3:D:595:LEU:HD13	1.82	0.60
3:A:12:ALA:HB2	3:A:105:ARG:HD2	1.84	0.60
3:D:516:GLY:HA2	3:D:613:ILE:HD12	1.85	0.59
3:D:512:ALA:HB2	3:D:605:ARG:HD2	1.86	0.58
2:L:1913:DA:OP2	3:J:1644:GLN:HA	2.03	0.57
3:A:149:ARG:HH21	3:A:149:ARG:HG2	1.68	0.57

All (169) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



		Interatomic	Clash overlap (Å)	
Atom-1	Atom-2	distance (Å)		
1:K:1821:DG:H2"	1:K:1822:DC:H5'	1.87	0.57	
3:D:712:ALA:HA	3:D:718:LYS:HG3	1.86	0.57	
3:A:53:ALA:HB3	3:A:54:PRO:HD3	1.86	0.57	
1:B:302:DC:H5"	3:A:213:LYS:HD2	1.87	0.56	
3:D:553:ALA:HB3	3:D:554:PRO:HD3	1.86	0.56	
2:L:1915:DA:H2"	2:L:1916:DC:O5'	2.05	0.56	
1:E:804:DA:OP2	3:D:678:ILE:HD13	2.06	0.55	
1:K:1814:DA:H2"	1:K:1815:DG:OP1	2.06	0.55	
1:H:1314:DA:C2'	1:H:1315:DG:H5"	2.38	0.54	
3:D:631:LYS:HE2	7:D:2246:HOH:O	2.08	0.54	
3:G:1089:TYR:HA	3:G:1092:ALA:HB3	1.90	0.54	
3:G:1152:LEU:HA	3:G:1155:LEU:CB	2.38	0.54	
3:D:539:VAL:HG13	3:D:579:GLU:HG3	1.90	0.54	
1:B:321:DG:O6	3:A:33:ARG:NH2	2.40	0.53	
2:C:408:DA:H5'	7:C:2256:HOH:O	2.08	0.53	
1:E:802:DC:H2'	3:D:630:TYR:CE2	2.43	0.53	
3:A:223:CYS:HA	3:A:226:VAL:HG13	1.90	0.53	
3:A:41:THR:HB	3:A:77:ARG:HG3	1.90	0.52	
3:A:179:LYS:HB2	4:A:770:GOL:C3	2.39	0.52	
1:E:802:DC:H2"	1:E:803:DA:C8	2.45	0.52	
1:K:1802:DC:H2"	1:K:1803:DA:C8	2.46	0.51	
3:A:161:VAL:HG12	3:A:162:GLY:N	2.25	0.51	
2:I:1420:DT:C6	2:I:1421:DT:H72	2.45	0.51	
1:K:1822:DC:H2"	1:K:1823:DG:C8	2.45	0.51	
3:D:506:ASN:O	3:D:510:ILE:HG12	2.11	0.50	
3:G:1149:ARG:O	3:G:1151:PHE:N	2.42	0.50	
2:L:1904:DC:H2"	2:L:1905:DG:C5'	2.31	0.50	
3:D:685:LEU:O	3:D:689:GLN:HB2	2.12	0.49	
1:K:1804:DA:H2"	1:K:1805:DA:OP2	2.12	0.49	
2:L:1903:DC:OP1	3:J:1584:SER:HA	2.12	0.49	
2:F:907:DA:H1'	7:F:2325:HOH:O	2.12	0.49	
3:D:517:LEU:HD13	3:D:540:ILE:HG21	1.95	0.49	
3:D:585:LYS:NZ	7:D:2362:HOH:O	2.38	0.49	
2:F:908:DA:H5'	7:F:2067:HOH:O	2.11	0.49	
1:K:1819:DC:H2"	1:K:1820:DG:C8	2.48	0.49	
3:A:16:GLY:HA2	3:A:113:ILE:CD1	2.43	0.49	
3:A:223:CYS:HA	3:A:226:VAL:CG1	2.43	0.48	
3:D:646:THR:O	3:D:649:ARG:HB2	2.13	0.48	
2:I:1414:DG:H3'	3:G:1118:GLY:O	2.12	0.48	
3:D:545:GLU:OE1	3:D:578:TYR:CE2	2.67	0.48	
1:K:1821:DG:H1'	1:K:1822:DC:H5"	1.95	0.48	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
3:D:541:THR:HB	3:D:577:ARG:HG3	1.96	0.48	
3:A:15:LEU:HD11	3:A:95:LEU:CD1	2.41	0.48	
1:B:302:DC:H2"	1:B:303:DA:C8	2.48	0.48	
1:B:321:DG:H2"	1:B:322:DC:H5'	1.95	0.48	
1:K:1814:DA:H4'	2:L:1914:DG:OP2	2.14	0.47	
3:D:558:PHE:O	3:D:562:GLU:HG2	2.14	0.47	
3:D:558:PHE:HB2	4:D:777:GOL:O3	2.14	0.47	
3:J:1709:LEU:O	3:J:1712:ALA:HB3	2.14	0.47	
3:A:178:ILE:HG23	3:A:206:ILE:HG23	1.97	0.47	
3:D:516:GLY:HA2	3:D:613:ILE:CD1	2.45	0.47	
2:I:1404:DC:C2'	2:I:1405:DG:H5'	2.30	0.47	
2:C:412:DG:H2"	2:C:413:DA:O4'	2.15	0.47	
2:L:1920:DT:H2'	2:L:1921:DT:H72	1.97	0.47	
3:A:126:PRO:HG2	7:A:2223:HOH:O	2.14	0.47	
1:E:814:DA:C2'	1:E:815:DG:H5"	2.45	0.46	
1:H:1315:DG:H2'	1:H:1316:DT:H71	1.97	0.46	
3:G:1147:GLU:C	3:G:1149:ARG:H	2.19	0.46	
2:C:414:DG:P	7:C:2411:HOH:O	2.73	0.46	
1:H:1314:DA:H2"	1:H:1315:DG:OP1	2.15	0.46	
2:I:1417:DA:OP1	3:G:1239:LYS:N	2.49	0.46	
2:F:916:DC:H2"	2:F:917:DA:H5'	1.96	0.46	
3:A:17:LEU:HD13	3:A:40:ILE:HG21	1.97	0.45	
3:A:101:PHE:CG	3:A:105:ARG:HG2	2.51	0.45	
3:A:80:LEU:C	3:A:80:LEU:HD23	2.37	0.45	
3:A:113:ILE:HG12	3:A:151:PHE:HZ	1.81	0.45	
3:G:1196:GLN:O	3:G:1199:ALA:HB3	2.17	0.45	
3:A:99:ARG:NH2	3:A:100:LEU:HD21	2.32	0.45	
3:J:1589:TYR:HA	3:J:1592:ALA:HB3	1.99	0.45	
3:D:630:TYR:CZ	3:D:635:GLN:HB2	2.51	0.44	
1:B:304:DA:OP2	3:A:178:ILE:HD13	2.17	0.44	
2:I:1420:DT:H2'	2:I:1421:DT:C7	2.48	0.44	
3:D:613:ILE:HG12	3:D:651:PHE:HZ	1.83	0.44	
2:F:904:DC:H2"	2:F:905:DG:H5"	1.99	0.44	
3:A:22:GLY:HA3	3:A:39:VAL:O	2.18	0.43	
3:A:149:ARG:NH2	3:A:153:ASP:OD2	2.52	0.43	
3:A:39:VAL:HG13	3:A:79:GLU:HG3	2.01	0.43	
3:D:723:CYS:HA	3:D:726:VAL:HG13	2.00	0.43	
2:C:404:DC:C2'	2:C:405:DG:H5'	2.40	0.43	
3:G:1194:PHE:C	3:G:1196:GLN:H	2.22	0.43	
2:F:914:DG:P	7:F:2410:HOH:O	2.76	0.43	
2:L:1919:DT:H2"	2:L:1920:DT:O5'	2.19	0.43	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
7:F:2218:HOH:O	3:D:532:ASN:HB3	2.20	0.42
3:D:650:TRP:HE3	3:D:654:LYS:HD2	1.84	0.42
3:D:708:GLN:OE1	3:D:718:LYS:NZ	2.52	0.42
1:B:302:DC:H5'	2:F:901:DC:H4'	2.00	0.42
3:A:209:LEU:N	3:A:210:PRO:HD2	2.34	0.42
3:D:517:LEU:HA	3:D:517:LEU:HD23	1.82	0.42
3:D:527:LEU:HD13	3:D:529:TYR:OH	2.19	0.42
3:D:661:VAL:HG12	3:D:662:GLY:H	1.84	0.42
2:C:410:DT:H2"	2:C:411:DT:O5'	2.20	0.42
3:A:6:ASN:O	3:A:10:ILE:HG12	2.19	0.42
3:A:189:GLN:HE21	3:A:189:GLN:HB3	1.58	0.42
3:J:1695:LYS:O	3:J:1699:ALA:HB2	2.20	0.42
1:B:302:DC:H5'	2:F:901:DC:C4'	2.49	0.42
1:K:1807:DT:H2"	1:K:1808:DG:OP2	2.19	0.42
3:D:650:TRP:CE3	3:D:654:LYS:HD2	2.55	0.42
1:H:1321:DG:H1'	1:H:1322:DC:H5"	2.02	0.42
3:J:1664:VAL:HA	3:J:1672:ASP:O	2.20	0.42
2:I:1413:DA:C2'	2:I:1414:DG:H5"	2.50	0.42
2:F:910:DT:H2"	2:F:911:DT:O5'	2.20	0.42
1:E:819:DC:H2"	1:E:820:DG:C8	2.55	0.41
3:A:212:ALA:HA	3:A:218:LYS:HG3	2.02	0.41
3:A:44:SER:HA	6:A:272:SO4:O4	2.19	0.41
4:B:775:GOL:H12	7:F:2106:HOH:O	2.20	0.41
3:A:75:ASP:OD1	3:A:76:THR:N	2.50	0.41
2:C:402:DG:O6	3:A:33:ARG:HD2	2.21	0.41
2:C:413:DA:C2'	2:C:414:DG:H5"	2.51	0.41
2:F:916:DC:H2'	2:F:917:DA:C8	2.55	0.41
2:I:1416:DC:H2"	2:I:1417:DA:H8	1.85	0.41
1:K:1805:DA:H1'	1:K:1806:DC:H5'	2.02	0.41
2:I:1415:DA:OP2	3:G:1119:SER:HA	2.21	0.41
2:L:1913:DA:H2"	2:L:1914:DG:OP1	2.20	0.41
2:C:416:DC:H2"	2:C:417:DA:H5'	2.02	0.41
3:A:144:GLN:HA	3:A:144:GLN:HE21	1.86	0.41
3:A:223:CYS:O	3:A:226:VAL:HG13	2.20	0.41
2:I:1419:DT:H2"	2:I:1420:DT:O5'	2.20	0.41
1:K:1814:DA:C2'	1:K:1815:DG:H5"	2.51	0.41
2:C:412:DG:H3'	3:A:145:LYS:HB3	2.04	0.40
3:A:179:LYS:CB	3:A:180:PRO:HD3	2.51	0.40
1:B:314:DA:C2'	1:B:315:DG:H5"	2.51	0.40
3:A:144:GLN:HE21	3:A:144:GLN:CA	2.34	0.40
3:D:522:GLY:HA3	3:D:539:VAL:O	2.20	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:712:ALA:HB2	3:D:722:VAL:HG21	2.03	0.40
1:E:823:DG:H3'	7:E:2397:HOH:O	2.21	0.40
1:K:1808:DG:H2"	1:K:1809:DT:OP2	2.21	0.40
2:I:1423:DG:O3'	1:K:1821:DG:N2	2.54	0.40
3:A:66:LYS:HD2	3:A:66:LYS:N	2.36	0.40
3:G:1212:ALA:HB1	3:G:1219:PHE:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
3	А	246/260~(95%)	239~(97%)	6 (2%)	1 (0%)	34	48
3	D	246/260~(95%)	238~(97%)	7(3%)	1 (0%)	34	48
3	G	219/260~(84%)	191 (87%)	22 (10%)	6 (3%)	5	5
3	J	216/260~(83%)	198 (92%)	17 (8%)	1 (0%)	29	41
All	All	927/1040~(89%)	866 (93%)	52 (6%)	9 (1%)	15	23

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	1102	ASN
3	D	603	GLY
3	G	1178	ILE
3	J	1678	ILE
3	G	1150	TRP
3	G	1195	LYS
3	G	1133	LYS
3	А	103	GLY
3	G	1103	GLY



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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	А	223/235~(95%)	210 (94%)	13~(6%)	20 32
3	D	221/235~(94%)	205~(93%)	16 (7%)	14 23
All	All	444/470~(94%)	415 (94%)	29~(6%)	17 27

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	А	17	LEU
3	А	47	LEU
3	А	77	ARG
3	А	95	LEU
3	А	105	ARG
3	А	141	GLN
3	А	144	GLN
3	А	165	ARG
3	А	189	GLN
3	А	198	GLN
3	А	203	LEU
3	А	209	LEU
3	А	226	VAL
3	D	517	LEU
3	D	568	LYS
3	D	577	ARG
3	D	595	LEU
3	D	602	ASN
3	D	605	ARG
3	D	628	GLN
3	D	644	GLN
3	D	665	ARG
3	D	689	GLN
3	D	698	GLN
3	D	703	LEU
3	D	709	LEU
3	D	711	SER



Continued from previous page...

Mol	Chain	Res	Type
3	D	724	THR
3	D	726	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	А	104	ASN
3	D	602	ASN
3	D	604	ASN
3	D	628	GLN

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 34 ligands modelled in this entry, 6 are monoatomic - leaving 28 for Mogul analysis.

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

Mol Tu	Turne	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Dec	Timle	B	ond len	gths	B	Bond ang	gles
INIOI	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2								
4	GOL	А	773	-	$5,\!5,\!5$	4.58	5 (100%)	$5,\!5,\!5$	5.78	3 (60%)								
4	GOL	D	776	-	5,5,5	4.52	5 (100%)	$5,\!5,\!5$	<mark>5.79</mark>	3 (60%)								



Mal	Type	Chain	Dog	Link	B	ond len	gths	Bond angles		
IVIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
6	SO4	А	280	-	4,4,4	0.25	0	$6,\!6,\!6$	0.04	0
6	SO4	D	274	-	4,4,4	0.29	0	$6,\!6,\!6$	0.07	0
4	GOL	Ε	771	-	$5,\!5,\!5$	4.52	5 (100%)	$5,\!5,\!5$	5.76	3 (60%)
6	SO4	А	271	-	4,4,4	0.26	0	$6,\!6,\!6$	0.05	0
6	SO4	D	273	-	4,4,4	0.25	0	$6,\!6,\!6$	0.07	0
4	GOL	В	775	-	$5,\!5,\!5$	4.57	5 (100%)	$5,\!5,\!5$	5.76	3 (60%)
4	GOL	D	764	-	$5,\!5,\!5$	4.57	5 (100%)	$5,\!5,\!5$	5.78	3 (60%)
6	SO4	А	277	-	4,4,4	0.26	0	$6,\!6,\!6$	0.10	0
6	SO4	D	278	-	4,4,4	0.27	0	$6,\!6,\!6$	0.04	0
6	SO4	А	272	-	4,4,4	0.25	0	$6,\!6,\!6$	0.07	0
4	GOL	D	761	-	$5,\!5,\!5$	4.54	5 (100%)	$5,\!5,\!5$	5.77	3 (60%)
4	GOL	А	770	-	$5,\!5,\!5$	4.55	5 (100%)	$5,\!5,\!5$	<mark>5.90</mark>	3 (60%)
6	SO4	А	276	-	4,4,4	0.25	0	$6,\!6,\!6$	0.06	0
4	GOL	А	765	-	$5,\!5,\!5$	4.56	5 (100%)	$5,\!5,\!5$	5.77	3 (60%)
4	GOL	D	763	-	$5,\!5,\!5$	4.52	5 (100%)	$5,\!5,\!5$	5.75	3 (60%)
4	GOL	D	766	-	$5,\!5,\!5$	4.62	5 (100%)	$5,\!5,\!5$	5.76	3 (60%)
4	GOL	F	774	-	$5,\!5,\!5$	4.52	5 (100%)	$5,\!5,\!5$	<mark>5.76</mark>	3 (60%)
4	GOL	А	767	-	5,5,5	4.66	5 (100%)	$5,\!5,\!5$	<mark>5.77</mark>	3 (60%)
4	GOL	D	778	-	5,5,5	4.58	5 (100%)	$5,\!5,\!5$	<mark>5.74</mark>	3 (60%)
6	SO4	А	275	-	4,4,4	0.22	0	$6,\!6,\!6$	0.08	0
6	SO4	D	279	-	4,4,4	0.24	0	$6,\!6,\!6$	0.08	0
4	GOL	А	772	_	$5,\!5,\!5$	4.52	5 (100%)	$5,\!5,\!5$	5.79	3 (60%)
4	GOL	D	777	-	5, 5, 5	4.61	5 (100%)	$5,\!5,\!5$	5.74	3(60%)
4	GOL	А	768	-	5,5,5	4.56	5 (100%)	5, 5, 5	5.75	3(60%)
4	GOL	А	769	-	$5,\!5,\!5$	4.51	5 (100%)	$5,\!5,\!5$	<mark>5.78</mark>	3 (60%)
4	GOL	В	762	-	$5,\!5,\!5$	4.59	5 (100%)	5, 5, 5	5.77	3 (60%)

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	GOL	А	770	-	-	2/4/4/4	-
4	GOL	D	778	-	-	3/4/4/4	-
4	GOL	А	772	-	-	2/4/4/4	-
4	GOL	А	773	-	-	2/4/4/4	-
4	GOL	А	765	-	-	3/4/4/4	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	В	775	-	-	2/4/4/4	-
4	GOL	D	763	-	-	2/4/4/4	-
4	GOL	D	776	-	-	3/4/4/4	-
4	GOL	D	766	-	-	3/4/4/4	-
4	GOL	F	774	-	-	2/4/4/4	-
4	GOL	D	777	-	-	3/4/4/4	-
4	GOL	А	768	-	-	3/4/4/4	-
4	GOL	А	767	-	-	3/4/4/4	-
4	GOL	В	762	-	-	2/4/4/4	-
4	GOL	А	769	-	-	3/4/4/4	-
4	GOL	Е	771	-	-	2/4/4/4	-
4	GOL	D	764	-	-	2/4/4/4	-
4	GOL	D	761	-	-	3/4/4/4	-

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
4	D	777	GOL	C3-C2	-7.77	1.19	1.51
4	А	770	GOL	C3-C2	-7.66	1.20	1.51
4	А	767	GOL	C3-C2	-7.66	1.20	1.51
4	А	773	GOL	C3-C2	-7.60	1.20	1.51
4	D	766	GOL	C3-C2	-7.57	1.20	1.51
4	D	763	GOL	C3-C2	-7.54	1.20	1.51
4	D	778	GOL	C3-C2	-7.53	1.20	1.51
4	А	768	GOL	C3-C2	-7.50	1.20	1.51
4	В	762	GOL	C3-C2	-7.50	1.20	1.51
4	В	775	GOL	C3-C2	-7.50	1.20	1.51
4	А	765	GOL	C3-C2	-7.49	1.20	1.51
4	Е	771	GOL	C3-C2	-7.48	1.21	1.51
4	D	764	GOL	C3-C2	-7.47	1.21	1.51
4	А	772	GOL	C3-C2	-7.43	1.21	1.51
4	F	774	GOL	C3-C2	-7.43	1.21	1.51
4	D	761	GOL	C3-C2	-7.38	1.21	1.51
4	А	769	GOL	C3-C2	-7.34	1.21	1.51
4	D	776	GOL	C3-C2	-7.32	1.21	1.51
4	А	770	GOL	01-C1	4.75	1.62	1.42
4	D	761	GOL	01-C1	4.63	1.61	1.42
4	Е	771	GOL	01-C1	4.62	1.61	1.42
4	А	768	GOL	O1-C1	4.59	1.61	1.42



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Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(A)			
4	В	762	GOL	O1-C1	4.58	1.61	1.42			
4	D	764	GOL	O1-C1	4.57	1.61	1.42			
4	A	772	GOL	O1-C1	4.55	1.61	1.42			
4	A	765	GOL	O1-C1	4.54	1.61	1.42			
4	В	775	GOL	O1-C1	4.51	1.61	1.42			
4	А	769	GOL	O1-C1	4.48	1.61	1.42			
4	А	773	GOL	O1-C1	4.47	1.61	1.42			
4	D	778	GOL	O1-C1	4.46	1.61	1.42			
4	D	776	GOL	O1-C1	4.44	1.61	1.42			
4	F	774	GOL	O1-C1	4.42	1.61	1.42			
4	D	777	GOL	O1-C1	4.37	1.60	1.42			
4	D	766	GOL	O1-C1	4.36	1.60	1.42			
4	А	767	GOL	O1-C1	4.35	1.60	1.42			
4	D	763	GOL	O1-C1	4.34	1.60	1.42			
4	D	776	GOL	O3-C3	3.43	1.56	1.42			
4	А	769	GOL	O3-C3	3.38	1.56	1.42			
4	Е	771	GOL	O3-C3	3.38	1.56	1.42			
4	D	766	GOL	C1-C2	-3.37	1.37	1.51			
4	D	761	GOL	O3-C3	3.36	1.56	1.42			
4	F	774	GOL	O3-C3	3.36	1.56	1.42			
4	А	772	GOL	O3-C3	3.34	1.56	1.42			
4	D	764	GOL	O3-C3	3.33	1.56	1.42			
4	В	775	GOL	O3-C3	3.30	1.56	1.42			
4	В	762	GOL	O3-C3	3.30	1.56	1.42			
4	А	765	GOL	O3-C3	3.29	1.56	1.42			
4	А	767	GOL	C1-C2	-3.26	1.38	1.51			
4	А	773	GOL	O3-C3	3.24	1.56	1.42			
4	D	763	GOL	O3-C3	3.24	1.56	1.42			
4	D	778	GOL	O3-C3	3.24	1.56	1.42			
4	А	768	GOL	O3-C3	3.23	1.56	1.42			
4	А	767	GOL	O2-C2	-3.19	1.33	1.43			
4	D	777	GOL	O3-C3	3.18	1.55	1.42			
4	A	770	GOL	O3-C3	3.18	1.55	1.42			
4	А	767	GOL	O3-C3	3.18	1.55	1.42			
4	D	766	GOL	O3-C3	3.11	1.55	1.42			
4	D	766	GOL	O2-C2	-3.08	1.34	1.43			
4	D	776	GOL	C1-C2	-3.05	1.39	1.51			
4	D	764	GOL	02-C2	-3.03	1.34	1.43			
4	D	778	GOL	02-C2	-3.01	1.34	1.43			
4	В	762	GOL	02-C2	-2.98	1.34	1.43			
4	A	768	GOL	02-C2	-2.96	1.34	1.43			
4	F	774	GOL	C1-C2	-2.95	1.39	1.51			

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	778	GOL	C1-C2	-2.94	1.39	1.51
4	А	773	GOL	C1-C2	-2.93	1.39	1.51
4	В	775	GOL	O2-C2	-2.93	1.34	1.43
4	В	762	GOL	C1-C2	-2.93	1.39	1.51
4	А	769	GOL	C1-C2	-2.90	1.39	1.51
4	D	777	GOL	C1-C2	-2.89	1.39	1.51
4	D	763	GOL	C1-C2	-2.89	1.39	1.51
4	D	761	GOL	O2-C2	-2.88	1.34	1.43
4	В	775	GOL	C1-C2	-2.86	1.39	1.51
4	А	773	GOL	O2-C2	-2.86	1.34	1.43
4	А	765	GOL	C1-C2	-2.85	1.40	1.51
4	D	777	GOL	O2-C2	-2.85	1.34	1.43
4	А	765	GOL	O2-C2	-2.83	1.34	1.43
4	D	776	GOL	O2-C2	-2.81	1.35	1.43
4	А	769	GOL	O2-C2	-2.79	1.35	1.43
4	А	772	GOL	O2-C2	-2.78	1.35	1.43
4	D	761	GOL	C1-C2	-2.77	1.40	1.51
4	D	764	GOL	C1-C2	-2.76	1.40	1.51
4	D	763	GOL	O2-C2	-2.75	1.35	1.43
4	А	768	GOL	C1-C2	-2.73	1.40	1.51
4	А	772	GOL	C1-C2	-2.73	1.40	1.51
4	F	774	GOL	O2-C2	-2.72	1.35	1.43
4	Е	771	GOL	C1-C2	-2.66	1.40	1.51
4	А	770	GOL	C1-C2	-2.61	1.41	1.51
4	Е	771	GOL	O2-C2	-2.56	1.35	1.43
4	А	770	GOL	O2-C2	-2.30	1.36	1.43

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All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	А	770	GOL	O3-C3-C2	10.68	161.43	110.20
4	D	776	GOL	O3-C3-C2	10.57	160.91	110.20
4	А	773	GOL	O3-C3-C2	10.55	160.78	110.20
4	В	762	GOL	O3-C3-C2	10.52	160.65	110.20
4	D	766	GOL	O3-C3-C2	10.51	160.61	110.20
4	А	772	GOL	O3-C3-C2	10.50	160.54	110.20
4	D	764	GOL	O3-C3-C2	10.50	160.53	110.20
4	А	769	GOL	O3-C3-C2	10.49	160.48	110.20
4	А	765	GOL	O3-C3-C2	10.49	160.47	110.20
4	D	761	GOL	O3-C3-C2	10.48	160.47	110.20
4	А	767	GOL	O3-C3-C2	10.46	160.37	110.20
4	F	774	GOL	O3-C3-C2	10.43	160.19	110.20



Mol

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Chain	Res	Type	Atoms		$Observed(^{o})$	$ $ Ideal(o)
А	768	GOL	O3-C3-C2	10.41	160.11	110.20
В	775	GOL	O3-C3-C2	10.40	160.04	110.20
D	763	GOL	O3-C3-C2	10.39	160.03	110.20
Ε	771	GOL	O3-C3-C2	10.38	159.98	110.20
D	778	GOL	O3-C3-C2	10.31	159.62	110.20
D	777	GOL	O3-C3-C2	10.24	159.31	110.20
А	770	GOL	O2-C2-C3	7.06	140.21	109.12
D	778	GOL	O2-C2-C3	6.87	139.39	109.12
D	777	GOL	O2-C2-C3	6.86	139.35	109.12
F	774	GOL	O2-C2-C3	6.85	139.28	109.12
D	766	GOL	O2-C2-C3	6.85	139.28	109.12
А	769	GOL	O2-C2-C3	6.84	139.23	109.12
А	767	GOL	O2-C2-C3	6.83	139.20	109.12
В	775	GOL	O2-C2-C3	6.80	139.09	109.12
D	763	GOL	O2-C2-C3	6.80	139.08	109.12
В	762	GOL	O2-C2-C3	6.78	138.97	109.12
Е	771	GOL	O2-C2-C3	6.77	138.94	109.12
А	765	GOL	O2-C2-C3	6.77	138.93	109.12
А	768	GOL	O2-C2-C3	6.77	138.92	109.12
D	776	GOL	O2-C2-C3	6.76	138.90	109.12
D	764	GOL	O2-C2-C3	6.73	138.78	109.12
А	772	GOL	O2-C2-C3	6.73	138.77	109.12
D	761	GOL	O2-C2-C3	6.72	138.74	109.12
А	773	GOL	O2-C2-C3	6.72	138.74	109.12
Е	771	GOL	O1-C1-C2	3.38	126.43	110.20
D	777	GOL	O1-C1-C2	3.36	126.31	110.20
А	772	GOL	O1-C1-C2	3.35	126.26	110.20
D		COT	01 01 02	0.01	100.07	110.00

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There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
4	В	762	GOL	C1-C2-C3-O3
4	В	775	GOL	C1-C2-C3-O3
4	Е	771	GOL	O1-C1-C2-C3
4	Е	771	GOL	C1-C2-C3-O3
4	F	774	GOL	C1-C2-C3-O3
4	А	765	GOL	C1-C2-C3-O3
4	А	767	GOL	C1-C2-C3-O3
4	А	768	GOL	C1-C2-C3-O3
4	А	769	GOL	O1-C1-C2-C3
4	А	769	GOL	C1-C2-C3-O3
4	А	770	GOL	C1-C2-C3-O3
4	А	772	GOL	C1-C2-C3-O3
4	А	773	GOL	C1-C2-C3-O3
4	D	761	GOL	C1-C2-C3-O3
4	D	763	GOL	C1-C2-C3-O3
4	D	764	GOL	C1-C2-C3-O3
4	D	766	GOL	O1-C1-C2-C3
4	D	766	GOL	C1-C2-C3-O3
4	D	776	GOL	O1-C1-C2-C3
4	D	776	GOL	C1-C2-C3-O3
4	D	777	GOL	O1-C1-C2-C3
4	D	777	GOL	C1-C2-C3-O3
4	D	778	GOL	O1-C1-C2-C3
4	D	778	GOL	C1-C2-C3-O3
4	А	765	GOL	O1-C1-C2-C3
4	А	773	GOL	O1-C1-C2-C3
4	В	762	GOL	O1-C1-C2-O2
4	D	763	GOL	O1-C1-C2-O2
4	В	775	GOL	O1-C1-C2-O2
4	F	774	GOL	O1-C1-C2-O2
4	А	768	GOL	O1-C1-C2-O2
4	А	770	GOL	O1-C1-C2-O2
4	А	772	GOL	O1-C1-C2-O2
4	D	764	GOL	O1-C1-C2-O2
4	D	761	GOL	O1-C1-C2-O2
4	D	766	GOL	O1-C1-C2-O2
4	А	767	GOL	O1-C1-C2-O2
4	А	769	GOL	O1-C1-C2-O2
4	D	776	GOL	O1-C1-C2-O2
4	D	777	GOL	O1-C1-C2-O2



Mol	Chain	Res	Type	Atoms
4	D	778	GOL	O1-C1-C2-O2
4	А	767	GOL	O1-C1-C2-C3
4	D	761	GOL	O1-C1-C2-C3
4	А	765	GOL	O1-C1-C2-O2
4	А	768	GOL	O1-C1-C2-C3

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	775	GOL	1	0
6	А	272	SO4	1	0
4	А	770	GOL	1	0
4	А	767	GOL	1	0
6	А	275	SO4	1	0
4	А	772	GOL	1	0
4	D	777	GOL	1	0

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	В	23/23~(100%)	-0.59	0 100 100	26, 39, 48, 52	0
1	Е	23/23~(100%)	-0.71	0 100 100	25, 38, 49, 54	0
1	Н	23/23~(100%)	0.50	0 100 100	120, 133, 144, 146	0
1	K	23/23~(100%)	0.52	0 100 100	130, 138, 151, 154	0
2	С	23/23~(100%)	-0.56	0 100 100	28, 39, 52, 55	0
2	F	23/23~(100%)	-0.64	0 100 100	27, 37, 53, 57	0
2	Ι	23/23~(100%)	0.44	1 (4%) 35 33	120, 132, 143, 145	0
2	L	23/23~(100%)	0.52	0 100 100	127, 136, 146, 149	0
3	А	248/260~(95%)	-0.52	0 100 100	22, 33, 55, 64	0
3	D	248/260~(95%)	-0.51	0 100 100	22, 33, 54, 64	0
3	G	233/260~(89%)	0.53	15 (6%) 19 18	103, 111, 117, 126	0
3	J	234/260~(90%)	0.41	11 (4%) 31 30	100, 108, 115, 118	0
All	All	$114\overline{7/1224} \ (93\%)$	-0.04	27 (2%) 59 57	22, 56, 133, 154	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	1512	ALA	3.9
3	J	1675	LEU	3.3
3	G	1144	GLN	3.1
3	J	1663	TYR	3.1
3	J	1662	GLY	3.0
3	J	1523	GLY	3.0
3	J	1699	ALA	2.9
3	G	1013	TYR	2.7
3	G	1211	SER	2.7
3	J	1589	TYR	2.6
3	G	1225	TRP	2.6



Mol	Chain	Res	Type	RSRZ
3	J	1650	TRP	2.5
3	G	1044	SER	2.4
3	G	1151	PHE	2.4
3	G	1173	TYR	2.3
3	G	1034	SER	2.3
3	G	1033	ARG	2.3
3	G	1072	VAL	2.2
3	G	1105	ARG	2.1
3	J	1581	ARG	2.1
3	G	1089	TYR	2.1
3	J	1544	SER	2.1
3	J	1547	LEU	2.1
2	Ι	1423	DG	2.0
3	G	1102	ASN	2.0
3	G	1132	PHE	2.0
3	G	1224	THR	2.0

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	$B-factors(Å^2)$	Q<0.9
6	SO4	А	275	5/5	0.63	0.28	$150,\!150,\!151,\!152$	0
4	GOL	В	775	6/6	0.74	0.26	91,97,99,103	0
4	GOL	D	763	6/6	0.76	0.22	84,86,90,92	0
4	GOL	А	770	6/6	0.76	0.28	54,85,86,87	0
4	GOL	А	769	6/6	0.77	0.26	64,75,79,87	0
4	GOL	D	761	6/6	0.77	0.23	79,86,89,90	0
6	SO4	А	277	5/5	0.78	0.26	126,127,130,131	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors($Å^2$)	Q<0.9
4	GOL	D	764	6/6	0.80	0.15	93,98,99,99	0
4	GOL	D	777	6/6	0.81	0.52	112,113,118,122	0
4	GOL	А	768	6/6	0.82	0.23	67,74,75,78	0
4	GOL	А	765	6/6	0.83	0.17	67,73,77,85	0
4	GOL	Е	771	6/6	0.84	0.14	62,68,72,74	0
4	GOL	D	776	6/6	0.85	0.28	79,81,83,90	0
4	GOL	F	774	6/6	0.86	0.13	62,67,71,73	0
5	MG	А	373	1/1	0.86	0.11	32,32,32,32	0
4	GOL	А	773	6/6	0.87	0.46	106,108,113,115	0
6	SO4	А	271	5/5	0.87	0.17	115,116,117,119	0
6	SO4	D	279	5/5	0.87	0.27	130,132,133,135	0
5	MG	Е	375	1/1	0.88	0.14	33,33,33,33	0
4	GOL	А	772	6/6	0.88	0.17	76,77,79,82	0
6	SO4	А	280	5/5	0.89	0.21	139,140,140,140	0
6	SO4	А	272	5/5	0.89	0.18	113,115,116,116	0
6	SO4	D	273	5/5	0.90	0.24	137,137,139,139	0
6	SO4	А	276	5/5	0.90	0.21	139,139,140,142	0
6	SO4	D	274	5/5	0.91	0.16	90,92,97,103	0
6	SO4	D	278	5/5	0.91	0.28	138,139,139,140	0
4	GOL	В	762	6/6	0.91	0.17	64,68,69,76	0
4	GOL	D	766	6/6	0.92	0.26	72,76,85,86	0
4	GOL	D	778	6/6	0.93	0.19	75, 76, 78, 79	0
5	MG	А	372	1/1	0.95	0.09	37,37,37,37	0
4	GOL	A	767	6/6	0.96	0.24	$5\overline{8,60,71,73}$	0
5	MG	D	374	1/1	0.96	0.14	20,20,20,20	0
5	MG	A	371	1/1	0.97	0.09	$1\overline{3,}13,13,13$	0
5	MG	D	376	1/1	0.99	0.16	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.

