

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	2BT4
Title	:	Type II Dehydroquinase inhibitor complex
Authors	:	Toscano, M.D.; Stewart, K.A.; Coggins, J.R.; Lapthorn, A.J.; Abell, C.
Deposited on	:	2005-05-26
Resolution	:	1.70 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:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
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-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	;	Percentile Ranks	Value	
Clashscore			11	
Ramachandran outliers			0	
	Worse		Better	
	Percentile relative to all X-ra	y structures		
	Percentile relative to X-ray s	tructures of similar resolution		
			~	

Matria	Whole archive	Similar resolution		
Metric	$(\# { m Entries})$	$(\# \text{Entries, resolution range}(\text{\AA}))$		
Clashscore	141614	4695 (1.70-1.70)		
Ramachandran outliers	138981	4610 (1.70-1.70)		

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain		
1	А	157	84%	11%	5%
1	В	157	87%	7%	• 5%
1	С	157	87%	8%	5%
1	D	157	83%	12%	5%
1	Е	157	81%	12%	• 5%
1	F	157	81%	13%	• 5%
1	G	157	87%	8%	• 5%
1	Н	157	85%	10%	5%
1	Ι	157	82%	13%	5%



Mol	Chain	Length	Quality of chain		
1	J	157	82%	13%	5%
1	K	157	83%	12%	5%
1	L	157	83%	11%	5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	А	2401	-	-	Х	-
5	GOL	В	2414	-	-	Х	-
5	GOL	С	2415	-	-	Х	-
5	GOL	D	2416	-	-	Х	-
5	GOL	Е	2419	-	-	Х	-
5	GOL	Е	2422	-	-	Х	-
5	GOL	F	2418	-	-	Х	-
5	GOL	G	2417	-	-	Х	-
5	GOL	Н	2411	-	-	Х	-
5	GOL	Ι	2420	-	-	Х	-
5	GOL	J	2412	-	-	Х	-
5	GOL	Κ	2421	-	-	Х	-



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 15641 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	oms			ZeroOcc	AltConf	Trace					
1	Δ	140	Total	С	Ν	0	S	0	2	0					
1	A	149	1127	701	210	211	5	0		0					
1	р	140	Total	С	Ν	0	S	0	1	0					
1	D	149	1126	701	210	210	5	0		0					
1	С	140	Total	С	Ν	0	S	0	1	0					
1	U	149	1126	701	210	210	5	0		0					
1	Л	140	Total	С	Ν	0	S	0	9	0					
T	D	149	1127	701	210	211	5	0	0		0				
1	F	140	Total	С	Ν	Ο	\mathbf{S}	0	1	0					
T	Ľ	143	1126	701	210	210	5	0	0	0	0	0	0	1	0
1	F	140	Total	С	Ν	Ο	\mathbf{S}	0	1	0					
1	I.	145	1126	701	210	210	5	0	I	0					
1	C	140	Total	С	Ν	0	\mathbf{S}	0	9	0					
T	G	143	1127	701	210	211	5	0	0	2	0				
1	н	140	Total	С	Ν	0	\mathbf{S}	0	1	0					
T	11	143	1126	701	210	210	5	0	T	0					
1	Т	140	Total	С	Ν	0	\mathbf{S}	0	1	0					
T	L	143	1126	701	210	210	5	0	T	0					
1	Т	140	Total	С	Ν	0	\mathbf{S}	0	9	0					
T	0	143	1132	704	213	210	5	0	2	0					
1	K	1/0	Total	С	Ν	Ο	S	0	1	0					
1	Γ	149	1126	701	210	210	5	U	I	0					
1	Т	140	Total	С	Ν	0	S	0	2	0					
		149	1127	701	210	211	5			U					

• Molecule 1 is a protein called 3-DEHYDROQUINATE DEHYDRATASE.

• Molecule 2 is (1S,3R,4R,5S)-1,3,4-TRIHYDROXY-5-(3-PHENOXYPROPYL)CYCLOHEX ANECARBOXYLIC ACID (three-letter code: CA2) (formula: C₁₆H₂₂O₆).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total C O 22 16 6	0	0
2	В	1	Total C O 22 16 6	0	0
2	С	1	Total C O 22 16 6	0	0
2	D	1	Total C O 22 16 6	0	0
2	Ε	1	Total C O 22 16 6	0	0
2	F	1	Total C O 22 16 6	0	0
2	G	1	Total C O 22 16 6	0	0
2	Н	1	Total C O 22 16 6	0	0
2	Ι	1	Total C O 22 16 6	0	0
2	J	1	Total C O 22 16 6	0	0
2	K	1	Total C O 22 16 6	0	0
2	L	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 22 & 16 & 6 \end{array}$	0	0

• Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).





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

• Molecule 4 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
4	А	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{N} & \text{O} \\ 8 & 4 & 1 & 3 \end{array}$	0	0
4	F	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{N} & \text{O} \\ 8 & 4 & 1 & 3 \end{array}$	0	0
4	Н	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{N} & \text{O} \\ 8 & 4 & 1 & 3 \end{array}$	0	0
4	L	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{N} & \text{O} \\ 8 & 4 & 1 & 3 \end{array}$	0	0

• Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
5	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
5	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
5	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
5	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
5	Ε	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
5	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
5	G	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
5	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
5	Ι	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
5	J	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
5	Κ	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	135	Total O 135 135	0	0
6	В	152	Total O 152 152	0	0
6	С	146	Total O 146 146	0	0
6	D	146	Total O 146 146	0	0
6	Ε	186	Total O 186 186	0	0
6	F	146	Total O 146 146	0	0
6	G	148	Total O 148 148	0	0
6	Н	124	Total O 124 124	0	0
6	Ι	156	Total O 156 156	0	0
6	J	120	Total O 120 120	0	0
6	К	123	Total O 123 123	0	0
6	L	149	Total O 149 149	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. 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. 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.

Note EDS was not executed.

• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE





Chain F:	81%	13%	• 5%
MET PRO R1002 A1007 A1007 C1020 C1020 P1025 P1025 F1025 T1027 T1027	D1031 D1055 D1055 D1055 D1052 E1068 A1069 A1069 A1071 D1098 D1125 A1116 H1117 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1116 H1117 H1117 H1116 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H1117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H117 H	SER ALA ARG ALA	
• Molecule 1: 3-DE	HYDROQUINATE DEHYDRATASE		
Chain G:	87%	8%	• 5%
MET PR0 11202 01222 F1225 E1226 D1231 D1231 N1265 W1265	81270 41281 11305 11325 11326 11324 11329 11327 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 11328 1138 113		
• Molecule 1: 3-DE	HYDROQUINATE DEHYDRATASE		
Chain H:	85%	10%	5%
MET PRO R1402 A1407 A1407 A1407 E1425 E1425 T1428 S1428 S1428 S1428 S1428 S1430 S1430 S1431	K 1442 A 1443 B 1447 R 1470 R 1470 R 1519 H 1519 D 1527 D 1527 C 1560 A 15 A 15 A 15 A 15 A 15 A 15 A 15 A 15		
• Molecule 1: 3-DE	HYDROQUINATE DEHYDRATASE		
Chain I:	82%	13%	5%
MET PRO R1602 81602 11604 11604 91622 91622 91625 11622 11627	K1642 A1643 H1647 H1647 H1658 H1658 H1658 C1674 D1692 P1701 F1719 P1701 F1719 C1770 C1750 C1750 C1750 A1A A1A A1A A1A A1A A1A A1A A1A A1A A1		
• Molecule 1: 3-DE	HYDROQUINATE DEHYDRATASE		
Chain J:	82%	13%	5%
MET PR0 R1815 P1815 P1823 Q1822 Q1822 Q1823 P1825 P1825 B1826 B1831	K1842 A1869 A1869 A1861 A1881 A1881 A1881 A1884 A188 A18956 A18926 A18926 A18926 A18926 A18926 A184 A18 A18 A18 A18 A18 A18 A18 A18 A18 A18		
• Molecule 1: 3-DE	HYDROQUINATE DEHYDRATASE		
Chain K:	83%	12%	5%
MET PR0 R2002 12004 12004 12007 P2008 12011 12011 12015 N2016	P2025 E2026 R2070 12071 V2077 V2077 V2077 V2071 R2014 R214 R2149 R2149 R2149 R2149 R2149 R2149 R2149 R2149 R2149 R2149 R14 R149 R149 R149 R149 R149 R149 R1		
• Molecule 1: 3-DE	HYDROQUINATE DEHYDRATASE		
Chain L:	83%	11%	5%
MET PRO R2202 82202 82202 12224 12226 12226 12226 12228 12228 12231	D2252 2284 2284 H2306 H2313 P2315 P2315 P2315 P2315 P2315 P2315 P2315 P2315 P2315 P2315 P2315 P2315 P2315 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P2325 P235 P23		



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	P 1	Depositor	
Cell constants	196.62Å 196.49Å 240.63Å	Depositor	
a, b, c, α , β , γ	65.91° 65.91° 90.01°	Depositor	
Resolution (Å)	27.00 - 1.70	Depositor	
% Data completeness	75.8 (27.00-1.70)	Depositor	
(in resolution range)	19.8 (21.00-1.10)	Depositor	
R_{merge}	0.17	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	REFMAC 5.2.0005	Depositor	
R, R_{free}	0.197 , 0.248	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	15641	wwPDB-VP	
Average B, all atoms $(Å^2)$	15.0	wwPDB-VP	



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: TRS, PO4, CA2, GOL

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	Bo	nd lengths	Bond angles		
WIOI	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	1.02	0/1161	1.04	4/1582~(0.3%)	
1	В	1.05	0/1155	0.99	4/1574~(0.3%)	
1	С	1.01	0/1155	0.95	3/1574~(0.2%)	
1	D	1.05	0/1161	0.95	2/1582~(0.1%)	
1	Е	1.01	2/1155~(0.2%)	0.94	3/1574~(0.2%)	
1	F	1.06	1/1155~(0.1%)	1.02	6/1574~(0.4%)	
1	G	1.03	1/1161~(0.1%)	1.01	3/1582~(0.2%)	
1	Н	1.04	0/1155	1.02	2/1574~(0.1%)	
1	Ι	1.00	0/1155	0.96	2/1574~(0.1%)	
1	J	1.02	1/1166~(0.1%)	0.98	3/1588~(0.2%)	
1	Κ	1.00	0/1155	0.93	0/1574	
1	L	1.02	0/1161	0.98	3/1582~(0.2%)	
All	All	1.03	5/13895~(0.0%)	0.98	35/18934~(0.2%)	

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	1083	TYR	CD1-CE1	6.32	1.48	1.39
1	G	1305	VAL	CB-CG2	-5.66	1.41	1.52
1	Е	828	TYR	CD2-CE2	-5.37	1.31	1.39
1	Е	939	VAL	CB-CG1	-5.24	1.41	1.52
1	J	1940	PHE	CD2-CE2	5.09	1.49	1.39

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	Н	1527	ASP	CB-CG-OD2	13.19	130.17	118.30
1	G	1327	ASP	CB-CG-OD2	8.20	125.68	118.30
1	С	527	ASP	CB-CG-OD2	7.63	125.17	118.30
1	В	252	ASP	CB-CG-OD1	7.24	124.82	118.30



Mol	Chain	Res	Type	Atoms Z		$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	D	631	ASP	CB-CG-OD2	7.06	124.65	118.30
1	С	525	ARG	NE-CZ-NH1	-6.91	116.85	120.30
1	J	1927	ASP	CB-CG-OD2	6.89	124.50	118.30
1	А	127	ASP	CB-CG-OD2	6.78	124.40	118.30
1	В	327	ASP	CB-CG-OD2	6.64	124.28	118.30
1	L	2327	ASP	CB-CG-OD2	6.41	124.06	118.30
1	А	92	ASP	CB-CG-OD1	6.39	124.05	118.30
1	В	292	ASP	CB-CG-OD1	6.33	123.99	118.30
1	А	64	ASP	CB-CG-OD2	6.31	123.98	118.30
1	F	1031	ASP	CB-CG-OD2	6.17	123.86	118.30
1	Ι	1631	ASP	CB-CG-OD2	6.14	123.83	118.30
1	G	1254	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	G	1231	ASP	CB-CG-OD2	6.06	123.75	118.30
1	F	1098	ASP	CB-CG-OD2	6.05	123.74	118.30
1	F	1035	ASP	CB-CG-OD2	5.94	123.64	118.30
1	С	431	ASP	CB-CG-OD2	5.87	123.58	118.30
1	Ι	1692	ASP	CB-CG-OD1	5.84	123.55	118.30
1	А	31	ASP	CB-CG-OD2	5.81	123.53	118.30
1	J	1831	ASP	CB-CG-OD2	5.72	123.45	118.30
1	F	1127	ASP	CB-CG-OD2	5.70	123.43	118.30
1	Н	1431	ASP	CB-CG-OD2	5.52	123.27	118.30
1	F	1117	ARG	NE-CZ-NH1	-5.51	117.55	120.30
1	Ε	835	ASP	CB-CG-OD2	5.42	123.18	118.30
1	L	2231	ASP	CB-CG-OD2	5.41	123.17	118.30
1	D	692	ASP	CB-CG-OD1	5.37	123.14	118.30
1	Ε	839	LEU	CB-CG-CD1	-5.28	102.03	111.00
1	F	1020	LEU	CB-CG-CD2	-5.26	102.05	111.00
1	J	1880	PRO	N-CD-CG	-5.26	95.31	103.20
1	Е	831	ASP	CB-CG-OD2	5.22	123.00	118.30
1	L	2252	ASP	CB-CG-OD1	5.21	122.99	118.30
1	В	298	ASP	CB-CG-OD2	5.12	122.91	118.30

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There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1127	0	1093	20	0
1	В	1126	0	1092	14	0
1	С	1126	0	1092	17	0
1	D	1127	0	1093	18	0
1	Е	1126	0	1092	38	0
1	F	1126	0	1092	36	0
1	G	1127	0	1093	16	0
1	Н	1126	0	1092	27	0
1	Ι	1126	0	1092	41	0
1	J	1132	0	1102	19	0
1	Κ	1126	0	1092	20	0
1	L	1127	0	1093	22	0
2	А	22	0	21	1	0
2	В	22	0	21	2	0
2	С	22	0	21	0	0
2	D	22	0	21	0	0
2	Ε	22	0	21	2	0
2	F	22	0	21	2	0
2	G	22	0	21	1	0
2	Н	22	0	21	1	0
2	Ι	22	0	21	0	0
2	J	22	0	21	1	0
2	K	22	0	21	0	0
2	L	22	0	21	0	0
3	А	5	0	0	2	0
3	D	5	0	0	1	0
3	Ι	5	0	0	1	0
3	L	5	0	0	0	0
4	А	8	0	12	0	0
4	F	8	0	12	0	0
4	Н	8	0	12	0	0
4	L	8	0	12	0	0
5	А	6	0	8	1	0
5	В	6	0	8	6	0
5	C	6	0	8	9	0
5	D	6	0	8	9	0
5	Е	12	0	16	15	0
5	F	6	0	8	13	0
5	G	6	0	8	7	0
5	H	6	0	8	7	0
5	I	6	0	8	21	0
5	J	6	0	8	4	0
5	K	6	0	8	12	0



$J \cdots J \cdots F J \cdots F J \cdots$							
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes	
6	А	135	0	0	10	0	
6	В	152	0	0	8	0	
6	С	146	0	0	10	0	
6	D	146	0	0	5	0	
6	Е	186	0	0	17	0	
6	F	146	0	0	10	0	
6	G	148	0	0	0	0	
6	Н	124	0	0	18	0	
6	Ι	156	0	0	22	0	
6	J	120	0	0	13	0	
6	K	123	0	0	2	0	
6	L	149	0	0	13	0	
All	All	15641	0	13514	305	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 11.

All (305) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:I:1719[A]:HIS:CD2	5:I:2420:GOL:H11	1.62	1.33
1:F:1098:ASP:CB	6:F:2109:HOH:O	1.68	1.31
1:H:1519[A]:HIS:CD2	5:H:2411:GOL:H12	1.72	1.25
5:B:2414:GOL:C1	6:B:2150:HOH:O	1.88	1.22
1:I:1602:ARG:N	6:I:2022:HOH:O	1.76	1.18
5:C:2415:GOL:H11	6:C:2146:HOH:O	1.03	1.18
1:J:1821:GLY:O	6:J:2016:HOH:O	1.56	1.17
1:J:1842:LYS:HE2	6:J:2046:HOH:O	1.41	1.17
1:B:271:LEU:CD2	6:B:2095:HOH:O	1.93	1.14
1:C:513:ARG:HG2	6:C:2111:HOH:O	1.43	1.13
1:F:1120:SER:H	5:F:2418:GOL:H12	1.05	1.12
1:F:1098:ASP:HB2	6:F:2109:HOH:O	1.32	1.12
5:D:2416:GOL:O1	6:D:2145:HOH:O	1.65	1.11
1:I:1750:GLY:HA3	6:I:2149:HOH:O	1.51	1.11
1:I:1719[A]:HIS:CD2	5:I:2420:GOL:C1	2.34	1.09
1:J:1821:GLY:C	6:J:2016:HOH:O	1.87	1.08
5:C:2415:GOL:C1	6:C:2146:HOH:O	1.64	1.08
1:F:1098:ASP:O	6:F:2109:HOH:O	1.70	1.07
1:E:914:GLU:CD	6:E:2155:HOH:O	1.91	1.06
5:B:2414:GOL:H11	6:B:2150:HOH:O	1.46	1.06
1:J:1842:LYS:HG2	6:J:2043:HOH:O	1.55	1.06



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:L:2319[B]:HIS:HD2	6:L:2101:HOH:O	1.39	1.05	
1:F:1071:LEU:HD12	6:F:2083:HOH:O	1.58	1.03	
1:G:1320:SER:H	5:G:2417:GOL:H12	1.20	1.02	
1:L:2225:PRO:HB3	6:L:2047:HOH:O	1.61	1.01	
1:I:1719[A]:HIS:CG	5:I:2420:GOL:H11	1.97	0.99	
1:L:2225:PRO:CB	6:L:2047:HOH:O	2.07	0.99	
5:E:2419:GOL:H2	6:E:2184:HOH:O	1.61	0.98	
1:I:1750:GLY:CA	6:I:2149:HOH:O	2.04	0.98	
1:C:425:PRO:HD2	1:C:426:GLU:OE2	1.62	0.97	
1:F:1098:ASP:C	6:F:2109:HOH:O	1.85	0.95	
5:H:2411:GOL:H32	6:H:2123:HOH:O	1.64	0.95	
1:H:1519[A]:HIS:HD2	5:H:2411:GOL:H12	1.30	0.94	
1:H:1519[A]:HIS:CD2	5:H:2411:GOL:C1	2.51	0.94	
1:H:1442:LYS:HG2	6:H:2046:HOH:O	1.65	0.94	
1:J:1842:LYS:HG3	6:J:2044:HOH:O	1.67	0.93	
5:B:2414:GOL:H12	6:B:2150:HOH:O	1.59	0.93	
1:I:1719[A]:HIS:HD2	5:I:2420:GOL:C2	1.81	0.92	
1:A:25:PRO:HB3	6:A:2023:HOH:O	1.68	0.92	
1:H:1442:LYS:HE3	6:H:2046:HOH:O	1.71	0.91	
1:G:1225:PRO:HD2	1:G:1226:GLU:OE2	1.69	0.91	
1:F:1120:SER:N	5:F:2418:GOL:H12	1.87	0.89	
5:H:2411:GOL:C3	6:H:2123:HOH:O	2.17	0.89	
1:F:1119[A]:HIS:CD2	5:F:2418:GOL:H31	2.07	0.89	
1:C:513:ARG:CD	6:C:2111:HOH:O	2.19	0.88	
3:D:2402:PO4:O2	6:D:2144:HOH:O	1.90	0.88	
1:E:919[A]:HIS:HD2	5:E:2419:GOL:C3	1.86	0.88	
1:B:319[A]:HIS:HD2	5:B:2414:GOL:H32	1.37	0.86	
6:B:2151:HOH:O	5:G:2417:GOL:H32	1.75	0.86	
1:I:1719[A]:HIS:CD2	5:I:2420:GOL:C2	2.58	0.86	
1:I:1750:GLY:N	6:I:2149:HOH:O	2.06	0.86	
1:E:919[A]:HIS:HD2	5:E:2419:GOL:H31	1.40	0.84	
1:C:513:ARG:NE	6:C:2111:HOH:O	2.10	0.84	
1:F:1052:ASP:OD1	6:F:2062:HOH:O	1.95	0.83	
1:L:2225:PRO:HG3	6:L:2047:HOH:O	1.79	0.83	
1:H:1442:LYS:HG3	6:H:2048:HOH:O	1.78	0.82	
1:A:111:HIS:HD1	5:D:2416:GOL:HO2	1.26	0.81	
1:A:25:PRO:CB	6:A:2023:HOH:O	2.26	0.81	
1:K:2120:SER:H	5:K:2421:GOL:C1	1.93	0.81	
5:E:2422:GOL:H12	1:L:2319[B]:HIS:ND1	1.97	0.80	
1:H:1519[A]:HIS:HD2	5:H:2411:GOL:C1	1.88	0.80	
1:I:1719[A]:HIS:HD2	5:I:2420:GOL:C3	1.94	0.79	



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:I:1749:ALA:C	6:I:2149:HOH:O	2.20	0.79
1:A:25:PRO:CG	6:A:2023:HOH:O	2.31	0.79
1:E:822:GLN:HE21	1:F:1070:ARG:HH22	1.29	0.78
1:H:1442:LYS:CE	6:H:2047:HOH:O	2.31	0.78
1:D:720:SER:H	5:D:2416:GOL:C1	1.96	0.78
1:D:720:SER:H	5:D:2416:GOL:H12	1.49	0.77
1:G:1320:SER:N	5:G:2417:GOL:H12	1.98	0.77
1:D:628:TYR:OH	1:D:713:ARG:NH1	2.17	0.77
1:E:914:GLU:OE2	6:E:2154:HOH:O	2.02	0.77
1:E:914:GLU:CG	6:E:2155:HOH:O	2.32	0.76
1:I:1668:GLU:OE1	6:I:2089:HOH:O	2.03	0.76
1:C:513:ARG:CG	6:C:2111:HOH:O	2.08	0.76
1:B:319[A]:HIS:CD2	5:B:2414:GOL:H32	2.21	0.75
1:E:919[A]:HIS:CD2	5:E:2419:GOL:H12	2.21	0.75
1:L:2247:HIS:CE1	6:L:2068:HOH:O	2.40	0.75
1:I:1674:CYS:O	6:I:2096:HOH:O	2.04	0.75
5:J:2412:GOL:C1	6:J:2098:HOH:O	2.35	0.74
1:F:1119[A]:HIS:HD2	5:F:2418:GOL:H31	1.50	0.74
1:G:1225:PRO:CD	1:G:1226:GLU:OE2	2.35	0.74
5:E:2422:GOL:H2	6:E:2149:HOH:O	1.88	0.73
1:L:2225:PRO:CG	6:L:2047:HOH:O	2.27	0.73
1:F:1119[A]:HIS:HD2	5:F:2418:GOL:C3	2.00	0.73
1:B:226:GLU:H	1:B:226:GLU:CD	1.91	0.73
1:B:271:LEU:HD23	6:B:2095:HOH:O	1.75	0.72
5:E:2419:GOL:C2	6:E:2184:HOH:O	2.29	0.72
1:G:1319[A]:HIS:ND1	5:G:2417:GOL:H31	2.04	0.72
1:I:1642:LYS:CE	6:I:2061:HOH:O	2.39	0.71
1:E:914:GLU:HG2	6:E:2155:HOH:O	1.91	0.71
1:F:1068:GLU:CD	6:F:2088:HOH:O	2.28	0.71
1:E:919[A]:HIS:CD2	5:E:2419:GOL:H31	2.24	0.70
1:F:1119[B]:HIS:HB3	5:F:2418:GOL:H31	1.72	0.70
1:H:1442:LYS:NZ	6:H:2047:HOH:O	2.09	0.70
1:L:2349:ALA:O	6:L:2147:HOH:O	2.09	0.69
1:L:2224:GLN:HA	1:L:2226:GLU:OE2	1.92	0.69
5:E:2422:GOL:C1	1:L:2319[B]:HIS:ND1	2.55	0.69
5:I:2420:GOL:H2	6:I:2155:HOH:O	1.91	0.69
1:C:519[B]:HIS:CD2	5:C:2415:GOL:H12	2.28	0.69
1:D:670:ARG:O	6:D:2097:HOH:O	2.11	0.69
1:L:2319[B]:HIS:CD2	6:L:2101:HOH:O	2.25	0.68
1:E:919[A]:HIS:CD2	5:E:2419:GOL:C3	2.74	0.68
1:F:1068:GLU:OE1	6:F:2088:HOH:O	2.12	0.67



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:I:1642:LYS:HE2	6:I:2061:HOH:O	1.94	0.67	
1:K:2119[A]:HIS:CD2	5:K:2421:GOL:C1	2.78	0.67	
1:L:2203:SER:HB2	6:L:2027:HOH:O	1.95	0.66	
1:D:668:GLU:OE1	6:D:2094:HOH:O	2.14	0.66	
1:H:1442:LYS:HE2	6:H:2047:HOH:O	1.92	0.65	
1:D:719[B]:HIS:ND1	6:D:2122:HOH:O	2.20	0.65	
5:A:2413:GOL:O1	6:A:2135:HOH:O	2.08	0.65	
6:A:2096:HOH:O	5:D:2416:GOL:H2	1.98	0.64	
1:K:2002:ARG:NH1	1:K:2071:LEU:O	2.32	0.63	
1:I:1719[A]:HIS:CD2	5:I:2420:GOL:H2	2.33	0.62	
1:E:822:GLN:NE2	1:F:1070:ARG:HH22	1.98	0.62	
1:I:1642:LYS:HE3	6:I:2059:HOH:O	1.99	0.61	
1:A:25:PRO:CD	6:A:2023:HOH:O	2.48	0.60	
1:H:1430:SER:HB3	6:H:2005:HOH:O	2.01	0.60	
1:I:1719[B]:HIS:ND1	5:I:2420:GOL:H31	2.17	0.60	
1:I:1719[A]:HIS:HD2	5:I:2420:GOL:H31	1.65	0.60	
1:E:802:ARG:NH1	6:E:2053:HOH:O	2.33	0.59	
1:D:626:GLU:H	1:D:626:GLU:CD	2.05	0.59	
5:J:2412:GOL:H11	6:J:2098:HOH:O	1.99	0.59	
1:C:448:GLY:HA3	6:C:2061:HOH:O	2.02	0.59	
1:H:1442:LYS:CE	6:H:2046:HOH:O	2.39	0.59	
1:L:2348:LEU:C	1:L:2350:GLY:H	2.05	0.59	
1:J:1842:LYS:CG	6:J:2043:HOH:O	2.30	0.58	
1:K:2120:SER:H	5:K:2421:GOL:H11	1.65	0.58	
1:F:1119[A]:HIS:CG	5:F:2418:GOL:H31	2.39	0.58	
1:E:935:VAL:HG22	6:E:2171:HOH:O	2.04	0.58	
5:J:2412:GOL:H12	6:J:2098:HOH:O	2.02	0.57	
1:D:670:ARG:HH22	1:F:1022:GLN:HE21	1.51	0.57	
1:E:823:ARG:NE	1:F:1098:ASP:OD2	2.36	0.57	
1:H:1442:LYS:CG	6:H:2046:HOH:O	2.38	0.57	
1:C:519[A]:HIS:ND1	5:C:2415:GOL:H31	2.19	0.57	
1:I:1719[A]:HIS:CD2	5:I:2420:GOL:H31	2.40	0.57	
1:K:2119[A]:HIS:CD2	5:K:2421:GOL:H11	2.40	0.56	
1:J:1842:LYS:CD	6:J:2046:HOH:O	2.50	0.56	
1:G:1319[A]:HIS:ND1	5:G:2417:GOL:C3	2.68	0.56	
5:C:2415:GOL:H12	6:C:2146:HOH:O	1.62	0.56	
1:A:25:PRO:HD3	6:A:2023:HOH:O	2.05	0.56	
1:H:1544:ARG:NH2	6:H:2117:HOH:O	2.15	0.56	
1:E:839:LEU:HD22	6:E:2093:HOH:O	2.07	0.55	
1:I:1627:ILE:HD13	6:I:2116:HOH:O	2.06	0.55	
5:I:2420:GOL:C2	6:I:2155:HOH:O	2.53	0.55	



Atom_1	Atom_2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:K:2026:GLU:H	1:K:2026:GLU:CD	2.10	0.55	
1:A:24:GLN:HA	1:A:26:GLU:OE2	2.07	0.55	
1:A:124:GLN:HE22	1:C:516:PHE:HE2	1.54	0.54	
1:I:1719[A]:HIS:CG	5:I:2420:GOL:C1	2.76	0.54	
1:E:822:GLN:HE22	1:F:1070:ARG:HH12	1.56	0.54	
1:E:914:GLU:OE2	6:E:2155:HOH:O	2.09	0.54	
1:L:2284:SER:OG	1:L:2306:HIS:HE1	1.91	0.54	
1:H:1430:SER:CB	6:H:2017:HOH:O	2.55	0.54	
1:I:1602:ARG:C	6:I:2022:HOH:O	2.47	0.54	
1:F:1068:GLU:OE2	6:F:2088:HOH:O	2.18	0.53	
1:A:113:ARG:HG2	6:A:2101:HOH:O	2.09	0.53	
1:E:802:ARG:NH2	6:E:2053:HOH:O	2.41	0.53	
1:I:1642:LYS:CE	6:I:2059:HOH:O	2.55	0.52	
1:E:822:GLN:HE21	1:F:1070:ARG:NH2	2.03	0.52	
1:F:1022:GLN:NE2	6:F:2030:HOH:O	2.41	0.52	
1:I:1720:SER:H	5:I:2420:GOL:C1	2.22	0.52	
3:A:2401:PO4:O4	1:C:458:HIS:ND1	2.40	0.52	
1:I:1719[B]:HIS:HB3	5:I:2420:GOL:H11	1.91	0.52	
1:K:2025:PRO:HD2	1:K:2026:GLU:OE2	2.10	0.52	
1:D:720:SER:N	5:D:2416:GOL:H12	2.21	0.52	
1:E:831:ASP:HB2	6:E:2078:HOH:O	2.10	0.52	
1:J:1842:LYS:HE3	6:J:2043:HOH:O	2.09	0.52	
1:J:1822:GLN:HE21	1:K:2070:ARG:HH22	1.58	0.51	
1:H:1424:GLN:HA	1:H:1426:GLU:OE2	2.10	0.51	
1:G:1222:GLN:HE21	1:H:1470:ARG:HH22	1.57	0.51	
1:E:919[A]:HIS:HD2	5:E:2419:GOL:C2	2.22	0.51	
1:B:319[A]:HIS:CD2	5:B:2414:GOL:H12	2.45	0.51	
1:K:2004:LEU:CD1	1:K:2149:ALA:HB3	2.40	0.51	
1:I:1642:LYS:HG2	6:I:2059:HOH:O	2.09	0.51	
5:K:2421:GOL:H2	6:K:3122:HOH:O	2.10	0.51	
1:A:2:ARG:NH2	6:A:2001:HOH:O	2.44	0.51	
1:G:1319[B]:HIS:HD2	5:G:2417:GOL:H2	1.77	0.50	
1:L:2315:PRO:HB2	6:L:2125:HOH:O	2.10	0.50	
1:L:2319[B]:HIS:CE1	6:L:2128:HOH:O	2.64	0.50	
1:G:1222:GLN:NE2	1:H:1470:ARG:HH22	2.09	0.50	
1:K:2119[A]:HIS:HD2	5:K:2421:GOL:C2	2.24	0.50	
1:H:1544:ARG:NE	6:H:2117:HOH:O	2.42	0.50	
1:J:1884:SER:OG	1:J:1906:HIS:HE1	1.95	0.50	
1:G:1281:ALA:HA	2:G:1360:CA2:HA	1.94	0.50	
1:B:224:GLN:N	1:B:225:PRO:CD	2.75	0.49	
1:G:1319[B]:HIS:CD2	5:G:2417:GOL:H2	2.47	0.49	



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:804:LEU:HD23	1:E:849:GLY:HA3	1.95	0.49
1:G:1270:ARG:HH22	1:I:1622:GLN:HE21	1.60	0.49
1:J:1826:GLU:H	1:J:1826:GLU:CD	2.16	0.49
1:I:1604:LEU:O	6:I:2024:HOH:O	2.20	0.49
1:E:828:TYR:CG	2:E:960:CA2:H13	2.48	0.48
1:F:1119[A]:HIS:HD2	5:F:2418:GOL:C2	2.26	0.48
1:A:111:HIS:ND1	5:D:2416:GOL:O2	2.31	0.48
1:E:919[A]:HIS:CD2	5:E:2419:GOL:C1	2.93	0.48
1:F:1028:TYR:CD1	2:F:1160:CA2:H13	2.48	0.48
1:K:2011:ILE:HD13	1:K:2077:VAL:HB	1.95	0.48
1:H:1519[A]:HIS:CG	5:H:2411:GOL:H12	2.38	0.48
1:A:28:TYR:OH	1:A:113:ARG:NH1	2.47	0.48
1:K:2015:PRO:O	1:K:2016:ASN:HB2	2.14	0.48
1:D:622:GLN:HE21	1:E:870:ARG:HH22	1.62	0.47
1:F:1025:PRO:HD2	1:F:1026:GLU:OE2	2.14	0.47
1:J:1842:LYS:HD3	6:J:2046:HOH:O	2.13	0.47
1:C:430:SER:HB3	6:C:2044:HOH:O	2.13	0.47
1:F:1119[A]:HIS:HB2	5:F:2418:GOL:H31	1.95	0.47
1:G:1226:GLU:CD	1:G:1226:GLU:H	2.14	0.47
1:I:1602:ARG:CA	6:I:2022:HOH:O	2.47	0.47
1:A:58:HIS:ND1	3:A:2401:PO4:O2	2.29	0.47
1:B:271:LEU:HD22	6:B:2095:HOH:O	1.85	0.47
1:K:2015:PRO:HD2	1:K:2081:ALA:HB3	1.95	0.47
1:I:1624:GLN:N	1:I:1625:PRO:CD	2.78	0.47
1:I:1642:LYS:NZ	6:I:2061:HOH:O	2.48	0.47
5:C:2415:GOL:O1	6:C:2144:HOH:O	2.21	0.47
1:E:828:TYR:CD1	2:E:960:CA2:H13	2.49	0.46
5:E:2422:GOL:H11	1:L:2319[B]:HIS:ND1	2.31	0.46
1:I:1658:HIS:HD1	3:I:2403:PO4:P	2.38	0.46
1:I:1627:ILE:O	6:I:2041:HOH:O	2.21	0.46
1:C:433:LEU:HD12	1:C:433:LEU:HA	1.87	0.46
1:F:1120:SER:H	5:F:2418:GOL:C1	1.98	0.46
1:G:1225:PRO:N	1:G:1226:GLU:OE2	2.49	0.46
1:D:604:LEU:HD12	1:D:674:CYS:SG	2.57	0.45
1:D:623:ARG:CD	1:E:896:THR:HA	2.47	0.45
1:I:1719[B]:HIS:HB3	5:I:2420:GOL:C1	2.47	0.45
1:J:1821:GLY:CA	6:J:2016:HOH:O	2.53	0.45
1:H:1428:TYR:CD1	2:H:1560:CA2:H13	2.51	0.45
1:L:2202:ARG:NH2	6:L:2098:HOH:O	2.39	0.45
1:E:927:ASP:OD1	6:E:2169:HOH:O	2.20	0.45
1:I:1701:PRO:HB2	1:I:1745:ILE:HD12	1.98	0.45



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:F:1026:GLU:CD	1:F:1026:GLU:H	2.19	0.44	
1:C:426:GLU:CD	1:C:426:GLU:H	2.20	0.44	
1:L:2226:GLU:CD	1:L:2226:GLU:H	2.21	0.44	
1:B:223:ARG:HG2	2:B:360:CA2:H15	1.99	0.44	
1:H:1519[A]:HIS:ND1	6:H:2098:HOH:O	2.14	0.44	
1:I:1643:ALA:O	1:I:1647:HIS:HD2	2.01	0.44	
5:K:2421:GOL:C2	6:K:3122:HOH:O	2.65	0.44	
1:A:25:PRO:HG3	6:A:2023:HOH:O	2.10	0.44	
1:F:1125:ARG:HD2	1:F:1125:ARG:O	2.18	0.44	
1:G:1324:GLN:HE22	1:I:1716:PHE:HE2	1.65	0.44	
1:I:1716:PHE:CB	6:I:2018:HOH:O	2.66	0.44	
1:B:269:ALA:HA	1:B:273:HIS:ND1	2.34	0.43	
1:H:1513:ARG:NH2	6:H:2029:HOH:O	2.51	0.43	
1:E:826:GLU:CD	1:E:826:GLU:H	2.21	0.43	
1:J:1824:GLN:N	1:J:1825:PRO:CD	2.81	0.43	
1:L:2228:TYR:OH	1:L:2313:ARG:NH1	2.44	0.43	
1:A:24:GLN:N	1:A:25:PRO:CD	2.82	0.43	
1:B:226:GLU:CD	1:B:226:GLU:N	2.67	0.43	
1:J:1919[B]:HIS:ND1	5:J:2412:GOL:H31	2.33	0.43	
1:D:622:GLN:HE22	1:E:870:ARG:HH12	1.66	0.43	
1:D:643:ALA:O	1:D:647:HIS:HD2	2.02	0.43	
1:J:1869:ALA:HA	1:J:1873:HIS:ND1	2.33	0.43	
1:J:1815:PRO:HD2	1:J:1881:ALA:HB3	2.01	0.42	
1:A:23:ARG:NH2	1:B:298:ASP:OD1	2.35	0.42	
1:D:707:ILE:HD13	1:D:707:ILE:HG21	1.84	0.42	
1:H:1443:ALA:O	1:H:1447:HIS:HD2	2.03	0.42	
1:D:624:GLN:N	1:D:625:PRO:CD	2.83	0.42	
1:D:627:ILE:HD13	1:D:627:ILE:HG21	1.83	0.42	
1:L:2348:LEU:C	1:L:2350:GLY:N	2.72	0.42	
1:E:911:HIS:HD1	5:E:2422:GOL:HO2	1.62	0.42	
1:A:2:ARG:HD3	1:A:7:ALA:HB2	2.02	0.42	
1:A:98:ASP:OD2	1:C:423:ARG:NE	2.40	0.42	
1:B:223:ARG:HD3	6:B:2036:HOH:O	2.19	0.42	
1:B:223:ARG:NH1	1:B:224:GLN:OE1	2.53	0.42	
1:G:1254:ARG:HB3	1:G:1265:TRP:CZ3	2.55	0.42	
1:K:2114:GLU:H	1:K:2114:GLU:CD	2.22	0.42	
1:K:2119[A]:HIS:HD2	5:K:2421:GOL:H31	1.84	0.42	
1:A:2:ARG:HB3	1:A:6:ASN:HD21	1.85	0.41	
1:J:1916:PHE:HE2	1:K:2124:GLN:HE22	1.68	0.41	
1:K:2119[A]:HIS:HD2	5:K:2421:GOL:C3	2.33	0.41	
1:C:519[B]:HIS:HD2	5:C:2415:GOL:H12	1.84	0.41	



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:E:950:GLY:CA	6:E:2181:HOH:O	2.68	0.41	
1:C:425:PRO:CD	1:C:426:GLU:OE2	2.51	0.41	
1:E:918:HIS:HE1	6:E:2158:HOH:O	2.03	0.41	
1:H:1430:SER:HB2	6:H:2017:HOH:O	2.17	0.41	
1:E:914:GLU:CD	6:E:2154:HOH:O	2.56	0.41	
1:F:1119[A]:HIS:HD2	5:F:2418:GOL:H2	1.85	0.41	
1:H:1402:ARG:HD3	1:H:1407:ALA:HB2	2.02	0.41	
1:H:1498:ASP:OD1	6:H:2083:HOH:O	2.22	0.41	
1:K:2119[A]:HIS:CD2	5:K:2421:GOL:C2	3.04	0.41	
1:L:2202:ARG:HA	6:L:2026:HOH:O	2.20	0.41	
1:E:824:GLN:HA	1:E:826:GLU:OE2	2.21	0.41	
1:E:919[A]:HIS:CD2	5:E:2419:GOL:C2	3.04	0.41	
2:J:1960:CA2:O4	1:K:2092:ASP:OD2	2.37	0.41	
2:A:160:CA2:H102	2:A:160:CA2:H17	1.83	0.41	
1:C:519[A]:HIS:ND1	5:C:2415:GOL:C3	2.83	0.40	
1:J:1925:ARG:O	1:J:1926:ALA:C	2.59	0.40	
1:F:1028:TYR:CG	2:F:1160:CA2:H13	2.56	0.40	
1:I:1749:ALA:O	6:I:2149:HOH:O	2.21	0.40	
1:E:822:GLN:NE2	1:F:1070:ARG:NH2	2.65	0.40	
1:E:914:GLU:HA	1:E:915:PRO:HD3	1.84	0.40	
1:F:1002:ARG:HD3	1:F:1007:ALA:HB2	2.04	0.40	
1:I:1720:SER:H	5:I:2420:GOL:H11	1.85	0.40	
1:K:2007:ALA:HB1	1:K:2008:PRO:HD2	2.03	0.40	
1:F:1114:GLU:HA	1:F:1115:PRO:HD3	1.93	0.40	
1:A:26:GLU:CD	1:A:26:GLU:H	2.24	0.40	
2:B:360:CA2:H2C1	2:B:360:CA2:H9C2	1.89	0.40	
1:D:670:ARG:HH22	1:F:1022:GLN:NE2	2.19	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
1	А	149/157~(95%)	146~(98%)	3~(2%)	0	100	100
1	В	148/157~(94%)	145~(98%)	3~(2%)	0	100	100
1	С	148/157~(94%)	145 (98%)	3~(2%)	0	100	100
1	D	149/157~(95%)	146 (98%)	3(2%)	0	100	100
1	Ε	148/157~(94%)	144 (97%)	4 (3%)	0	100	100
1	F	148/157~(94%)	145 (98%)	3(2%)	0	100	100
1	G	149/157~(95%)	145~(97%)	4(3%)	0	100	100
1	Н	148/157~(94%)	145~(98%)	3~(2%)	0	100	100
1	Ι	148/157~(94%)	145~(98%)	3~(2%)	0	100	100
1	J	148/157~(94%)	144 (97%)	4(3%)	0	100	100
1	Κ	148/157~(94%)	145~(98%)	3~(2%)	0	100	100
1	L	149/157~(95%)	145 (97%)	4 (3%)	0	100	100
All	All	1780/1884~(94%)	1740 (98%)	40 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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)

32 ligands are modelled in this entry.



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

Mal	Turne	Chain	Dec	Tink	Bo	Bond lengths		Bond angles		
	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	CA2	В	360	-	23,23,23	1.00	2 (8%)	28,32,32	2.74	10 (35%)
4	TRS	F	2406	-	7,7,7	0.62	0	$9,\!9,\!9$	0.69	0
2	CA2	L	2360	-	23,23,23	1.30	1 (4%)	28,32,32	1.91	6 (21%)
2	CA2	G	1360	-	23,23,23	1.79	4 (17%)	28,32,32	2.71	9 (32%)
5	GOL	Е	2422	-	5,5,5	0.92	0	$5,\!5,\!5$	0.43	0
5	GOL	Ι	2420	-	$5,\!5,\!5$	0.55	0	$5,\!5,\!5$	0.77	0
2	CA2	Е	960	-	23,23,23	1.08	1 (4%)	$28,\!32,\!32$	2.50	8 (28%)
5	GOL	С	2415	-	$5,\!5,\!5$	0.77	0	$5,\!5,\!5$	0.80	0
5	GOL	J	2412	-	$5,\!5,\!5$	0.51	0	$5,\!5,\!5$	1.01	0
2	CA2	K	2160	-	23,23,23	0.84	1 (4%)	$28,\!32,\!32$	2.22	8 (28%)
5	GOL	F	2418	-	5,5,5	0.96	0	$5,\!5,\!5$	1.97	3 (60%)
2	CA2	Н	1560	-	23,23,23	1.44	1 (4%)	28,32,32	1.96	9 (32%)
3	PO4	Ι	2403	-	4,4,4	1.40	1 (25%)	6,6,6	1.67	2 (33%)
2	CA2	F	1160	-	23,23,23	1.67	2 (8%)	28,32,32	2.11	8 (28%)
3	PO4	А	2401	-	4,4,4	1.62	1 (25%)	$6,\!6,\!6$	1.78	2 (33%)
5	GOL	Н	2411	-	$5,\!5,\!5$	0.41	0	$5,\!5,\!5$	0.60	0
4	TRS	Н	2407	-	7,7,7	0.91	0	$9,\!9,\!9$	0.83	0
3	PO4	L	2404	-	4,4,4	1.06	0	$6,\!6,\!6$	2.15	2 (33%)
5	GOL	G	2417	-	$5,\!5,\!5$	0.77	0	$5,\!5,\!5$	1.41	1 (20%)
2	CA2	D	760	-	23,23,23	1.01	2 (8%)	28,32,32	2.47	10 (35%)
4	TRS	L	2408	-	7,7,7	0.45	0	$9,\!9,\!9$	0.97	0
5	GOL	В	2414	-	5,5,5	0.53	0	$5,\!5,\!5$	0.49	0
5	GOL	K	2421	-	$5,\!5,\!5$	0.64	0	$5,\!5,\!5$	0.91	0
4	TRS	А	2405	-	7,7,7	0.68	0	$9,\!9,\!9$	1.47	3 (33%)
5	GOL	Е	2419	-	$5,\!5,\!5$	0.72	0	$5,\!5,\!5$	0.86	0
3	PO4	D	2402	-	4,4,4	1.50	1 (25%)	$6,\!6,\!6$	0.76	0
5	GOL	D	2416	-	5,5,5	0.56	0	$5,\!5,\!5$	0.55	0
2	CA2	J	1960	-	23,23,23	1.50	4 (17%)	28,32,32	1.96	8 (28%)
2	CA2	С	560	-	23,23,23	1.25	2 (8%)	28,32,32	1.72	8 (28%)
2	CA2	A	160	-	23,23,23	1.61	4 (17%)	28,32,32	2.15	8 (28%)
2	CA2	I	1760	-	23,23,23	1.29	2 (8%)	$28,\!32,\!32$	1.99	9 (32%)



Mol Type Chain		Dog	Link	Bond lengths			Bond lengths Bond angles			gles
	туре	Unaim	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	А	2413	-	$5,\!5,\!5$	0.76	0	$5,\!5,\!5$	0.69	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
2	CA2	В	360	-	-	2/13/31/31	0/2/2/2
4	TRS	F	2406	-	-	0/9/9/9	-
2	CA2	L	2360	-	-	3/13/31/31	0/2/2/2
2	CA2	G	1360	-	-	1/13/31/31	0/2/2/2
5	GOL	Е	2422	-	-	4/4/4/4	-
5	GOL	Ι	2420	-	-	3/4/4/4	-
2	CA2	Е	960	-	_	1/13/31/31	0/2/2/2
5	GOL	С	2415	-	-	3/4/4/4	-
5	GOL	J	2412	-	-	4/4/4/4	-
2	CA2	K	2160	-	-	3/13/31/31	0/2/2/2
5	GOL	F	2418	-	-	0/4/4/4	-
2	CA2	Н	1560	-	-	3/13/31/31	0/2/2/2
2	CA2	F	1160	-	_	2/13/31/31	0/2/2/2
5	GOL	Н	2411	-	_	0/4/4/4	-
4	TRS	Н	2407	-	-	0/9/9/9	-
5	GOL	G	2417	-	-	1/4/4/4	-
2	CA2	D	760	-	-	1/13/31/31	0/2/2/2
4	TRS	L	2408	-	-	0/9/9/9	-
5	GOL	В	2414	-	-	2/4/4/4	-
5	GOL	K	2421	-	-	2/4/4/4	-
4	TRS	А	2405	-	-	0/9/9/9	-
5	GOL	Е	2419	-	-	2/4/4/4	-
5	GOL	D	2416	-	-	4/4/4/4	-
2	CA2	J	1960	-	_	2/13/31/31	0/2/2/2
2	CA2	С	560	-	-	4/13/31/31	0/2/2/2
2	CA2	А	160	-	-	1/13/31/31	0/2/2/2
2	CA2	Ι	1760	-	-	2/13/31/31	0/2/2/2
5	GOL	А	2413	-	-	4/4/4/4	-

All (29) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1360	CA2	C1-C7	-6.45	1.46	1.53
2	F	1160	CA2	C1-C7	-6.40	1.46	1.53
2	Н	1560	CA2	C1-C7	-5.35	1.47	1.53
2	L	2360	CA2	C1-C7	-4.84	1.48	1.53
2	А	160	CA2	C1-C7	-4.78	1.48	1.53
2	Ι	1760	CA2	C1-C7	-4.33	1.48	1.53
2	С	560	CA2	C1-C7	-4.16	1.49	1.53
2	J	1960	CA2	C1-C7	-4.08	1.49	1.53
2	А	160	CA2	O3-C1	3.45	1.50	1.43
2	В	360	CA2	C1-C7	-3.19	1.50	1.53
2	Е	960	CA2	O3-C1	3.16	1.49	1.43
3	А	2401	PO4	P-O2	-2.79	1.46	1.54
2	J	1960	CA2	O5-C5	2.75	1.49	1.43
2	D	760	CA2	C1-C7	-2.68	1.50	1.53
2	С	560	CA2	C5-C4	-2.61	1.48	1.52
3	Ι	2403	PO4	P-O3	-2.54	1.47	1.54
2	G	1360	CA2	C2-C1	-2.49	1.48	1.53
2	D	760	CA2	C6-C5	2.45	1.56	1.53
2	F	1160	CA2	C6-C5	2.34	1.56	1.53
2	G	1360	CA2	C6-C5	-2.31	1.49	1.53
2	Κ	2160	CA2	C1-C7	-2.26	1.51	1.53
2	А	160	CA2	C3-C4	2.23	1.56	1.53
3	D	2402	PO4	P-O4	-2.15	1.48	1.54
2	А	160	CA2	O4-C4	2.13	1.48	1.43
2	J	1960	CA2	C3-C4	-2.11	1.50	1.53
2	J	1960	CA2	O2-C7	2.03	1.28	1.22
2	В	360	CA2	O5-C5	2.01	1.47	1.43
2	Ι	1760	CA2	C6-C5	2.01	1.56	1.53
2	G	1360	CA2	O3-C1	-2.00	1.39	1.43

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
2	В	360	CA2	C6-C1-C2	8.22	115.99	110.72
2	G	1360	CA2	O2-C7-C1	-7.44	111.72	122.25
2	Е	960	CA2	C6-C1-C2	-6.62	106.48	110.72
2	А	160	CA2	C2-C3-C4	6.46	117.40	109.20
2	Н	1560	CA2	C2-C3-C4	6.01	116.83	109.20
2	K	2160	CA2	C6-C1-C2	5.68	114.36	110.72
2	K	2160	CA2	C6-C5-C4	-5.51	105.45	110.84
2	G	1360	CA2	C6-C1-C2	5.38	114.17	110.72
2	D	760	CA2	C6-C5-C4	-5.33	105.62	110.84
2	G	1360	CA2	C2-C3-C8	-5.23	102.23	111.99



Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
2	L	2360	CA2	C2-C3-C4	4.99	115.54	109.20
2	В	360	CA2	O2-C7-C1	-4.85	115.38	122.25
2	D	760	CA2	C2-C3-C4	4.81	115.31	109.20
2	D	760	CA2	C6-C1-C2	4.73	113.75	110.72
2	F	1160	CA2	C6-C1-C2	-4.71	107.70	110.72
2	G	1360	CA2	O1-C7-C1	4.69	121.20	113.05
2	J	1960	CA2	O2-C7-C1	-4.66	115.66	122.25
2	F	1160	CA2	C2-C1-C7	-4.65	99.75	109.96
2	L	2360	CA2	O2-C7-C1	-4.61	115.73	122.25
2	Е	960	CA2	O2-C7-C1	-4.59	115.75	122.25
2	D	760	CA2	O1-C7-C1	4.57	120.99	113.05
2	В	360	CA2	C2-C1-C7	-4.55	99.96	109.96
2	В	360	CA2	O5-C5-C6	4.50	120.38	109.91
2	Ι	1760	CA2	O1-C7-C1	4.45	120.77	113.05
2	Е	960	CA2	O1-C7-C1	4.36	120.63	113.05
2	F	1160	CA2	O2-C7-C1	-4.36	116.09	122.25
3	L	2404	PO4	O2-P-O1	-4.32	95.08	110.89
2	Е	960	CA2	O4-C4-C3	-4.29	102.84	110.08
2	G	1360	CA2	C6-C5-C4	-4.23	106.70	110.84
2	С	560	CA2	O2-C7-C1	-4.19	116.32	122.25
2	Е	960	CA2	C2-C3-C4	4.17	114.50	109.20
2	L	2360	CA2	C2-C1-C7	-4.13	100.89	109.96
2	Κ	2160	CA2	O2-C7-C1	-4.05	116.52	122.25
2	D	760	CA2	O2-C7-C1	-4.02	116.56	122.25
2	D	760	CA2	C2-C3-C8	-3.97	104.59	111.99
2	Ι	1760	CA2	O2-C7-C1	-3.96	116.64	122.25
2	J	1960	CA2	O1-C7-C1	3.95	119.92	113.05
2	Е	960	CA2	C2-C1-C7	-3.92	101.35	109.96
2	J	1960	CA2	C2-C1-C7	-3.82	101.58	109.96
2	В	360	CA2	C2-C3-C4	3.80	114.02	109.20
2	G	1360	CA2	C2-C3-C4	3.78	114.00	109.20
2	J	1960	CA2	C6-C1-C2	3.75	113.12	110.72
2	Н	1560	CA2	C2-C1-C7	-3.74	101.75	109.96
2	F	1160	CA2	C2-C3-C4	3.67	113.86	109.20
2	В	360	CA2	O5-C5-C4	-3.61	102.90	110.14
2	F	1160	CA2	O1-C7-C1	3.61	119.31	113.05
2	А	160	CA2	O1-C7-C1	3.54	119.20	113.05
2	А	160	CA2	C6-C5-C4	-3.53	107.38	110.84
2	D	760	CA2	O4-C4-C5	-3.53	103.24	109.99
2	Κ	2160	CA2	O1-C7-C1	3.51	119.14	113.05
2	Ι	1760	CA2	O4-C4-C5	-3.47	103.35	109.99
2	J	1960	CA2	C2-C3-C4	3.42	113.54	109.20



Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
2	В	360	CA2	C1-C6-C5	-3.39	106.32	112.54
2	Ι	1760	CA2	C6-C1-C7	3.35	117.31	109.96
2	С	560	CA2	O5-C5-C4	-3.31	103.52	110.14
2	В	360	CA2	O4-C4-C5	-3.29	103.70	109.99
2	Ι	1760	CA2	C2-C1-C7	-3.26	102.79	109.96
2	Ι	1760	CA2	C6-C5-C4	3.26	114.02	110.84
2	Κ	2160	CA2	C2-C3-C4	3.22	113.29	109.20
2	А	160	CA2	O3-C1-C2	3.22	116.69	109.41
2	Κ	2160	CA2	O4-C4-C5	-3.21	103.84	109.99
2	Е	960	CA2	O3-C1-C6	3.21	116.66	109.41
3	А	2401	PO4	O3-P-O2	3.20	118.22	107.97
2	А	160	CA2	O2-C7-C1	-3.14	117.81	122.25
2	А	160	CA2	O5-C5-C4	-3.09	103.94	110.14
2	Ι	1760	CA2	O5-C5-C4	-3.00	104.12	110.14
2	L	2360	CA2	O1-C7-C1	2.89	118.07	113.05
5	F	2418	GOL	O1-C1-C2	2.88	124.03	110.20
2	Н	1560	CA2	O4-C4-C5	-2.87	104.50	109.99
2	С	560	CA2	O1-C7-C1	2.86	118.02	113.05
2	Κ	2160	CA2	C2-C1-C7	-2.83	103.74	109.96
2	F	1160	CA2	O5-C5-C6	2.80	116.43	109.91
2	G	1360	CA2	O4-C4-C3	2.77	114.77	110.08
2	Κ	2160	CA2	C2-C3-C8	-2.70	106.96	111.99
2	Н	1560	CA2	C6-C1-C7	2.69	115.87	109.96
2	С	560	CA2	C2-C1-C7	-2.69	104.05	109.96
2	D	760	CA2	C6-C1-C7	2.68	115.83	109.96
2	Н	1560	CA2	O1-C7-C1	2.66	117.67	113.05
4	А	2405	TRS	O1-C1-C	2.66	119.42	111.00
5	G	2417	GOL	O1-C1-C2	2.65	122.91	110.20
2	Н	1560	CA2	O5-C5-C4	-2.59	104.95	110.14
2	С	560	CA2	O4-C4-C5	-2.55	105.11	109.99
2	L	2360	CA2	O4-C4-C5	-2.54	105.13	109.99
3	А	2401	PO4	O3-P-O1	-2.54	101.59	110.89
2	D	760	CA2	C10-O11-C12	2.54	124.55	117.93
2	J	1960	CA2	O5-C5-C4	-2.50	105.13	110.14
2	D	760	CA2	O3-C1-C6	-2.46	103.86	109.41
2	F	1160	CA2	O5-C5-C4	-2.46	105.22	110.14
2	G	1360	CA2	C2-C1-C7	-2.45	104.58	109.96
2	G	1360	CA2	C8-C9-C10	-2.45	105.54	113.27
2	J	1960	CA2	C6-C1-C7	2.41	115.24	109.96
2	C	560	CA2	C2-C3-C8	-2.40	107.51	111.99
2	В	360	CA2	C6-C5-C4	-2.39	108.50	110.84
2	А	160	CA2	C2-C1-C7	-2.36	104.77	109.96



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	560	CA2	C6-C1-C2	2.34	112.22	110.72
2	А	160	CA2	O4-C4-C5	-2.34	105.51	109.99
2	Н	1560	CA2	O2-C7-C1	-2.30	119.00	122.25
2	Ι	1760	CA2	C10-O11-C12	2.29	123.92	117.93
3	Ι	2403	PO4	O3-P-O2	2.25	115.20	107.97
3	Ι	2403	PO4	O4-P-O1	2.20	118.96	110.89
2	L	2360	CA2	O5-C5-C4	-2.20	105.73	110.14
4	А	2405	TRS	C3-C-N	2.18	114.48	107.98
2	Н	1560	CA2	O3-C1-C2	2.15	114.28	109.41
2	Н	1560	CA2	C1-C6-C5	2.15	116.48	112.54
4	А	2405	TRS	O3-C3-C	2.14	117.78	111.00
2	J	1960	CA2	O3-C1-C2	2.13	114.22	109.41
5	F	2418	GOL	O2-C2-C3	-2.08	99.96	109.12
2	Е	960	CA2	O4-C4-C5	-2.08	106.01	109.99
5	F	2418	GOL	C3-C2-C1	2.06	119.72	111.70
2	С	560	CA2	C2-C3-C4	2.06	111.81	109.20
2	Ι	1760	CA2	C6-C1-C2	2.05	112.04	110.72
3	L	2404	PO4	04-P-01	2.01	118.26	110.89
2	В	360	CA2	C9-C8-C3	-2.00	108.38	115.17
2	F	1160	CA2	C6-C1-C7	2.00	114.35	109.96

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	2360	CA2	O3-C1-C7-O1
5	А	2413	GOL	C1-C2-C3-O3
5	В	2414	GOL	C1-C2-C3-O3
5	С	2415	GOL	C1-C2-C3-O3
5	Ε	2419	GOL	C1-C2-C3-O3
5	Е	2422	GOL	O1-C1-C2-C3
5	Е	2422	GOL	C1-C2-C3-O3
5	Е	2422	GOL	O2-C2-C3-O3
5	Ι	2420	GOL	O1-C1-C2-C3
5	J	2412	GOL	O1-C1-C2-C3
5	J	2412	GOL	C1-C2-C3-O3
5	Κ	2421	GOL	O1-C1-C2-C3
5	Κ	2421	GOL	O1-C1-C2-O2
5	А	2413	GOL	O1-C1-C2-C3
5	С	2415	GOL	O1-C1-C2-C3
5	D	2416	GOL	O1-C1-C2-C3
5	G	2417	GOL	O1-C1-C2-C3



Mol	Chain	Res	Type	Atoms
2	В	360	CA2	O11-C10-C9-C8
5	А	2413	GOL	O1-C1-C2-O2
5	А	2413	GOL	O2-C2-C3-O3
5	В	2414	GOL	O2-C2-C3-O3
5	Е	2422	GOL	O1-C1-C2-O2
5	J	2412	GOL	O1-C1-C2-O2
5	J	2412	GOL	O2-C2-C3-O3
5	D	2416	GOL	O1-C1-C2-O2
5	Е	2419	GOL	O2-C2-C3-O3
2	F	1160	CA2	O11-C10-C9-C8
2	J	1960	CA2	O11-C10-C9-C8
5	Ι	2420	GOL	O1-C1-C2-O2
2	Ι	1760	CA2	O11-C10-C9-C8
2	А	160	CA2	O3-C1-C7-O2
2	В	360	CA2	O3-C1-C7-O2
2	С	560	CA2	O3-C1-C7-O2
2	D	760	CA2	O3-C1-C7-O2
2	Е	960	CA2	O3-C1-C7-O2
2	F	1160	CA2	O3-C1-C7-O2
2	G	1360	CA2	O3-C1-C7-O2
2	Н	1560	CA2	O3-C1-C7-O2
2	Ι	1760	CA2	O3-C1-C7-O2
2	J	1960	CA2	O3-C1-C7-O2
5	D	2416	GOL	O2-C2-C3-O3
2	K	2160	CA2	O11-C10-C9-C8
2	С	560	CA2	O11-C10-C9-C8
2	Н	1560	CA2	C13-C12-O11-C10
5	Ι	2420	GOL	C1-C2-C3-O3
2	С	560	CA2	C13-C12-O11-C10
2	С	560	CA2	C17-C12-O11-C10
2	Н	1560	CA2	C17-C12-O11-C10
5	С	2415	GOL	O2-C2-C3-O3
2	L	2360	CA2	C13-C12-O11-C10
2	L	2360	CA2	C17-C12-O11-C10
5	D	2416	GOL	C1-C2-C3-O3
2	K	2160	CA2	O3-C1-C7-O2
2	K	2160	CA2	C13-C12-O11-C10

Continued from previous page...

There are no ring outliers.

22 monomers are involved in 118 short contacts:



Mol	Chain	\mathbf{Res}	Type	Clashes	Symm-Clashes
2	В	360	CA2	2	0
2	G	1360	CA2	1	0
5	Е	2422	GOL	5	0
5	Ι	2420	GOL	21	0
2	Е	960	CA2	2	0
5	С	2415	GOL	9	0
5	J	2412	GOL	4	0
5	F	2418	GOL	13	0
2	Н	1560	CA2	1	0
3	Ι	2403	PO4	1	0
2	F	1160	CA2	2	0
3	А	2401	PO4	2	0
5	Н	2411	GOL	7	0
5	G	2417	GOL	7	0
5	В	2414	GOL	6	0
5	Κ	2421	GOL	12	0
5	Е	2419	GOL	10	0
3	D	2402	PO4	1	0
5	D	2416	GOL	9	0
2	J	1960	CA2	1	0
2	А	160	CA2	1	0
5	А	2413	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and sufficient 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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

