

Full wwPDB X-ray Structure Validation Report (i)

Mar 8, 2025 – 12:42 pm GMT

PDB ID	:	8S88
Title	:	Crystal structure of human L-lactate Dehydrogenase B protein in complex
		with NADH, oxamate and fluoxetine
Authors	:	Van Gysel, M.; Wouters, J.
Deposited on	:	2024-03-06
Resolution	:	2.07 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 as 541 be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7(2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

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 2.07 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	$\begin{array}{c} {\rm Whole \ archive} \\ (\#{\rm Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	164625	3436 (2.08-2.04)
Clashscore	180529	3661 (2.08-2.04)
Ramachandran outliers	177936	3649 (2.08-2.04)
Sidechain outliers	177891	3649 (2.08-2.04)
RSRZ outliers	164620	3436 (2.08-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
1	٨	240	5%		
	A	349	71%	24%	5%
			3%		
1	В	349	70%	25%	• 5%
			5%		
1	С	349	79%	17%	·
			6%		
1	D	349	73%	22%	5%
			7%		
1	E	349	69%	26%	5%



001000								
Mol	Chain	Length	Quality of chain					
			6%					
1	F	349	71%	24%	•			
			2%					
1	G	349	73%	22%	5%			
			5%					
1	Н	349	72%	23%	• •			
			3%					
1	Ι	349	77%	17%	• 5%			
			4%					
1	J	349	72%	22%	• 5%			
			8%					
1	Κ	349	66%	29%	• •			
			17%					
1	L	349	68%	27%	• •			

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SFX	В	401	-	-	Х	-
2	SFX	F	401	-	-	Х	-
3	OXM	А	402	-	-	Х	-
3	OXM	F	402	-	-	Х	-
3	OXM	L	401	-	-	Х	-
7	GOL	Κ	405	-	-	Х	-



2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 33474 atoms, of which 356 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	222	Total	С	Ν	0	S	4	0	0
1	A	ააა	2560	1628	431	487	14	4	0	0
1	D	222	Total	С	Ν	0	S	0	0	0
1	D	ააა	2560	1628	431	487	14	0	0	0
1	C	224	Total	С	Ν	0	S	2	1	0
		- 334	2580	1639	436	491	14	5	1	0
1	П	220	Total	С	Ν	0	S	4	0	0
	D	332	2552	1622	430	486	14	4	0	0
1	F	220	Total	С	Ν	0	S	0	0	0
1	Ľ	552	2555	1625	430	486	14	0	0	
1	F	F 334	Total	С	Ν	Ο	S	0	0	0
1	I.		2569	1633	432	490	14	0	0	U
1	С	222	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	G	000	2560	1628	431	487	14	0	0	0
1	н	224	Total	\mathbf{C}	Ν	0	\mathbf{S}	1	1	0
1	11		2578	1639	434	491	14	T	T	0
1	Т	222	Total	\mathbf{C}	Ν	0	\mathbf{S}	0	0	0
1	L	000	2560	1628	431	487	14	0	0	0
1	Т	330	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	3	0	0
1	5	002	2552	1622	430	486	14	5	0	0
1	K	334	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
	17	004	2569	1633	432	490	14	0	0 0	
1	L	334	Total	С	Ν	0	S	14	0	0
1		004	2569	1633	432	490	14	1.4	U	U

• Molecule 1 is a protein called L-lactate dehydrogenase B chain.

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	334	GLU	-	expression tag	UNP P07195
А	335	ASN	-	expression tag	UNP P07195
А	336	LEU	-	expression tag	UNP P07195
А	337	TYR	-	expression tag	UNP P07195
А	338	PHE	-	expression tag	UNP P07195



Continu	eu jioni pre	orous puye			-
Chain	Residue	Modelled	Actual	Comment	Reference
A	339	GLN	-	expression tag	UNP P07195
А	340	GLY	-	expression tag	UNP P07195
А	341	LEU	-	expression tag	UNP P07195
А	342	GLU	-	expression tag	UNP P07195
А	343	HIS	-	expression tag	UNP P07195
А	344	HIS	-	expression tag	UNP P07195
А	345	HIS	-	expression tag	UNP P07195
А	346	HIS	-	expression tag	UNP P07195
А	347	HIS	-	expression tag	UNP P07195
А	348	HIS	-	expression tag	UNP P07195
В	334	GLU	-	expression tag	UNP P07195
В	335	ASN	-	expression tag	UNP P07195
В	336	LEU	-	expression tag	UNP P07195
В	337	TYR	-	expression tag	UNP P07195
В	338	PHE	-	expression tag	UNP P07195
В	339	GLN	-	expression tag	UNP P07195
В	340	GLY	-	expression tag	UNP P07195
В	341	LEU	-	expression tag	UNP P07195
В	342	GLU	-	expression tag	UNP P07195
В	343	HIS	-	expression tag	UNP P07195
В	344	HIS	-	expression tag	UNP P07195
В	345	HIS	-	expression tag	UNP P07195
В	346	HIS	-	expression tag	UNP P07195
В	347	HIS	-	expression tag	UNP P07195
В	348	HIS	-	expression tag	UNP P07195
С	334	GLU	-	expression tag	UNP P07195
С	335	ASN	-	expression tag	UNP P07195
С	336	LEU	-	expression tag	UNP P07195
С	337	TYR	-	expression tag	UNP P07195
С	338	PHE	-	expression tag	UNP P07195
С	339	GLN	-	expression tag	UNP P07195
С	340	GLY	-	expression tag	UNP P07195
С	341	LEU	-	expression tag	UNP P07195
С	342	GLU	-	expression tag	UNP P07195
С	343	HIS	-	expression tag	UNP P07195
С	344	HIS	-	expression tag	UNP P07195
С	345	HIS	-	expression tag	UNP P07195
С	346	HIS	-	expression tag	UNP P07195
С	347	HIS	-	expression tag	UNP P07195
С	348	HIS	-	expression tag	UNP P07195
D	334	GLU	-	expression tag	UNP P07195
D	335	ASN	-	expression tag	UNP P07195



Chain	Residue	Modelled	Actual	Comment	Reference
D	336	LEU	-	expression tag	UNP P07195
D	337	TYR	-	expression tag	UNP P07195
D	338	PHE	-	expression tag	UNP P07195
D	339	GLN	-	expression tag	UNP P07195
D	340	GLY	-	expression tag	UNP P07195
D	341	LEU	-	expression tag	UNP P07195
D	342	GLU	-	expression tag	UNP P07195
D	343	HIS	-	expression tag	UNP P07195
D	344	HIS	-	expression tag	UNP P07195
D	345	HIS	-	expression tag	UNP P07195
D	346	HIS	-	expression tag	UNP P07195
D	347	HIS	-	expression tag	UNP P07195
D	348	HIS	-	expression tag	UNP P07195
E	334	GLU	-	expression tag	UNP P07195
Е	335	ASN	-	expression tag	UNP P07195
Е	336	LEU	-	expression tag	UNP P07195
Е	337	TYR	-	expression tag	UNP P07195
Е	338	PHE	-	expression tag	UNP P07195
Е	339	GLN	-	expression tag	UNP P07195
Е	340	GLY	-	expression tag	UNP P07195
Е	341	LEU	-	expression tag	UNP P07195
Е	342	GLU	-	expression tag	UNP P07195
Е	343	HIS	-	expression tag	UNP P07195
Е	344	HIS	-	expression tag	UNP P07195
Е	345	HIS	-	expression tag	UNP P07195
Е	346	HIS	-	expression tag	UNP P07195
Е	347	HIS	-	expression tag	UNP P07195
Е	348	HIS	-	expression tag	UNP P07195
F	334	GLU	-	expression tag	UNP P07195
F	335	ASN	-	expression tag	UNP P07195
F	336	LEU	-	expression tag	UNP P07195
F	337	TYR	-	expression tag	UNP P07195
F	338	PHE	-	expression tag	UNP P07195
F	339	GLN	-	expression tag	UNP P07195
F	340	GLY	-	expression tag	UNP P07195
F	341	LEU	-	expression tag	UNP P07195
F	342	GLU	-	expression tag	UNP P07195
F	343	HIS	-	expression tag	UNP P07195
F	344	HIS	-	expression tag	UNP P07195
F	345	HIS	-	expression tag	UNP P07195
F	346	HIS	-	expression tag	UNP P07195
F	347	HIS	-	expression tag	UNP P07195

Continued from previous page...



Chain	Residue	Modelled	Actual	Comment	Beference
F	348	HIS	-	expression tag	UNP P07195
G	334	GLU		expression tag	UNP P07195
G	335	ASN		expression tag	UNP P07195
G	336	LEU	_	expression tag	UNP P07195
G	337	TVR	_	expression tag	UNP P07195
G	338	PHE		expression tag	UNP P07195
G	330	GLN	_	expression tag	UNP P07195
G	340	GLN		expression tag	UNP P07195
G	3/1	LEU	_	expression tag	UNP P07195
G	342	GLU		expression tag	UNP P07195
G	3/3	HIS		expression tag	UNP P07195
G	344	HIS		expression tag	UNP P07195
G	345	HIS	_	ovpression tag	UNP P07105
	346	HIS	_	expression tag	UNP P07105
G	340	HIS	-	expression tag	UNP P07105
G	248	HIS	-	expression tag	UND D07105
и Ц	224		-	expression tag	UNI 107195
	225	ASN	-	expression tag	UNI 107195
		ASN	-	expression tag	UNF F07195
П	330 227		-	expression tag	UNP P07195
П			-	expression tag	UNP P07195
П			-	expression tag	UNP P07195
П		GLN	-	expression tag	UNP P07195
	340		-	expression tag	UNP P07195
П	341		-	expression tag	UNP P07195
H	342	GLU	-	expression tag	UNP P07195
H II	343	HIS	-	expression tag	UNP P07195
H II	344	HIS	-	expression tag	UNP P07195
H	345	HIS	-	expression tag	UNP P07195
	340	HIS	-	expression tag	UNP P07195
H	347	HIS	-	expression tag	UNP P07195
H	348	HIS	-	expression tag	UNP P07195
	334	GLU	-	expression tag	UNP P07195
	335	ASN	-	expression tag	UNP P07195
I	336		-	expression tag	UNP P07195
	337	TYR	-	expression tag	UNP P07195
	338	PHE	-	expression tag	UNP P07195
	339	GLN	-	expression tag	UNP P07195
	340	GLY	-	expression tag	UNP P07195
	341	LEU	-	expression tag	UNP P07195
I	342	GLU	-	expression tag	UNP P07195
	343	HIS	-	expression tag	UNP P07195
I	344	HIS	-	expression tag	UNP P07195



Chain	Residue	Modelled	Actual	Comment	Reference
Ι	345	HIS	-	expression tag	UNP P07195
Ι	346	HIS	-	expression tag	UNP P07195
Ι	347	HIS	-	expression tag	UNP P07195
Ι	348	HIS	-	expression tag	UNP P07195
J	334	GLU	-	expression tag	UNP P07195
J	335	ASN	-	expression tag	UNP P07195
J	336	LEU	-	expression tag	UNP P07195
J	337	TYR	-	expression tag	UNP P07195
J	338	PHE	-	expression tag	UNP P07195
J	339	GLN	-	expression tag	UNP P07195
J	340	GLY	-	expression tag	UNP P07195
J	341	LEU	-	expression tag	UNP P07195
J	342	GLU	-	expression tag	UNP P07195
J	343	HIS	-	expression tag	UNP P07195
J	344	HIS	-	expression tag	UNP P07195
J	345	HIS	-	expression tag	UNP P07195
J	346	HIS	-	expression tag	UNP P07195
J	347	HIS	-	expression tag	UNP P07195
J	348	HIS	-	expression tag	UNP P07195
К	334	GLU	-	expression tag	UNP P07195
K	335	ASN	-	expression tag	UNP P07195
K	336	LEU	-	expression tag	UNP P07195
K	337	TYR	-	expression tag	UNP P07195
K	338	PHE	-	expression tag	UNP P07195
K	339	GLN	-	expression tag	UNP P07195
К	340	GLY	-	expression tag	UNP P07195
К	341	LEU	-	expression tag	UNP P07195
К	342	GLU	-	expression tag	UNP P07195
K	343	HIS	-	expression tag	UNP P07195
К	344	HIS	-	expression tag	UNP P07195
K	345	HIS	-	expression tag	UNP P07195
К	346	HIS	-	expression tag	UNP P07195
К	347	HIS	-	expression tag	UNP P07195
K	348	HIS	-	expression tag	UNP P07195
L	334	GLU	-	expression tag	UNP P07195
L	335	ASN	-	expression tag	UNP P07195
L	336	LEU	-	expression tag	UNP P07195
L	337	TYR	-	expression tag	UNP P07195
L	338	PHE	-	expression tag	UNP P07195
L	339	GLN	-	expression tag	UNP P07195
L	340	GLY	-	expression tag	UNP P07195
L	341	LEU	-	expression tag	UNP P07195



Chain	Residue	Modelled	Actual	Comment	Reference
L	342	GLU	-	expression tag	UNP P07195
L	343	HIS	-	expression tag	UNP P07195
L	344	HIS	-	expression tag	UNP P07195
L	345	HIS	-	expression tag	UNP P07195
L	346	HIS	-	expression tag	UNP P07195
L	347	HIS	-	expression tag	UNP P07195
L	348	HIS	-	expression tag	UNP P07195

• Molecule 2 is (3S)-N-methyl-3-phenyl-3-[4-(trifluoromethyl)phenoxy]propan-1-am ine (three-letter code: SFX) (formula: $C_{17}H_{18}F_3NO$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
0	Λ	1	Total C F N O	0	0
	A	1	22 17 3 1 1	0	0
0	В	1	Total C F N O	0	0
	D	1	22 17 3 1 1	0	0
0	C	C 1	Total C F N O	0	0
	U		22 17 3 1 1	0	
0	Б	1	Total C F N O	0	0
	Г	1	22 17 3 1 1	0	0
0	т	1	Total C F N O	0	0
			22 17 3 1 1	0	

• Molecule 3 is OXAMIC ACID (three-letter code: OXM) (formula: $C_2H_3NO_3$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
9	٨	1	Total	С	Η	Ν	0	0	0
5	Л	1	8	2	2	1	3	0	0
2	р	1	Total	С	Η	Ν	0	0	0
່ <u>ບ</u>	D	1	8	2	2	1	3	0	0
3	C	1	Total	С	Η	Ν	Ο	0	0
5	U	1	8	2	2	1	3	0	0
3	Л	1	Total	С	Η	Ν	Ο	0	0
0	D	1	8	2	2	1	3	0	0
3	E	1	Total	С	Η	Ν	Ο	0	0
0	Ц	I	8	2	2	1	3	0	0
3	F	1	Total	С	Η	Ν	Ο	0	0
	1	1	8	2	2	1	3	0	
3	G	1	Total	С	Η	Ν	Ο	0	0
		-	8	2	2	1	3		<u> </u>
3	Н	1	Total	С	Η	Ν	0	0	0
		-	8	2	2	1	3		
3	Ι	1	Total	С	Н	Ν	Ο	0	0
	-	-	8	2	2	1	3		
3	J	1	Total	С	Н	Ν	0	0	0
		-	8	2	2	1	3		
3	K 1	1	Total	С	Н	Ν	0	0	0
		-	8	2	2	1	3		Ň
3	L	1	Total	С	Н	Ν	0	0	0
	-	-	8	2	2	1	3		Ĭ

• Molecule 4 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		A	Aton	ıs			ZeroOcc	AltConf		
4	٨	1	Total	С	Η	Ν	0	Р	0	0		
4	A	1	71	21	27	7	14	2	0	0		
4	D	1	Total	С	Η	Ν	0	Р	0	0		
4	D	1	71	21	27	7	14	2	0	0		
4	C	1	Total	С	Η	Ν	Ο	Р	0	0		
4	U	1	71	21	27	7	14	2	0	0		
4	л	1	Total	С	Η	Ν	Ο	Р	0	0		
4	D	1	71	21	27	7	14	2	0	0		
4	E	1	Total	С	Η	Ν	Ο	Р	0	0		
-1	Ľ	L	71	21	27	7	14	2	0	0		
4	F	1	Total	С	Η	Ν	Ο	Р	0	0		
т	Ľ	I	71	21	27	7	14	2		0		
4	G	1	Total	С	Η	Ν	Ο	Р	0	0		
Ŧ	u	I	71	21	27	7	14	2	0	0		
4	н	1	Total	С	Η	Ν	Ο	Р	0	0		
т	11	I	71	21	27	7	14	2	0	0		
4	Т	1	Total	С	Η	Ν	Ο	Р	0	0		
т	T	I	71	21	27	7	14	2	0	0		
4	Т	1	Total	С	Η	Ν	Ο	Р	0	0		
	0	I	71	21	27	7	14	2	0	0		
4	K	1	Total	$\overline{\mathbf{C}}$	Η	N	Ο	Р	0	0		
±	17	IX I	П	T	71	21	27	7	14	2	0	0
	т	1	Total	\mathbf{C}	Η	Ν	Ο	Р	0	0		
- '		L	71	21	27	7	14	2	U			

• Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C₈H₁₉NO₅).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Λ	1	Total C N O	0	0
0	Л	1	14 8 1 5	0	0
5	С	1	Total C N O	0	0
0	U	1	14 8 1 5	0	0
5	F	1	Total C N O	0	0
0	Ľ	T	14 8 1 5	0	0
5	G	1	Total C N O	0	Ο
0	G	1	14 8 1 5	0	0
5	K	1	Total C N O	0	Ο
0	IX	T	14 8 1 5	0	0
5	T.	1	Total C N O	0	0
			14 8 1 5	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	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
6	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
6	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
6	С	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	G	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
6	J	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
6	J	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
6	L	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
6	L	1	$\begin{array}{c cc} \text{Total} & \text{O} & \text{S} \\ \hline 5 & 4 & 1 \end{array}$	0	0





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	В	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	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	F	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
7	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	Ι	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	J	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	Κ	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	K	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	L	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	L	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	L	1	Total C H O 14 3 8 3	0	0

• Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
8	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
8	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
8	Е	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
8	Н	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
8	J	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0



Continued from previous page...

Mol	Chain	Residues	Atom	s	ZeroOcc	AltConf
8	J	1	Total C 7 4	O 3	0	0

• Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	А	122	Total O 122 122	0	0
9	В	133	Total O 133 133	0	0
9	С	134	Total O 134 134	0	0
9	D	121	Total O 121 121	0	0
9	Е	119	Total O 119 119	0	0
9	F	98	Total O 98 98	0	0
9	G	119	Total O 119 119	0	0
9	Н	101	Total O 101 101	0	0
9	Ι	141	Total O 141 141	0	0
9	J	99	Total O 99 99	0	0
9	К	96	Total O 96 96	0	0
9	L	54	$\begin{array}{cc} \text{Total} & \text{O} \\ 54 & 54 \end{array}$	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.













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• Molecule 1: L-lactate dehydrogenase B chain







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	66.53Å 413.96Å 85.30Å	Depositor
a, b, c, α , β , γ	90.00° 109.57° 90.00°	Depositor
Bosolution(A)	48.67 - 2.07	Depositor
Resolution (A)	48.67 - 2.07	EDS
% Data completeness	99.3 (48.67-2.07)	Depositor
(in resolution range)	99.3 (48.67 - 2.07)	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.51 (at 2.08 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
P. P.	0.213 , 0.264	Depositor
n, n_{free}	0.212 , 0.263	DCC
R_{free} test set	14069 reflections (5.00%)	wwPDB-VP
Wilson B-factor $(Å^2)$	34.4	Xtriage
Anisotropy	0.756	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.36, 39.6	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	33474	wwPDB-VP
Average B, all atoms $(Å^2)$	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.44% 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: SFX, GOL, SO4, PEG, BTB, NAI, OXM

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).

Mol Chain		Bond lengths		Bond angles		
MOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.42	0/2601	0.60	0/3526	
1	В	0.42	0/2601	0.58	0/3526	
1	С	0.47	0/2621	0.61	0/3552	
1	D	0.43	0/2593	0.58	0/3515	
1	Ε	0.41	0/2596	0.60	1/3519~(0.0%)	
1	F	0.44	0/2610	0.60	0/3538	
1	G	0.41	0/2601	0.58	0/3526	
1	Н	0.39	0/2619	0.58	1/3549~(0.0%)	
1	Ι	0.45	0/2601	0.59	0/3526	
1	J	0.38	0/2593	0.56	0/3515	
1	K	0.38	0/2610	0.59	0/3538	
1	L	0.37	0/2610	0.54	0/3538	
All	All	0.42	0/31256	0.58	2/42368~(0.0%)	

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Н	276	MET	CA-CB-CG	-6.49	102.27	113.30
1	Е	174	MET	CA-CB-CG	5.84	123.23	113.30

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2560	0	2633	74	0
1	В	2560	0	2633	81	0
1	С	2580	0	2651	50	0
1	D	2552	0	2622	60	0
1	Е	2555	0	2625	70	0
1	F	2569	0	2639	69	0
1	G	2560	0	2633	67	0
1	Н	2578	0	2651	70	0
1	Ι	2560	0	2633	48	0
1	J	2552	0	2622	53	0
1	Κ	2569	0	2639	91	0
1	L	2569	0	2639	89	0
2	А	22	0	18	8	0
2	В	22	0	18	12	0
2	С	22	0	18	4	0
2	F	22	0	18	11	0
2	Ι	22	0	18	7	0
3	А	6	2	2	2	0
3	В	6	2	2	1	0
3	С	6	2	2	0	0
3	D	6	2	2	1	0
3	Е	6	2	2	0	0
3	F	6	2	2	4	0
3	G	6	2	2	0	0
3	Н	6	2	2	0	0
3	Ι	6	2	2	1	0
3	J	6	2	2	1	0
3	Κ	6	2	2	1	0
3	L	6	2	2	4	0
4	А	44	27	27	5	0
4	В	44	27	27	6	0
4	С	44	27	27	3	0
4	D	44	27	27	3	0
4	Е	44	27	27	1	0
4	F	44	27	27	2	0
4	G	44	27	27	1	0
4	Н	44	27	27	3	0
4	Ι	44	27	27	2	0
4	J	44	27	27	2	0
4	K	44	27	27	2	0
4	L	44	27	27	12	0

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.



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	А	14	0	19	2	0
5	С	14	0	19	4	0
5	F	14	0	19	5	0
5	G	14	0	19	2	0
5	K	14	0	19	1	0
5	L	14	0	19	4	0
6	А	5	0	0	0	0
6	В	10	0	0	0	0
6	С	10	0	0	0	0
6	D	10	0	0	0	0
6	G	5	0	0	0	0
6	J	10	0	0	0	0
6	L	10	0	0	0	0
7	В	12	0	16	1	0
7	С	6	0	8	0	0
7	D	6	0	8	0	0
7	F	12	0	16	1	0
7	G	12	0	16	0	0
7	Н	24	0	32	1	0
7	Ι	6	0	8	1	0
7	J	6	0	8	0	0
7	K	12	0	16	7	0
7	L	18	8	24	3	0
8	В	7	0	10	0	0
8	D	14	0	20	0	0
8	Е	7	0	10	1	0
8	Н	7	0	10	1	0
8	J	14	0	20	3	0
9	А	122	0	0	5	0
9	В	133	0	0	4	0
9	С	134	0	0	7	0
9	D	121	0	0	2	0
9	E	119	0	0	1	0
9	F	98	0	0	2	0
9	G	119	0	0	2	0
9	H	101	0	0	4	0
9	I	141	0	0	2	0
9	J	99	0	0	4	0
9	K	96	0	0	4	0
9	L	54	0	0	1	0
All	All	33118	356	32394	817	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 13.

All (817) 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:H:204:VAL:HG12	1:H:211:LEU:HD12	1.41	1.03
1:F:23:ILE:HD12	1:F:45:ALA:HB2	1.40	0.98
1:J:217:GLU:HG3	1:J:223:ASP:HA	1.49	0.94
1:F:311:ASP:OD1	1:F:315:GLN:NE2	2.04	0.91
1:C:149:LYS:HD2	1:C:334:GLU:HG2	1.53	0.90
1:D:294:ILE:HD12	1:D:302:SER:HB2	1.52	0.88
3:A:402:OXM:C1	4:A:403:NAI:H42N	2.06	0.86
1:K:192:GLU:HB2	1:K:323:LEU:HD11	1.59	0.84
1:K:123:GLN:NE2	9:K:501:HOH:O	2.07	0.84
1:A:211:LEU:HD13	1:B:3:LEU:HD21	1.59	0.84
1:I:155:LYS:HG3	2:I:401:SFX:H3	1.58	0.83
1:A:243:LYS:NZ	9:A:501:HOH:O	2.11	0.83
1:J:175:ALA:HB1	1:J:180:ILE:O	1.79	0.82
1:J:7:LEU:HD23	1:J:8:ILE:HD11	1.60	0.81
1:F:294:ILE:HD12	1:F:302:SER:HB2	1.63	0.81
1:B:294:ILE:HD12	1:B:302:SER:HB2	1.64	0.80
1:K:175:ALA:HB1	1:K:180:ILE:O	1.82	0.79
1:I:155:LYS:HE2	2:I:401:SFX:H11	1.64	0.79
1:E:173:LEU:HD13	1:E:233:MET:HE2	1.64	0.79
3:F:402:OXM:C1	4:F:403:NAI:H42N	2.13	0.79
1:A:151:SER:HB2	1:A:153:LEU:HD12	1.65	0.78
1:L:31:VAL:HG21	4:L:402:NAI:H51N	1.63	0.77
1:F:134:ILE:HD11	1:F:263:MET:CE	2.14	0.77
1:A:175:ALA:HB1	1:A:180:ILE:O	1.85	0.77
1:L:28:VAL:HG22	1:L:61:GLU:HG3	1.66	0.77
4:C:403:NAI:O2A	9:C:501:HOH:O	2.02	0.77
1:B:210:SER:CB	1:B:213:GLU:HG2	2.14	0.76
1:D:134:ILE:HD11	1:D:263:MET:CE	2.15	0.76
1:F:134:ILE:HD11	1:F:263:MET:HE3	1.68	0.76
1:H:114:VAL:HG12	1:H:118:LYS:HE3	1.67	0.75
1:H:204:VAL:CG1	1:H:211:LEU:HD12	2.17	0.74
1:G:82:ASP:O	1:G:85:VAL:HG22	1.87	0.74
1:D:173:LEU:HD13	1:D:233:MET:HE2	1.71	0.73
1:B:210:SER:OG	1:B:213:GLU:HG2	1.88	0.73
1:G:19:PRO:HG3	1:G:47:GLU:OE1	1.89	0.73
1:B:210:SER:HB3	1:B:213:GLU:HG2	1.69	0.73
1:F:155:LYS:HG3	2:F:401:SFX:H17	1.71	0.72
1:K:28:VAL:HG22	1:K:61:GLU:HG3	1.71	0.72



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:J:82:ASP:O	1:J:85:VAL:HG22	1.89	0.72	
1:J:98:VAL:HG23	1:J:109:LEU:HD22	1.69	0.72	
1:C:149:LYS:HD2	1:C:334:GLU:CG	2.19	0.72	
1:C:110:VAL:HG22	1:C:139:PRO:HG3	1.72	0.71	
1:B:268:SER:HA	1:B:295:LEU:O	1.89	0.71	
1:F:117:PHE:CE1	1:F:143:LEU:HD13	2.26	0.71	
1:C:236:GLU:OE1	5:C:404:BTB:H81	1.91	0.71	
1:A:211:LEU:HB2	1:A:218:MET:HE1	1.72	0.71	
1:H:241:VAL:CG1	1:H:248:THR:HG22	2.20	0.71	
1:E:134:ILE:HD11	1:E:263:MET:CE	2.21	0.70	
1:H:219:GLY:HA2	1:H:228:LYS:HD3	1.71	0.70	
1:L:286:GLU:O	1:L:327:GLN:NE2	2.25	0.70	
1:G:175:ALA:HB1	1:G:180:ILE:O	1.91	0.70	
3:I:402:OXM:C1	4:I:403:NAI:H42N	2.22	0.70	
1:L:23:ILE:HD12	1:L:45:ALA:HB2	1.73	0.70	
1:E:173:LEU:HD22	1:E:233:MET:HE1	1.74	0.70	
1:H:309:LYS:O	1:H:313:VAL:HG23	1.92	0.70	
1:A:267:LEU:O	1:G:181:HIS:HB2	1.91	0.69	
1:K:210:SER:OG	1:K:213:GLU:HG3	1.92	0.69	
1:K:319:SER:O	1:K:323:LEU:HD13	1.91	0.69	
1:A:23:ILE:HD12	1:A:45:ALA:HB2	1.74	0.69	
1:K:134:ILE:HD11	1:K:263:MET:CE	2.22	0.69	
1:F:138:ASN:HD21	3:F:402:OXM:HN1	1.41	0.69	
1:E:215:ASN:OD1	1:E:217:GLU:HG2	1.93	0.69	
1:I:210:SER:HB3	1:I:213:GLU:HG3	1.73	0.68	
1:L:110:VAL:HG13	1:L:111:GLN:N	2.07	0.68	
1:A:151:SER:CB	1:A:153:LEU:HD12	2.23	0.68	
1:G:121:ILE:HD12	1:G:147:THR:HG23	1.74	0.68	
1:B:155:LYS:HG3	2:B:401:SFX:H3	1.76	0.68	
1:L:276:MET:HE3	1:L:278:LYS:H	1.57	0.68	
1:L:164:ASN:HB3	9:L:523:HOH:O	1.93	0.68	
1:L:118:LYS:HA	1:L:150:LEU:HD21	1.76	0.68	
1:F:42:LYS:HE3	9:F:564:HOH:O	1.92	0.68	
1:K:265:LYS:NZ	7:K:405:GOL:H2	2.09	0.68	
1:A:20:ASN:O	1:A:90:LYS:HE3	1.95	0.67	
1:C:107:LEU:O	1:C:110:VAL:HG23	1.93	0.67	
1:G:268:SER:HA	1:G:295:LEU:O	1.93	0.67	
1:J:7:LEU:C	1:J:8:ILE:HD13	2.14	0.67	
5:F:404:BTB:H61	5:F:404:BTB:H32	1.77	0.67	
1:C:154:PRO:HB3	2:C:401:SFX:H7	1.75	0.67	
1:F:155:LYS:HG3	2:F:401:SFX:C17	2.25	0.67	



	io ao pagon	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:I:210:SER:CB	1:I:213:GLU:HG3	2.25	0.66
3:K:401:OXM:C1	4:K:402:NAI:H42N	2.25	0.66
1:B:2:THR:O	1:B:6:LYS:HG3	1.95	0.66
1:K:134:ILE:HD11	1:K:263:MET:HE2	1.78	0.66
1:E:173:LEU:HD22	1:E:233:MET:CE	2.25	0.66
3:L:401:OXM:C1	4:L:402:NAI:H42N	2.25	0.66
1:C:8:ILE:HG22	1:D:302:SER:HB3	1.78	0.66
1:A:211:LEU:CB	1:A:218:MET:HE1	2.26	0.65
1:J:80:ASP:HB2	1:J:85:VAL:HG11	1.78	0.65
1:C:134:ILE:HD11	1:C:263:MET:CE	2.27	0.65
1:J:184:SER:O	9:J:501:HOH:O	2.14	0.65
1:E:175:ALA:HB1	1:E:180:ILE:O	1.97	0.65
1:D:134:ILE:HD11	1:D:263:MET:HE1	1.78	0.65
1:L:174:MET:HG3	1:L:227:TRP:HH2	1.61	0.65
1:B:107:LEU:O	1:B:110:VAL:HG23	1.96	0.65
1:L:175:ALA:HB1	1:L:180:ILE:O	1.96	0.65
1:L:112:ARG:O	1:L:116:VAL:HG23	1.97	0.64
1:G:23:ILE:HD12	1:G:45:ALA:HB2	1.77	0.64
1:H:82:ASP:O	1:H:85:VAL:HG12	1.97	0.64
1:A:92:VAL:HG11	1:A:124:ILE:HD13	1.80	0.64
1:B:7:LEU:C	1:B:8:ILE:HD13	2.18	0.64
1:I:148:TRP:HE1	2:I:401:SFX:H2	1.61	0.64
1:C:175:ALA:HB1	1:C:180:ILE:O	1.97	0.64
1:I:180:ILE:HD11	1:I:185:CYS:SG	2.38	0.64
1:H:107:LEU:O	1:H:110:VAL:HG12	1.97	0.64
1:J:23:ILE:HD12	1:J:45:ALA:HB2	1.80	0.63
1:L:276:MET:HE1	1:L:278:LYS:HB3	1.79	0.63
1:A:154:PRO:HA	2:A:401:SFX:H2A	1.79	0.63
1:F:175:ALA:HB1	1:F:180:ILE:O	1.98	0.63
1:A:236:GLU:OE1	5:A:404:BTB:H81	1.97	0.63
1:D:136:VAL:O	4:D:402:NAI:H2N	1.99	0.63
1:D:175:ALA:HB1	1:D:180:ILE:O	1.98	0.63
2:F:401:SFX:N4	1:I:13:GLU:OE1	2.31	0.63
1:A:154:PRO:HA	2:A:401:SFX:H17	1.81	0.63
1:C:236:GLU:OE2	5:C:404:BTB:H61	1.98	0.63
1:J:174:MET:HG2	1:J:185:CYS:HB3	1.79	0.63
1:H:114:VAL:CG1	1:H:118:LYS:HE3	2.28	0.63
1:K:28:VAL:CG2	1:K:61:GLU:HG3	2.28	0.62
1:L:190:LEU:HD22	1:L:291:LEU:HA	1.81	0.62
1:H:23:ILE:HD12	1:H:45:ALA:HB2	1.81	0.62
1:H:294:ILE:HD12	1:H:302:SER:HB2	1.81	0.62



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:175:ALA:HB1	1:B:180:ILE:O	1.99	0.62
1:A:134:ILE:HD11	1:A:263:MET:CE	2.29	0.62
1:H:281:TYR:CE1	1:H:308:LEU:HD12	2.33	0.62
1:G:281:TYR:CE1	1:G:308:LEU:HD12	2.34	0.62
1:B:22:LYS:HB3	1:B:89:SER:HA	1.80	0.62
1:A:155:LYS:HG2	2:A:401:SFX:H2	1.82	0.62
1:K:265:LYS:HE2	7:K:405:GOL:H31	1.82	0.62
1:B:99:ARG:HH12	7:B:404:GOL:HO2	1.45	0.61
1:G:3:LEU:HD13	1:H:227:TRP:CZ2	2.35	0.61
1:A:269:ARG:HD2	9:A:593:HOH:O	2.01	0.61
1:D:215:ASN:ND2	1:D:225:GLU:HG3	2.15	0.61
1:F:201:TRP:HB3	1:F:218:MET:HE2	1.82	0.61
1:B:8:ILE:HD12	1:G:304:ILE:HD13	1.83	0.61
1:L:22:LYS:HB3	1:L:89:SER:HA	1.81	0.61
1:L:198:VAL:HG22	1:L:315:GLN:HB2	1.83	0.61
1:F:22:LYS:HG3	1:F:47:GLU:HG2	1.81	0.61
1:K:46:ASP:HB3	9:K:557:HOH:O	1.99	0.61
1:L:311:ASP:O	1:L:315:GLN:HG2	2.01	0.61
1:L:7:LEU:C	1:L:8:ILE:HD13	2.21	0.60
9:C:564:HOH:O	1:D:265:LYS:HE3	1.99	0.60
1:E:2:THR:HG22	1:E:4:LYS:N	2.16	0.60
1:C:2:THR:OG1	1:C:5:GLU:HG3	2.01	0.60
1:L:28:VAL:CG2	1:L:61:GLU:HG3	2.32	0.60
1:G:180:ILE:HD11	1:G:185:CYS:SG	2.41	0.60
1:L:174:MET:HG3	1:L:227:TRP:CH2	2.35	0.60
1:L:332:ASP:O	1:L:333:LEU:HD23	2.02	0.60
1:L:27:GLY:O	1:L:32:GLY:HA3	2.01	0.60
1:C:252:ILE:O	1:C:256:VAL:HG23	2.00	0.60
1:H:219:GLY:CA	1:H:228:LYS:HD3	2.32	0.60
1:D:121:ILE:HB	1:D:122:PRO:HD3	1.84	0.59
1:A:53:VAL:HG13	4:A:403:NAI:C2A	2.32	0.59
1:A:294:ILE:HD11	1:H:8:ILE:CD1	2.32	0.59
1:D:157:ARG:HD2	9:D:555:HOH:O	2.03	0.59
1:E:7:LEU:HD22	1:E:7:LEU:O	2.02	0.59
1:J:192:GLU:HB2	1:J:323:LEU:HD21	1.84	0.59
1:F:46:ASP:O	1:F:75:PRO:HD2	2.03	0.59
1:J:221:ASP:OD1	9:J:502:HOH:O	2.16	0.59
1:D:141:ASP:HB3	1:D:288:PHE:O	2.03	0.59
1:G:14:GLU:OE2	1:G:15:GLU:N	2.35	0.59
1:A:238:ALA:O	1:A:242:ILE:HG13	2.02	0.59
1:F:309:LYS:HE3	1:F:309:LYS:HA	1.84	0.59



	te de pagetti	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:G:309:LYS:O	1:G:313:VAL:HG23	2.01	0.59
1:K:15:GLU:HG2	1:K:16:ALA:N	2.17	0.59
1:D:110:VAL:HG13	1:D:111:GLN:N	2.18	0.59
1:D:192:GLU:HB2	1:D:323:LEU:HD21	1.85	0.58
1:L:154:PRO:HB2	1:L:156:HIS:CD2	2.37	0.58
1:F:309:LYS:HA	1:F:309:LYS:CE	2.31	0.58
1:I:210:SER:HB2	7:I:404:GOL:H32	1.85	0.58
1:L:110:VAL:CG1	1:L:111:GLN:N	2.66	0.58
1:L:280:MET:O	1:L:283:ILE:HD13	2.04	0.58
1:F:311:ASP:O	1:F:315:GLN:NE2	2.33	0.58
1:L:236:GLU:OE1	5:L:403:BTB:H81	2.02	0.58
1:E:174:MET:HE3	1:E:204:VAL:HG13	1.83	0.58
1:L:53:VAL:HG13	4:L:402:NAI:N1A	2.18	0.58
1:F:155:LYS:HG3	2:F:401:SFX:C18	2.32	0.58
1:J:121:ILE:HD12	1:J:147:THR:HG23	1.86	0.58
1:K:98:VAL:HA	9:K:555:HOH:O	2.04	0.58
1:B:154:PRO:HA	2:B:401:SFX:C21	2.33	0.58
1:F:17:THR:HG23	1:F:17:THR:O	2.04	0.58
1:F:148:TRP:HE1	2:F:401:SFX:H18	1.69	0.58
1:K:15:GLU:HG2	1:K:16:ALA:H	1.68	0.58
1:E:113:ASN:HB3	1:E:143:LEU:HD11	1.86	0.58
1:E:277:VAL:CG2	1:E:283:ILE:HD13	2.34	0.58
1:G:266:ASN:OD1	1:G:296:ASN:HB2	2.04	0.57
1:G:136:VAL:O	4:G:402:NAI:H2N	2.03	0.57
1:I:128:SER:HB3	1:I:131:CYS:HB3	1.87	0.57
1:I:175:ALA:HB1	1:I:180:ILE:O	2.04	0.57
1:C:273:VAL:O	1:C:290:SER:HA	2.04	0.57
2:F:401:SFX:H1	2:F:401:SFX:H7	1.84	0.57
1:B:156:HIS:ND1	2:B:401:SFX:H22	2.19	0.57
1:L:155:LYS:H	7:L:406:GOL:H2	1.70	0.57
1:F:98:VAL:HG23	1:F:109:LEU:HD22	1.85	0.57
1:L:276:MET:CE	1:L:278:LYS:HB3	2.34	0.57
1:C:23:ILE:HD12	1:C:45:ALA:HB2	1.85	0.57
1:D:59:LYS:O	1:D:63:MET:HG3	2.04	0.57
1:E:214:LEU:HB3	1:K:6:LYS:HD2	1.87	0.57
2:F:401:SFX:H1A	9:I:599:HOH:O	2.03	0.57
1:L:141:ASP:HB3	1:L:288:PHE:O	2.04	0.57
1:J:113:ASN:HB3	1:J:143:LEU:HD11	1.87	0.57
1:L:268:SER:HA	1:L:295:LEU:O	2.05	0.57
1:L:278:LYS:HE3	1:L:286:GLU:HG3	1.86	0.57
1:B:174:MET:SD	1:B:185:CYS:HB3	2.45	0.57



	lo do pagom	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:L:53:VAL:HG13	4:L:402:NAI:C6A	2.35	0.57	
1:L:134:ILE:HD11	1:L:263:MET:CE	2.34	0.57	
1:L:309:LYS:HB2	1:L:312:GLU:CD	2.26	0.57	
1:F:155:LYS:HG3	2:F:401:SFX:H18	1.87	0.57	
1:K:122:PRO:HG2	9:K:519:HOH:O	2.05	0.57	
1:D:134:ILE:HD11	1:D:263:MET:HE2	1.87	0.56	
1:G:273:VAL:O	1:G:290:SER:HA	2.05	0.56	
1:H:29:GLY:HA3	4:H:402:NAI:O5B	2.05	0.56	
1:K:23:ILE:HG21	1:K:39:ILE:HD13	1.86	0.56	
1:C:1:ALA:HB1	1:C:5:GLU:OE1	2.06	0.56	
1:I:266:ASN:OD1	1:I:296:ASN:HB2	2.05	0.56	
1:K:110:VAL:HG13	1:K:111:GLN:H	1.69	0.56	
1:G:294:ILE:HD12	1:G:302:SER:HB2	1.87	0.56	
1:H:122:PRO:O	1:H:125:VAL:HG22	2.05	0.56	
1:C:46:ASP:HA	9:C:564:HOH:O	2.06	0.56	
1:F:154:PRO:HB3	2:F:401:SFX:H22A	1.86	0.56	
1:E:134:ILE:HD11	1:E:263:MET:HE2	1.85	0.56	
1:E:190:LEU:HD11	1:E:306:GLN:HE22	1.70	0.56	
1:L:241:VAL:CG1	1:L:248:THR:HG22	2.36	0.56	
1:L:52:ASP:HA	4:L:402:NAI:H2A	1.87	0.56	
1:B:22:LYS:HG3	1:B:47:GLU:HG2	1.87	0.55	
1:H:20:ASN:C	1:H:90:LYS:HZ2	2.08	0.55	
1:I:174:MET:SD	1:I:185:CYS:HB3	2.45	0.55	
1:C:134:ILE:HD11	1:C:263:MET:HE3	1.87	0.55	
1:I:210:SER:OG	1:I:213:GLU:HG3	2.07	0.55	
1:G:39:ILE:HG23	1:G:44:LEU:HB2	1.89	0.55	
1:E:191:GLY:HA2	1:E:289:LEU:HD13	1.89	0.55	
1:G:229:GLU:O	1:G:233:MET:HG3	2.06	0.55	
1:K:27:GLY:O	1:K:32:GLY:HA3	2.07	0.55	
1:A:252:ILE:HD13	4:A:403:NAI:O7N	2.07	0.55	
1:B:294:ILE:HD12	1:B:302:SER:CB	2.35	0.55	
1:I:170:PHE:CE2	1:I:174:MET:HE1	2.42	0.55	
1:A:268:SER:HA	1:A:295:LEU:O	2.07	0.55	
1:F:130:ASP:HA	1:F:157:ARG:NH2	2.22	0.55	
1:H:53:VAL:HG13	4:H:402:NAI:N1A	2.22	0.55	
1:J:110:VAL:HG13	1:J:111:GLN:N	2.22	0.55	
1:B:210:SER:HB3	1:B:213:GLU:CG	2.36	0.55	
1:L:273:VAL:O	1:L:290:SER:HA	2.07	0.55	
1:K:319:SER:O	1:K:323:LEU:CD1	2.55	0.54	
1:E:280:MET:HE1	1:E:303:VAL:HG11	1.87	0.54	
1:J:293:CYS:SG	1:J:300:LEU:HD21	2.47	0.54	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:286:GLU:OE2	2:B:401:SFX:F15	2.15	0.54	
1:K:33:MET:CE	1:K:65:LEU:HD11	2.37	0.54	
1:K:154:PRO:HG2	1:K:157:ARG:HG3	1.88	0.54	
1:K:44:LEU:HD21	1:K:261:GLU:HG3	1.88	0.54	
1:A:57:LYS:NZ	1:A:61:GLU:OE2	2.40	0.54	
1:A:134:ILE:HD11	1:A:263:MET:HE1	1.88	0.54	
1:E:266:ASN:OD1	1:E:296:ASN:HB2	2.07	0.54	
1:I:273:VAL:O	1:I:290:SER:HA	2.08	0.54	
1:C:148:TRP:HZ2	2:C:401:SFX:H17	1.73	0.54	
1:J:107:LEU:HD22	1:J:326:ILE:CD1	2.37	0.54	
1:F:87:ALA:O	1:F:88:ASN:HB2	2.07	0.54	
1:K:20:ASN:O	1:K:90:LYS:HE2	2.07	0.54	
1:K:211:LEU:HB3	1:K:218:MET:HE3	1.90	0.54	
1:K:283:ILE:HG13	1:K:317:LYS:HD3	1.89	0.54	
1:A:270:ILE:HA	1:A:293:CYS:O	2.07	0.54	
1:F:128:SER:HB3	1:F:131:CYS:HB3	1.90	0.54	
1:G:110:VAL:HG23	1:G:111:GLN:N	2.23	0.54	
1:G:262:SER:HA	1:G:267:LEU:HD12	1.88	0.53	
1:H:156:HIS:HB2	1:H:300:LEU:O	2.08	0.53	
1:I:46:ASP:HA	9:I:542:HOH:O	2.08	0.53	
1:E:19:PRO:HG3	1:E:47:GLU:OE1	2.07	0.53	
1:B:20:ASN:O	1:B:90:LYS:HD2	2.09	0.53	
1:C:239:TYR:CE2	5:C:404:BTB:H72	2.43	0.53	
1:I:188:TRP:CZ3	1:I:272:PRO:HD3	2.43	0.53	
1:C:29:GLY:HA3	4:C:403:NAI:O5B	2.08	0.53	
1:G:7:LEU:C	1:G:8:ILE:HD13	2.29	0.53	
1:K:39:ILE:HD11	1:K:260:ILE:CD1	2.39	0.53	
1:L:276:MET:HE3	1:L:278:LYS:N	2.23	0.53	
1:D:42:LYS:HB3	1:D:44:LEU:HG	1.90	0.53	
1:E:28:VAL:HG23	1:E:28:VAL:O	2.08	0.53	
1:K:190:LEU:HD12	1:K:200:VAL:HG21	1.89	0.53	
1:A:247:TYR:HA	9:A:525:HOH:O	2.08	0.53	
1:E:2:THR:HG22	1:E:4:LYS:H	1.74	0.53	
1:F:55:GLU:OE2	1:F:81:LYS:HE3	2.09	0.53	
1:L:7:LEU:HG	1:L:8:ILE:HD13	1.90	0.53	
1:L:31:VAL:CG2	4:L:402:NAI:H51N	2.35	0.53	
1:D:153:LEU:N	1:D:153:LEU:HD23	2.24	0.53	
1:F:113:ASN:HB3	1:F:143:LEU:HD11	1.90	0.53	
1:C:108:ASN:OD1	9:C:502:HOH:O	2.19	0.53	
1:B:82:ASP:O	1:B:85:VAL:HG12	2.09	0.52	
4:B:403:NAI:H52A	9:B:501:HOH:O	2.08	0.52	



	te de pagetti	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:270:ILE:HA	1:E:293:CYS:O	2.09	0.52
1:B:136:VAL:O	4:B:403:NAI:H2N	2.09	0.52
1:C:223:ASP:CG	1:C:225:GLU:O	2.48	0.52
1:D:204:VAL:HG12	1:D:211:LEU:HD12	1.91	0.52
1:H:146:VAL:HG12	1:H:150:LEU:HD12	1.91	0.52
1:H:240:GLU:HG3	9:H:584:HOH:O	2.09	0.52
1:K:294:ILE:HD12	1:K:302:SER:HB2	1.89	0.52
1:B:151:SER:HB2	1:B:153:LEU:HG	1.91	0.52
1:E:277:VAL:HG23	1:E:283:ILE:HD13	1.91	0.52
1:K:112:ARG:O	1:K:115:ASN:HB2	2.10	0.52
1:E:49:ALA:HA	1:E:78:VAL:O	2.10	0.52
1:K:19:PRO:HG3	1:K:47:GLU:OE1	2.10	0.52
1:D:212:GLN:HG3	1:D:218:MET:HB3	1.92	0.52
1:D:289:LEU:C	1:D:289:LEU:HD12	2.30	0.52
1:L:99:ARG:HD3	4:L:402:NAI:O3	2.10	0.52
1:H:53:VAL:HG13	4:H:402:NAI:C2A	2.40	0.52
1:D:277:VAL:HG11	1:D:289:LEU:CD1	2.40	0.52
1:D:308:LEU:HB2	1:D:313:VAL:HG23	1.91	0.52
1:G:110:VAL:HG12	1:G:139:PRO:HG3	1.91	0.52
1:L:46:ASP:O	1:L:75:PRO:HD2	2.10	0.52
1:E:173:LEU:CD1	1:E:233:MET:HE2	2.38	0.52
1:H:191:GLY:HA2	1:H:289:LEU:HD13	1.92	0.52
1:K:190:LEU:HD22	1:K:291:LEU:HA	1.91	0.52
1:L:111:GLN:HG3	1:L:112:ARG:H	1.74	0.52
1:B:155:LYS:HE2	2:B:401:SFX:H7	1.90	0.52
1:K:22:LYS:HB3	1:K:89:SER:HA	1.92	0.52
1:A:155:LYS:H	2:A:401:SFX:C2	2.23	0.51
1:D:287:VAL:HA	1:D:327:GLN:HE22	1.75	0.51
1:C:289:LEU:HD12	1:C:289:LEU:C	2.31	0.51
1:L:210:SER:HB2	7:L:404:GOL:H2	1.91	0.51
1:F:163:CYS:HA	1:F:166:ASP:OD1	2.09	0.51
1:F:262:SER:HA	1:F:267:LEU:HD12	1.92	0.51
1:B:7:LEU:O	1:B:8:ILE:HD13	2.11	0.51
1:H:128:SER:HB3	1:H:131:CYS:HB3	1.92	0.51
1:L:52:ASP:HA	4:L:402:NAI:C2A	2.40	0.51
1:A:110:VAL:HG13	1:A:111:GLN:N	2.26	0.51
1:F:35:CYS:O	1:F:39:ILE:HG13	2.10	0.51
1:A:40:LEU:HD11	1:A:65:LEU:HD13	1.91	0.51
1:B:273:VAL:O	1:B:290:SER:HA	2.09	0.51
1:F:101:GLN:HG3	1:F:104:GLU:OE1	2.10	0.51
1:G:22:LYS:HG3	1:G:47:GLU:HG2	1.93	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:L:121:ILE:N	1:L:122:PRO:HD2	2.26	0.51
1:A:214:LEU:HD23	1:G:307:LYS:HE3	1.93	0.51
1:E:20:ASN:O	1:E:90:LYS:HE2	2.09	0.51
1:J:325:ASP:OD1	9:J:503:HOH:O	2.19	0.51
1:K:107:LEU:O	1:K:110:VAL:HG12	2.10	0.51
1:K:265:LYS:HZ1	7:K:405:GOL:H2	1.76	0.51
1:A:294:ILE:HD11	1:H:8:ILE:HD11	1.91	0.51
1:F:27:GLY:O	1:F:32:GLY:HA3	2.11	0.51
1:A:113:ASN:HB3	1:A:143:LEU:HD11	1.92	0.51
3:A:402:OXM:C2	4:A:403:NAI:H42N	2.40	0.51
1:B:323:LEU:O	1:B:327:GLN:HG3	2.11	0.51
1:B:160:GLY:HA3	1:B:274:SER:HB3	1.92	0.51
1:E:174:MET:HE3	1:E:204:VAL:CG1	2.40	0.51
1:F:180:ILE:HD11	1:F:185:CYS:SG	2.51	0.51
1:I:155:LYS:HD3	2:I:401:SFX:H21	1.92	0.51
1:B:22:LYS:HE3	1:B:47:GLU:OE2	2.10	0.50
1:H:155:LYS:HG3	7:H:404:GOL:H2	1.92	0.50
1:J:53:VAL:HG23	1:J:54:LEU:HD23	1.92	0.50
1:K:273:VAL:O	1:K:290:SER:HA	2.11	0.50
1:A:134:ILE:HD11	1:A:263:MET:HE2	1.92	0.50
1:A:174:MET:SD	1:A:185:CYS:HB3	2.51	0.50
9:F:553:HOH:O	1:I:11:VAL:HG22	2.10	0.50
1:H:245:LYS:HA	8:H:407:PEG:H21	1.94	0.50
1:I:44:LEU:HD13	1:I:260:ILE:HG22	1.93	0.50
1:J:281:TYR:CZ	8:J:406:PEG:H22	2.46	0.50
1:F:270:ILE:HA	1:F:293:CYS:O	2.12	0.50
1:G:139:PRO:HG2	1:G:142:ILE:HB	1.93	0.50
1:B:259:LEU:O	1:B:263:MET:HG3	2.11	0.50
1:D:19:PRO:HG3	1:D:47:GLU:OE1	2.12	0.50
1:F:156:HIS:CG	1:I:12:ALA:HB2	2.46	0.50
1:D:110:VAL:HG13	1:D:111:GLN:H	1.76	0.50
1:I:134:ILE:HA	1:I:159:ILE:O	2.11	0.50
1:F:304:ILE:HD13	1:I:8:ILE:HD12	1.94	0.50
1:G:268:SER:CA	1:G:295:LEU:O	2.59	0.50
1:A:180:ILE:HG22	1:A:184:SER:HB2	1.92	0.50
1:E:126:LYS:HE3	1:E:127:TYR:CE1	2.46	0.50
1:F:20:ASN:O	1:F:90:LYS:HE2	2.11	0.50
1:K:136:VAL:O	4:K:402:NAI:H2N	2.12	0.50
1:K:156:HIS:HB2	1:K:300:LEU:O	2.12	0.50
1:L:309:LYS:O	1:L:313:VAL:HG23	2.12	0.50
1:B:109:LEU:HD23	1:B:112:ARG:NH2	2.27	0.50



	lo de pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:K:7:LEU:C	1:K:8:ILE:HD13	2.32	0.50
1:K:212:GLN:O	1:K:212:GLN:HG2	2.12	0.50
1:D:326:ILE:O	1:D:330:LEU:HD13	2.11	0.50
1:H:20:ASN:O	1:H:90:LYS:NZ	2.41	0.50
1:H:219:GLY:C	1:H:228:LYS:HD3	2.31	0.50
1:K:42:LYS:O	7:K:405:GOL:H32	2.11	0.50
1:L:134:ILE:HD11	1:L:263:MET:HE1	1.93	0.50
1:A:117:PHE:CE1	1:A:143:LEU:HD13	2.47	0.49
1:G:134:ILE:HD11	1:G:263:MET:CE	2.42	0.49
1:H:180:ILE:HD11	1:H:185:CYS:SG	2.52	0.49
1:I:114:VAL:HG22	1:I:146:VAL:HG21	1.94	0.49
1:I:170:PHE:CE2	1:I:174:MET:CE	2.95	0.49
1:K:265:LYS:CE	7:K:405:GOL:H31	2.41	0.49
1:K:291:LEU:HB3	1:K:292:PRO:CD	2.42	0.49
1:L:111:GLN:HG3	1:L:112:ARG:N	2.27	0.49
1:E:110:VAL:HG13	1:E:111:GLN:N	2.26	0.49
1:I:110:VAL:HG13	1:I:111:GLN:N	2.27	0.49
1:K:125:VAL:HG23	1:K:153:LEU:HD21	1.93	0.49
1:A:180:ILE:CG2	1:A:184:SER:HB2	2.42	0.49
1:B:213:GLU:HA	1:B:213:GLU:OE1	2.12	0.49
1:I:277:VAL:HG22	1:I:287:VAL:O	2.12	0.49
1:K:211:LEU:HB3	1:K:218:MET:CE	2.42	0.49
1:L:28:VAL:HG22	1:L:33:MET:SD	2.52	0.49
1:A:67:HIS:CG	1:B:169:ARG:HG2	2.48	0.49
1:E:3:LEU:HD21	1:K:211:LEU:HD13	1.93	0.49
1:G:27:GLY:O	1:G:32:GLY:HA3	2.12	0.49
1:G:324:TRP:O	1:G:328:LYS:HG2	2.12	0.49
1:K:266:ASN:OD1	1:K:296:ASN:HB2	2.13	0.49
1:E:118:LYS:HA	1:E:150:LEU:CD1	2.43	0.49
1:F:218:MET:HG3	1:F:227:TRP:CG	2.48	0.49
1:D:27:GLY:O	1:D:32:GLY:HA3	2.13	0.49
1:J:50:LEU:O	1:J:79:ALA:HA	2.12	0.49
1:L:283:ILE:HD12	1:L:283:ILE:N	2.27	0.49
1:D:308:LEU:HB2	1:D:313:VAL:CG2	2.43	0.49
1:J:47:GLU:HG3	1:J:76:LYS:HB3	1.95	0.49
1:J:195:ASP:HA	1:J:235:VAL:HG13	1.95	0.49
1:K:28:VAL:HG13	1:K:28:VAL:O	2.13	0.49
1:K:33:MET:HE1	1:K:65:LEU:HD11	1.95	0.49
1:B:267:LEU:O	1:H:181:HIS:HB2	2.13	0.49
1:G:241:VAL:CG1	1:G:248:THR:HG22	2.42	0.49
1:H:119:PHE:HD1	9:H:594:HOH:O	1.96	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:K:174:MET:SD	1:K:185:CYS:HB3	2.53	0.49
1:J:58:LEU:HG	1:J:79:ALA:HB1	1.95	0.48
1:K:265:LYS:HZ3	7:K:405:GOL:H2	1.78	0.48
1:L:198:VAL:HG22	1:L:315:GLN:CB	2.41	0.48
1:A:218:MET:HA	1:A:223:ASP:OD2	2.13	0.48
1:E:280:MET:CE	1:E:303:VAL:HG11	2.43	0.48
1:B:18:VAL:CG2	1:B:19:PRO:HD2	2.43	0.48
1:D:326:ILE:O	1:D:330:LEU:CD1	2.61	0.48
1:G:110:VAL:CG1	1:G:139:PRO:HG3	2.43	0.48
1:L:28:VAL:O	1:L:28:VAL:HG13	2.12	0.48
1:J:293:CYS:SG	1:J:303:VAL:HG22	2.53	0.48
1:B:126:LYS:HE2	1:B:127:TYR:CZ	2.49	0.48
3:J:401:OXM:C1	4:J:402:NAI:H42N	2.44	0.48
1:L:287:VAL:HA	1:L:327:GLN:HE22	1.78	0.48
1:F:13:GLU:OE2	1:F:13:GLU:HA	2.14	0.48
1:F:148:TRP:NE1	2:F:401:SFX:H18	2.28	0.48
1:H:241:VAL:HG12	1:H:248:THR:HG22	1.93	0.48
1:J:128:SER:HB3	1:J:131:CYS:HB3	1.95	0.48
1:L:156:HIS:HB2	1:L:300:LEU:O	2.13	0.48
1:E:22:LYS:HG3	1:E:47:GLU:HG2	1.94	0.48
1:H:201:TRP:HB3	1:H:218:MET:HE3	1.96	0.48
1:I:190:LEU:HD12	1:I:200:VAL:HG21	1.96	0.48
1:F:302:SER:HB3	1:I:8:ILE:CG2	2.44	0.48
1:K:127:TYR:C	1:K:129:PRO:HD3	2.34	0.48
1:L:151:SER:HB2	1:L:153:LEU:HG	1.96	0.48
1:D:170:PHE:CE2	1:D:174:MET:HE1	2.49	0.48
3:L:401:OXM:C2	4:L:402:NAI:H42N	2.43	0.48
1:B:311:ASP:O	1:B:315:GLN:HG2	2.13	0.47
1:J:191:GLY:HA2	1:J:289:LEU:HD13	1.96	0.47
1:L:274:SER:HA	1:L:290:SER:HA	1.96	0.47
1:K:145:TYR:CD2	1:K:327:GLN:HG2	2.49	0.47
1:B:8:ILE:HG23	1:G:302:SER:HB3	1.96	0.47
1:B:128:SER:HB3	1:B:131:CYS:HB3	1.95	0.47
1:E:27:GLY:O	1:E:32:GLY:HA3	2.15	0.47
1:G:198:VAL:HG22	1:G:315:GLN:HB2	1.95	0.47
1:G:198:VAL:HG22	1:G:315:GLN:CB	2.44	0.47
1:K:134:ILE:HD11	1:K:263:MET:HE1	1.96	0.47
1:F:18:VAL:O	1:F:18:VAL:HG13	2.14	0.47
1:G:100:GLN:HG3	9:G:537:HOH:O	2.13	0.47
1:H:293:CYS:SG	1:H:300:LEU:HD11	2.55	0.47
1:J:80:ASP:HB2	1:J:85:VAL:CG1	2.44	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:151:SER:HB2	1:A:153:LEU:CD1	2.40	0.47
1:A:281:TYR:O	1:A:317:LYS:HE3	2.13	0.47
1:B:268:SER:CA	1:B:295:LEU:O	2.60	0.47
1:D:112:ARG:HG3	9:D:565:HOH:O	2.13	0.47
1:J:154:PRO:HB2	1:J:156:HIS:CD2	2.49	0.47
1:A:46:ASP:HA	9:A:532:HOH:O	2.15	0.47
1:A:181:HIS:HB2	1:G:267:LEU:O	2.13	0.47
1:C:110:VAL:HG22	1:C:139:PRO:CG	2.44	0.47
1:A:266:ASN:OD1	1:A:296:ASN:HB2	2.15	0.47
1:A:273:VAL:O	1:A:290:SER:HA	2.15	0.47
5:F:404:BTB:C8	5:F:404:BTB:H11	2.40	0.47
1:G:324:TRP:CE2	1:G:328:LYS:HB3	2.49	0.47
1:H:228:LYS:HA	1:H:228:LYS:HD2	1.52	0.47
1:I:7:LEU:HG	1:I:8:ILE:HD13	1.97	0.47
1:I:262:SER:HA	1:I:267:LEU:HD12	1.97	0.47
1:J:51:VAL:HG22	1:J:80:ASP:O	2.14	0.47
1:E:280:MET:CE	1:E:291:LEU:HD13	2.45	0.47
1:F:256:VAL:O	1:F:260:ILE:HG13	2.15	0.47
1:D:148:TRP:CZ3	1:D:149:LYS:HE2	2.50	0.47
1:D:223:ASP:OD1	1:D:225:GLU:N	2.47	0.47
1:K:202:SER:HB3	1:K:309:LYS:HE2	1.97	0.47
1:A:58:LEU:HG	1:A:79:ALA:HB1	1.96	0.46
1:D:125:VAL:HG11	1:D:153:LEU:HD21	1.97	0.46
1:L:309:LYS:HB2	1:L:312:GLU:OE1	2.14	0.46
1:A:121:ILE:HB	1:A:122:PRO:HD3	1.96	0.46
1:B:191:GLY:HA2	1:B:289:LEU:HD13	1.97	0.46
1:C:149:LYS:CE	1:C:334:GLU:OE2	2.63	0.46
1:F:188:TRP:CZ3	1:F:272:PRO:HD3	2.50	0.46
1:G:19:PRO:HB2	1:G:22:LYS:HB2	1.96	0.46
1:G:308:LEU:HB2	1:G:313:VAL:HG22	1.96	0.46
1:H:276:MET:HG2	1:H:277:VAL:N	2.30	0.46
1:H:270:ILE:HA	1:H:293:CYS:O	2.15	0.46
1:K:28:VAL:HG23	1:K:33:MET:SD	2.56	0.46
5:K:403:BTB:O4	5:K:403:BTB:O1	2.34	0.46
1:L:28:VAL:CG2	1:L:33:MET:SD	3.03	0.46
1:B:155:LYS:HE2	2:B:401:SFX:H1A	1.97	0.46
1:G:110:VAL:HG12	1:G:139:PRO:CG	2.46	0.46
1:J:280:MET:HB3	8:J:406:PEG:H31	1.97	0.46
1:K:262:SER:OG	1:K:269:ARG:NH1	2.48	0.46
1:A:98:VAL:HG23	1:A:109:LEU:HD22	1.98	0.46
1:C:241:VAL:CG1	1:C:248:THR:HG22	2.46	0.46


		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:E:84:SER:HA	1:E:127:TYR:CD2	2.51	0.46	
1:A:311:ASP:O	1:A:315:GLN:HG2	2.15	0.46	
1:B:96:ALA:HB1	4:B:403:NAI:C4A	2.45	0.46	
1:G:8:ILE:HD13	1:G:8:ILE:N	2.31	0.46	
1:H:155:LYS:HB2	1:H:155:LYS:HE3	1.66	0.46	
1:E:250:TRP:CZ2	1:K:33:MET:HB3	2.50	0.46	
1:I:218:MET:HE2	1:I:227:TRP:CE2	2.51	0.46	
1:L:142:ILE:HD12	1:L:327:GLN:HG3	1.98	0.46	
3:B:402:OXM:C1	4:B:403:NAI:H42N	2.45	0.46	
1:F:8:ILE:HG23	1:I:302:SER:HB3	1.97	0.46	
1:B:155:LYS:H	2:B:401:SFX:H171	1.64	0.45	
1:C:307:LYS:HB3	1:C:307:LYS:HE2	1.75	0.45	
1:E:308:LEU:HB2	1:E:313:VAL:HG23	1.98	0.45	
5:G:403:BTB:H41	5:G:403:BTB:H71	1.13	0.45	
1:J:21:ASN:HA	1:J:90:LYS:HG3	1.98	0.45	
1:K:226:ASN:HB3	1:K:229:GLU:HB2	1.98	0.45	
1:B:17:THR:HG22	1:B:18:VAL:N	2.32	0.45	
1:E:80:ASP:HB2	1:E:85:VAL:HG11	1.98	0.45	
1:B:47:GLU:OE1	1:B:76:LYS:HD3	2.17	0.45	
3:D:401:OXM:C1	4:D:402:NAI:H42N	2.46	0.45	
1:F:177:LYS:HD2	1:F:177:LYS:HA	1.73	0.45	
1:F:217:GLU:O	1:F:223:ASP:HB2	2.15	0.45	
1:H:293:CYS:SG	1:H:300:LEU:HD21	2.57	0.45	
1:K:2:THR:O	1:K:6:LYS:HB2	2.16	0.45	
1:E:280:MET:HE1	1:E:291:LEU:CD1	2.46	0.45	
1:H:256:VAL:O	1:H:260:ILE:HG13	2.16	0.45	
1:L:155:LYS:HG3	7:L:406:GOL:H2	1.98	0.45	
1:E:126:LYS:HG2	1:E:127:TYR:CE1	2.52	0.45	
1:F:91:ILE:HD12	1:F:260:ILE:HG23	1.97	0.45	
1:F:239:TYR:CZ	5:F:404:BTB:H41	2.51	0.45	
1:K:283:ILE:HA	1:K:317:LYS:HE2	1.99	0.45	
1:C:27:GLY:O	1:C:32:GLY:HA3	2.16	0.45	
1:D:277:VAL:HG11	1:D:289:LEU:HD11	1.98	0.45	
1:F:289:LEU:C	1:F:289:LEU:HD12	2.37	0.45	
1:J:270:ILE:HA	1:J:293:CYS:O	2.17	0.45	
1:A:53:VAL:HG13	4:A:403:NAI:N1A	2.31	0.45	
1:B:18:VAL:HG22	1:B:19:PRO:HD2	1.98	0.45	
1:C:149:LYS:NZ	1:C:334:GLU:OE2	2.47	0.45	
1:E:58:LEU:HG	1:E:79:ALA:HB1	1.99	0.45	
1:H:58:LEU:HG	1:H:79:ALA:HB1	1.99	0.45	
1:H:189:ILE:HD13	1:H:199:ALA:HA	1.99	0.45	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:I:110:VAL:HG13	1:I:111:GLN:H	1.81	0.45	
1:J:229:GLU:O	1:J:233:MET:HG3	2.17	0.45	
1:B:20:ASN:ND2	1:G:20:ASN:OD1	2.50	0.45	
1:J:147:THR:O	1:J:151:SER:HB3	2.17	0.45	
1:L:159:ILE:HG23	1:L:300:LEU:HD12	1.99	0.45	
1:L:214:LEU:HD12	1:L:214:LEU:N	2.31	0.45	
1:L:239:TYR:CE2	5:L:403:BTB:H72	2.52	0.45	
4:L:402:NAI:H6N	4:L:402:NAI:H2D	1.77	0.45	
1:A:263:MET:HE3	1:A:263:MET:HB2	1.83	0.45	
1:E:84:SER:HA	1:E:127:TYR:CE2	2.51	0.45	
1:G:309:LYS:HA	1:G:309:LYS:HD2	1.69	0.45	
1:J:96:ALA:HB1	4:J:402:NAI:C4A	2.47	0.45	
1:L:193:HIS:HE1	3:L:401:OXM:O3	2.00	0.45	
1:D:29:GLY:HA3	4:D:402:NAI:O5B	2.17	0.45	
1:J:289:LEU:HD12	1:J:289:LEU:C	2.37	0.45	
5:A:404:BTB:H31	5:A:404:BTB:H71	1.85	0.44	
1:D:323:LEU:HD13	1:D:323:LEU:HA	1.87	0.44	
1:J:121:ILE:HB	1:J:122:PRO:HD3	1.99	0.44	
1:D:125:VAL:CG1	1:D:153:LEU:HD21	2.47	0.44	
1:E:108:ASN:OD1	1:F:115:ASN:HB3	2.17	0.44	
1:G:289:LEU:C	1:G:289:LEU:HD12	2.37	0.44	
1:I:84:SER:HA	1:I:127:TYR:CD2	2.52	0.44	
1:K:180:ILE:HD11	1:K:185:CYS:SG	2.58	0.44	
1:D:273:VAL:O	1:D:290:SER:HA	2.17	0.44	
1:F:148:TRP:CZ3	1:F:149:LYS:HE2	2.52	0.44	
1:G:276:MET:HB2	1:G:288:PHE:CZ	2.52	0.44	
1:K:110:VAL:HG13	1:K:111:GLN:N	2.31	0.44	
1:K:111:GLN:HE21	1:K:112:ARG:HG3	1.83	0.44	
1:L:210:SER:O	1:L:214:LEU:HD13	2.17	0.44	
1:C:2:THR:HG23	1:C:5:GLU:OE1	2.18	0.44	
1:D:42:LYS:HE3	1:D:261:GLU:OE1	2.17	0.44	
1:G:7:LEU:HG	1:G:8:ILE:HD13	2.00	0.44	
1:G:191:GLY:HA2	1:G:289:LEU:HD13	2.00	0.44	
1:J:240:GLU:O	1:J:244:LEU:HG	2.17	0.44	
1:L:218:MET:HE2	1:L:227:TRP:CD1	2.53	0.44	
1:E:126:LYS:HG2	1:E:127:TYR:CD1	2.53	0.44	
1:G:83:TYR:OH	1:G:120:ILE:HG12	2.18	0.44	
1:H:192:GLU:HG3	1:H:323:LEU:HD21	1.99	0.44	
1:L:241:VAL:HG11	1:L:248:THR:HG22	2.00	0.44	
2:A:401:SFX:H2A	2:A:401:SFX:H17	1.67	0.44	
1:C:180:ILE:HD11	1:C:185:CYS:SG	2.56	0.44	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:174:MET:CE	1:E:204:VAL:HG13	2.46	0.44
1:E:331:LYS:HG2	1:E:332:ASP:N	2.33	0.44
1:A:155:LYS:H	2:A:401:SFX:H2A	1.82	0.44
1:B:130:ASP:HB2	9:B:541:HOH:O	2.17	0.44
1:E:39:ILE:HG23	1:E:44:LEU:HB2	1.99	0.44
1:F:85:VAL:HA	7:F:405:GOL:H31	1.99	0.44
1:G:80:ASP:HB2	1:G:85:VAL:HG11	1.99	0.44
1:G:270:ILE:HB	9:G:555:HOH:O	2.16	0.44
1:H:218:MET:HG3	1:H:227:TRP:CD1	2.53	0.44
1:C:20:ASN:HD21	1:D:20:ASN:HD21	1.65	0.44
1:H:130:ASP:HA	1:H:157:ARG:NH1	2.32	0.44
1:H:186:HIS:O	1:H:204:VAL:HA	2.18	0.44
1:K:8:ILE:HD13	1:K:8:ILE:N	2.33	0.44
1:L:106:ARG:HH21	3:L:401:OXM:C1	2.31	0.44
1:E:146:VAL:HG22	1:E:333:LEU:HD11	2.00	0.44
1:F:266:ASN:OD1	1:F:296:ASN:HB2	2.18	0.44
5:F:404:BTB:H11	5:F:404:BTB:H71	1.73	0.44
1:G:174:MET:HE2	1:G:227:TRP:CZ3	2.53	0.44
1:L:110:VAL:CG1	1:L:111:GLN:H	2.30	0.44
1:A:160:GLY:HA3	1:A:274:SER:HB3	2.00	0.43
1:B:139:PRO:HB2	1:B:142:ILE:HD12	2.00	0.43
1:E:33:MET:HB3	1:K:250:TRP:CZ2	2.53	0.43
8:E:403:PEG:H31	9:E:604:HOH:O	2.18	0.43
1:F:13:GLU:HG2	2:I:401:SFX:F15	2.08	0.43
1:H:241:VAL:HG11	1:H:248:THR:HG22	1.97	0.43
1:L:8:ILE:HD13	1:L:8:ILE:N	2.33	0.43
1:C:275:THR:O	1:C:288:PHE:HA	2.19	0.43
1:F:14:GLU:C	1:F:15:GLU:HG2	2.39	0.43
1:G:110:VAL:HG23	1:G:111:GLN:H	1.83	0.43
1:H:293:CYS:HB3	1:H:300:LEU:HD21	2.00	0.43
1:L:136:VAL:O	4:L:402:NAI:H2N	2.18	0.43
1:A:180:ILE:HD13	1:G:270:ILE:HD11	1.99	0.43
1:B:148:TRP:CZ2	2:B:401:SFX:H17	2.53	0.43
1:C:8:ILE:CG2	1:D:302:SER:HB3	2.48	0.43
1:C:110:VAL:CG2	1:C:139:PRO:HG3	2.44	0.43
1:C:142:ILE:HD13	1:C:326:ILE:HG21	1.99	0.43
1:J:307:LYS:HE3	9:J:558:HOH:O	2.18	0.43
1:A:37:ILE:HD12	1:A:37:ILE:HA	1.90	0.43
1:A:180:ILE:HG22	1:A:181:HIS:N	2.33	0.43
2:C:401:SFX:H3	9:C:503:HOH:O	2.18	0.43
1:H:62:MET:O	1:H:66:GLN:HG3	2.18	0.43



	A L O	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:I:155:LYS:HE2	2:I:401:SFX:C11	2.41	0.43	
1:J:27:GLY:HA2	1:J:52:ASP:OD2	2.18	0.43	
1:J:273:VAL:O	1:J:290:SER:HA	2.17	0.43	
1:B:125:VAL:HG21	1:B:151:SER:HB2	2.01	0.43	
1:C:111:GLN:O	1:C:112:ARG:C	2.57	0.43	
1:E:119:PHE:HD2	1:E:120:ILE:HG23	1.83	0.43	
1:E:252:ILE:O	1:E:256:VAL:HG23	2.18	0.43	
1:F:308:LEU:HB2	1:F:313:VAL:CG2	2.49	0.43	
1:H:219:GLY:O	1:H:228:LYS:HD3	2.18	0.43	
1:H:273:VAL:O	1:H:290:SER:HA	2.18	0.43	
8:J:407:PEG:H22	8:J:407:PEG:H41	1.74	0.43	
1:K:289:LEU:C	1:K:289:LEU:HD12	2.39	0.43	
1:L:204:VAL:HG12	1:L:211:LEU:HD12	2.00	0.43	
1:L:308:LEU:HD23	1:L:308:LEU:HA	1.83	0.43	
1:B:304:ILE:CD1	1:G:8:ILE:HD12	2.49	0.43	
1:E:7:LEU:HD13	1:E:8:ILE:HD13	2.00	0.43	
1:G:3:LEU:HD12	1:H:215:ASN:HD22	1.84	0.43	
1:G:280:MET:O	1:G:283:ILE:HD12	2.19	0.43	
1:K:308:LEU:HB2	1:K:313:VAL:HG23	1.99	0.43	
1:A:20:ASN:O	1:A:90:LYS:HG3	2.18	0.43	
1:E:37:ILE:HD12	1:E:37:ILE:HA	1.80	0.43	
1:E:120:ILE:HD13	1:E:120:ILE:HG21	1.72	0.43	
1:B:278:LYS:HB2	1:B:286:GLU:HA	2.01	0.43	
1:B:318:LYS:HG2	9:B:520:HOH:O	2.19	0.43	
1:D:218:MET:HE2	1:D:227:TRP:CD1	2.54	0.43	
1:K:47:GLU:CD	1:K:76:LYS:HD3	2.37	0.43	
1:K:275:THR:O	1:K:288:PHE:HA	2.18	0.43	
1:L:198:VAL:CG2	1:L:315:GLN:HB2	2.48	0.43	
1:L:309:LYS:HD2	1:L:309:LYS:HA	1.92	0.43	
1:A:276:MET:HB2	1:A:288:PHE:CZ	2.54	0.43	
1:B:44:LEU:HD13	1:B:260:ILE:HG22	2.00	0.43	
1:C:189:ILE:O	1:C:190:LEU:HD23	2.19	0.43	
1:D:252:ILE:O	1:D:256:VAL:HG23	2.18	0.43	
1:H:293:CYS:HB3	1:H:300:LEU:CD2	2.49	0.43	
1:H:308:LEU:HB2	1:H:313:VAL:HG22	2.00	0.43	
1:J:237:SER:O	1:J:241:VAL:HG23	2.19	0.43	
1:K:195:ASP:HA	1:K:235:VAL:HG13	1.99	0.43	
1:K:273:VAL:HG23	1:K:300:LEU:HD11	2.01	0.43	
1:L:47:GLU:CD	1:L:76:LYS:HD3	2.39	0.43	
1:L:117:PHE:CD2	1:L:143:LEU:HD22	2.54	0.43	
1:B:98:VAL:HG23	1:B:109:LEU:HD22	2.01	0.42	



	A L O	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:B:226:ASN:O	1:B:229:GLU:HB3	2.19	0.42	
1:B:289:LEU:C	1:B:289:LEU:HD12	2.39	0.42	
5:C:404:BTB:H12	9:C:615:HOH:O	2.19	0.42	
1:D:277:VAL:HG22	1:D:287:VAL:O	2.18	0.42	
1:H:81:LYS:HD3	9:H:553:HOH:O	2.19	0.42	
1:C:94:VAL:HG11	1:C:117:PHE:CZ	2.54	0.42	
1:C:149:LYS:HE3	1:C:334:GLU:OE2	2.19	0.42	
1:D:28:VAL:HG11	1:D:58:LEU:HD12	2.01	0.42	
1:G:134:ILE:HD11	1:G:263:MET:HE3	2.01	0.42	
1:H:165:LEU:HD12	1:H:165:LEU:O	2.19	0.42	
1:L:193:HIS:O	1:L:193:HIS:CG	2.72	0.42	
1:A:155:LYS:H	2:A:401:SFX:H2	1.84	0.42	
1:B:111:GLN:HE22	4:L:402:NAI:H61A	1.68	0.42	
1:E:277:VAL:HG21	1:E:283:ILE:HD13	2.01	0.42	
1:I:189:ILE:HD13	1:I:199:ALA:HA	2.00	0.42	
1:J:19:PRO:HB2	1:J:22:LYS:HB2	2.00	0.42	
1:K:175:ALA:HB2	1:K:182:PRO:HA	2.01	0.42	
1:A:106:ARG:O	1:A:139:PRO:HD3	2.19	0.42	
1:B:304:ILE:HD13	1:G:8:ILE:HD12	2.01	0.42	
1:C:148:TRP:CZ2	2:C:401:SFX:H17	2.54	0.42	
1:F:138:ASN:ND2	3:F:402:OXM:HN1	2.11	0.42	
1:F:189:ILE:O	1:F:190:LEU:HD23	2.20	0.42	
1:K:164:ASN:HA	1:K:272:PRO:HG2	2.00	0.42	
1:A:56:ASP:O	1:B:244:LEU:HB3	2.20	0.42	
1:A:225:GLU:HB3	1:A:227:TRP:CD1	2.55	0.42	
1:C:3:LEU:HD12	1:C:3:LEU:O	2.20	0.42	
1:C:331:LYS:O	1:C:332:ASP:HB3	2.19	0.42	
1:E:275:THR:O	1:E:288:PHE:HA	2.19	0.42	
1:F:294:ILE:HD12	1:F:302:SER:CB	2.43	0.42	
1:H:289:LEU:HD12	1:H:289:LEU:C	2.40	0.42	
1:K:33:MET:HE3	1:K:65:LEU:HD11	2.00	0.42	
1:E:110:VAL:CG2	1:E:142:ILE:HG21	2.49	0.42	
1:I:138:ASN:HD22	1:I:140:VAL:H	1.67	0.42	
1:L:15:GLU:CG	1:L:16:ALA:N	2.81	0.42	
1:L:44:LEU:HD13	1:L:260:ILE:HG22	2.01	0.42	
1:A:172:TYR:CZ	1:B:66:GLN:HB3	2.55	0.42	
1:C:52:ASP:HA	4:C:403:NAI:H2A	2.01	0.42	
1:K:188:TRP:CZ3	1:K:272:PRO:HD3	2.54	0.42	
1:D:23:ILE:HG21	1:D:39:ILE:HD13	2.02	0.42	
1:G:236:GLU:O	1:G:240:GLU:HG3	2.20	0.42	
1:G:270:ILE:HA	1:G:293:CYS:O	2.20	0.42	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
5:G:403:BTB:H31	5:G:403:BTB:H52	1.60	0.42	
1:J:61:GLU:HA	1:J:61:GLU:OE1	2.19	0.42	
1:L:215:ASN:OD1	1:L:217:GLU:HG2	2.20	0.42	
1:A:294:ILE:HD13	1:G:180:ILE:HG22	2.02	0.42	
1:B:155:LYS:N	2:B:401:SFX:H171	2.18	0.42	
4:B:403:NAI:O2N	9:B:501:HOH:O	2.21	0.42	
1:E:280:MET:HE1	1:E:291:LEU:HD13	2.02	0.42	
1:F:148:TRP:HE1	2:F:401:SFX:C18	2.30	0.42	
1:G:177:LYS:CE	1:G:225:GLU:OE1	2.67	0.42	
1:I:23:ILE:HG21	1:I:39:ILE:HD13	2.02	0.42	
1:A:278:LYS:NZ	9:A:506:HOH:O	2.35	0.42	
1:C:264:LEU:HA	1:C:264:LEU:HD23	1.81	0.42	
1:E:268:SER:HA	1:E:295:LEU:O	2.19	0.42	
1:G:324:TRP:HA	1:G:327:GLN:HB2	2.02	0.42	
1:J:230:VAL:O	1:J:234:VAL:HG23	2.19	0.42	
1:B:39:ILE:HG23	1:B:44:LEU:HB2	2.01	0.41	
1:D:226:ASN:HB3	1:D:229:GLU:HB3	2.02	0.41	
1:E:51:VAL:HG21	1:E:86:THR:CG2	2.50	0.41	
1:J:293:CYS:HB3	1:J:300:LEU:HD21	2.01	0.41	
1:K:98:VAL:HG22	1:K:113:ASN:OD1	2.20	0.41	
1:L:316:LEU:HD12	1:L:316:LEU:HA	1.91	0.41	
5:L:403:BTB:H71	5:L:403:BTB:H31	1.78	0.41	
1:A:244:LEU:HD13	1:B:59:LYS:HG2	2.01	0.41	
1:A:265:LYS:HB3	1:A:267:LEU:HD21	2.02	0.41	
1:D:319:SER:O	1:D:323:LEU:HD23	2.20	0.41	
1:E:178:LEU:N	1:E:178:LEU:HD23	2.35	0.41	
1:E:218:MET:HG3	1:E:227:TRP:CD1	2.55	0.41	
1:F:37:ILE:HD12	1:F:37:ILE:HA	1.91	0.41	
1:F:49:ALA:HA	1:F:78:VAL:O	2.21	0.41	
1:G:141:ASP:HB3	1:G:288:PHE:O	2.20	0.41	
1:J:109:LEU:HD23	1:J:112:ARG:NH2	2.35	0.41	
1:K:111:GLN:HG2	1:K:112:ARG:N	2.35	0.41	
1:K:198:VAL:HG22	1:K:315:GLN:HB3	2.02	0.41	
1:A:155:LYS:HE2	2:A:401:SFX:H7	2.02	0.41	
1:B:29:GLY:HA3	4:B:403:NAI:H52A	2.01	0.41	
1:D:189:ILE:HD13	1:D:199:ALA:HA	2.01	0.41	
1:H:14:GLU:HG2	1:H:15:GLU:N	2.35	0.41	
2:I:401:SFX:C11	2:I:401:SFX:C16	2.99	0.41	
1:J:117:PHE:CE1	1:J:143:LEU:HD13	2.55	0.41	
1:L:22:LYS:O	1:L:90:LYS:N	2.53	0.41	
1:F:100:GLN:HB3	1:F:104:GLU:HB3	2.03	0.41	



	A L O	Interatomic	Clash
Atom-1	Atom-1 Atom-2		overlap (Å)
1:F:201:TRP:HB3	1:F:218:MET:CE	2.46	0.41
1:I:98:VAL:HG22	1:I:113:ASN:OD1	2.21	0.41
1:I:268:SER:HA	1:I:295:LEU:O	2.20	0.41
1:K:28:VAL:CG2	1:K:33:MET:SD	3.08	0.41
1:L:163:CYS:HA	1:L:166:ASP:OD1	2.20	0.41
1:L:218:MET:HA	1:L:223:ASP:OD2	2.20	0.41
1:A:110:VAL:O	1:A:114:VAL:HG23	2.21	0.41
1:A:192:GLU:HG3	1:A:323:LEU:HD21	2.02	0.41
1:B:286:GLU:OE2	2:B:401:SFX:F13	2.28	0.41
1:C:303:VAL:HG23	1:D:11:VAL:CG2	2.51	0.41
1:J:110:VAL:CG1	1:J:111:GLN:N	2.84	0.41
1:C:177:LYS:HE2	1:C:227:TRP:CZ2	2.55	0.41
1:F:309:LYS:HE3	1:F:309:LYS:CA	2.47	0.41
1:I:237:SER:O	1:I:241:VAL:HG23	2.21	0.41
1:K:211:LEU:CB	1:K:218:MET:HE1	2.51	0.41
1:K:330:LEU:HD23	1:K:330:LEU:HA	1.85	0.41
1:B:152:GLY:O	2:B:401:SFX:H19	2.21	0.41
1:H:163:CYS:HA	1:H:166:ASP:OD1	2.21	0.41
1:I:44:LEU:HD13	1:I:260:ILE:CG2	2.51	0.41
1:K:121:ILE:N	1:K:122:PRO:HD2	2.35	0.41
1:K:265:LYS:NZ	7:K:405:GOL:C2	2.82	0.41
1:B:140:VAL:O	1:B:144:THR:OG1	2.33	0.41
1:B:156:HIS:HB2	1:B:300:LEU:O	2.21	0.41
1:C:236:GLU:O	1:C:240:GLU:HG3	2.21	0.41
1:D:174:MET:HE2	1:D:174:MET:HB2	1.81	0.41
1:E:29:GLY:HA3	4:E:402:NAI:O5B	2.21	0.41
1:E:111:GLN:O	1:E:112:ARG:C	2.59	0.41
1:E:177:LYS:C	1:E:178:LEU:HD23	2.41	0.41
1:H:134:ILE:HD11	1:H:263:MET:CE	2.50	0.41
1:I:42:LYS:HB2	1:I:42:LYS:HE2	1.93	0.41
1:J:155:LYS:HE3	1:J:155:LYS:HB2	1.81	0.41
1:J:294:ILE:HD12	1:J:302:SER:HB2	2.03	0.41
1:K:143:LEU:HD23	1:K:143:LEU:HA	1.85	0.41
1:K:211:LEU:HB2	1:K:218:MET:HE1	2.02	0.41
1:K:231:HIS:O	1:K:235:VAL:HG23	2.20	0.41
1:L:239:TYR:CZ	5:L:403:BTB:H72	2.56	0.41
1:A:7:LEU:C	1:A:8:ILE:HD13	2.41	0.41
1:D:37:ILE:HD12	1:D:37:ILE:HA	1.87	0.41
1:D:291:LEU:HB3	1:D:292:PRO:CD	2.51	0.41
1:H:173:LEU:HD22	1:H:233:MET:HE2	2.03	0.41
1:J:18:VAL:O	1:J:18:VAL:HG13	2.20	0.41



	io de pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:K:106:ARG:O	1:K:139:PRO:HD3	2.21	0.41
1:K:120:ILE:HG21	1:K:120:ILE:HD13	1.76	0.41
1:C:242:ILE:HG12	9:C:532:HOH:O	2.20	0.40
1:E:117:PHE:HA	1:E:120:ILE:HG12	2.03	0.40
1:E:174:MET:HE2	1:E:185:CYS:HB3	2.02	0.40
3:F:402:OXM:N1	4:F:403:NAI:H42N	2.36	0.40
1:H:218:MET:HG3	1:H:227:TRP:CG	2.56	0.40
1:L:276:MET:SD	1:L:286:GLU:HG2	2.62	0.40
1:B:142:ILE:O	1:B:146:VAL:HG23	2.21	0.40
1:B:269:ARG:HG2	1:H:181:HIS:HB3	2.03	0.40
1:D:110:VAL:CG1	1:D:111:GLN:N	2.84	0.40
1:F:215:ASN:OD1	1:F:217:GLU:OE1	2.38	0.40
1:A:151:SER:OG	1:A:153:LEU:HD12	2.21	0.40
1:B:27:GLY:O	1:B:32:GLY:HA3	2.21	0.40
1:B:47:GLU:CD	1:B:76:LYS:HD3	2.42	0.40
1:B:181:HIS:HB2	1:H:267:LEU:O	2.21	0.40
1:B:308:LEU:HB2	1:B:313:VAL:HG23	2.03	0.40
1:D:155:LYS:HE2	1:D:155:LYS:HB2	1.85	0.40
1:E:164:ASN:HA	1:E:272:PRO:HG2	2.03	0.40
1:E:204:VAL:HG12	1:E:211:LEU:HD12	2.03	0.40
1:G:56:ASP:O	1:H:244:LEU:HB3	2.21	0.40
1:H:2:THR:OG1	1:H:5:GLU:HG3	2.21	0.40
1:H:283:ILE:HG13	1:H:317:LYS:HD2	2.04	0.40
1:I:14:GLU:HG3	1:I:15:GLU:N	2.35	0.40
1:L:117:PHE:HA	1:L:120:ILE:HG12	2.02	0.40
1:B:154:PRO:HB3	2:B:401:SFX:H2	2.04	0.40
1:C:188:TRP:CZ3	1:C:272:PRO:HD3	2.56	0.40
5:F:404:BTB:H42	5:F:404:BTB:H52	1.60	0.40
1:G:189:ILE:HD13	1:G:199:ALA:HA	2.04	0.40
1:A:51:VAL:HG21	1:A:86:THR:CG2	2.51	0.40
1:A:227:TRP:HZ2	1:B:3:LEU:HD23	1.87	0.40
1:D:236:GLU:O	1:D:240:GLU:HG3	2.21	0.40
1:D:265:LYS:HA	1:D:265:LYS:HD2	1.57	0.40
1:D:300:LEU:HD23	1:D:300:LEU:C	2.42	0.40
1:E:35:CYS:SG	1:E:256:VAL:HG21	2.62	0.40
1:F:61:GLU:HA	1:F:61:GLU:OE1	2.22	0.40
1:H:240:GLU:HB2	9:H:584:HOH:O	2.21	0.40
1:I:40:LEU:HD11	1:I:65:LEU:HD13	2.04	0.40
1:I:136:VAL:O	4:I:403:NAI:H2N	2.22	0.40
1:I:331:LYS:HE2	1:I:331:LYS:HB2	1.89	0.40
1:K:210:SER:CB	1:K:213:GLU:HG3	2.51	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	Percer	ntiles
1	А	331/349~(95%)	318~(96%)	13 (4%)	0	100	100
1	В	331/349~(95%)	320 (97%)	10 (3%)	1 (0%)	37	31
1	С	333/349~(95%)	315~(95%)	18 (5%)	0	100	100
1	D	330/349~(95%)	320~(97%)	9~(3%)	1 (0%)	37	31
1	Ε	330/349~(95%)	318 (96%)	11 (3%)	1 (0%)	37	31
1	F	332/349~(95%)	317~(96%)	14 (4%)	1 (0%)	37	31
1	G	331/349~(95%)	317~(96%)	13~(4%)	1 (0%)	37	31
1	Η	333/349~(95%)	320 (96%)	13~(4%)	0	100	100
1	Ι	331/349~(95%)	317~(96%)	14 (4%)	0	100	100
1	J	330/349~(95%)	315~(96%)	14 (4%)	1 (0%)	37	31
1	Κ	332/349~(95%)	318~(96%)	10 (3%)	4 (1%)	11	4
1	L	332/349~(95%)	314 (95%)	17 (5%)	1 (0%)	37	31
All	All	3976/4188~(95%)	3809 (96%)	156 (4%)	11 (0%)	37	31

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	226	ASN
1	F	69	SER
1	Κ	332	ASP
1	Е	249	ASN
1	G	249	ASN
1	Κ	249	ASN
1	D	249	ASN
1	L	16	ALA
1	Κ	28	VAL



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Mol	Chain	Res	Type
1	В	110	VAL
1	Κ	110	VAL

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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	289/304~(95%)	287~(99%)	2(1%)	81 82
1	В	289/304~(95%)	286~(99%)	3 (1%)	73 73
1	С	291/304~(96%)	289~(99%)	2(1%)	81 82
1	D	288/304~(95%)	287 (100%)	1 (0%)	91 92
1	Ε	289/304~(95%)	287~(99%)	2(1%)	81 82
1	F	290/304~(95%)	288~(99%)	2(1%)	81 82
1	G	289/304~(95%)	288 (100%)	1 (0%)	91 92
1	Н	291/304~(96%)	288~(99%)	3~(1%)	73 73
1	Ι	289/304~(95%)	285~(99%)	4 (1%)	62 62
1	J	288/304~(95%)	284 (99%)	4 (1%)	62 62
1	Κ	290/304~(95%)	288~(99%)	2(1%)	81 82
1	L	$29\overline{0}/304~(95\%)$	287 (99%)	$\overline{3(1\%)}$	73 73
All	All	3473/3648~(95%)	3444 (99%)	29 (1%)	79 80

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

Mol	Chain	Res	Type
1	А	81	LYS
1	А	226	ASN
1	В	221	ASP
1	В	318	LYS
1	В	325	ASP
1	С	101	GLN
1	С	325	ASP
1	D	81	LYS



Mol	Chain	Res	Type
1	Е	5	GLU
1	Е	81	LYS
1	F	3	LEU
1	F	100	GLN
1	G	14	GLU
1	Н	21	ASN
1	Н	119	PHE
1	Н	240	GLU
1	Ι	3	LEU
1	Ι	42	LYS
1	Ι	174	MET
1	Ι	317	LYS
1	J	85	VAL
1	J	119	PHE
1	J	226	ASN
1	J	248	THR
1	Κ	237	SER
1	Κ	317	LYS
1	L	217	GLU
1	L	255	SER
1	L	321	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	20	ASN
1	В	111	GLN
1	В	285	ASN
1	С	20	ASN
1	С	222	ASN
1	D	215	ASN
1	D	327	GLN
1	Е	306	GLN
1	F	100	GLN
1	F	108	ASN
1	F	138	ASN
1	Н	20	ASN
1	Н	111	GLN
1	Ι	138	ASN
1	Κ	111	GLN
1	L	123	GLN
1	L	156	HIS



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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

73 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).

Mol	Type	Chain	Bos	Link	В	Bond lengths			Bond angles		
	Type	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
2	SFX	С	401	-	23,23,23	1.11	2 (8%)	30,31,31	1.00	1 (3%)	
2	SFX	В	401	-	23,23,23	1.18	1 (4%)	30,31,31	1.35	3 (10%)	
3	OXM	G	401	-	$5,\!5,\!5$	2.75	3 (60%)	4,6,6	1.51	1 (25%)	
4	NAI	D	402	-	42,48,48	2.02	9 (21%)	47,73,73	2.46	15 (31%)	
7	GOL	L	405	-	$5,\!5,\!5$	0.52	0	$5,\!5,\!5$	0.41	0	
7	GOL	F	406	-	$5,\!5,\!5$	0.56	0	$5,\!5,\!5$	0.24	0	
4	NAI	L	402	-	42,48,48	2.21	10 (23%)	47,73,73	2.88	18 (38%)	
4	NAI	С	403	-	42,48,48	1.96	9 (21%)	47,73,73	2.23	15 (31%)	
3	OXM	С	402	-	$5,\!5,\!5$	<mark>3.10</mark>	3 (60%)	4,6,6	1.42	1 (25%)	
5	BTB	L	403	-	13,13,13	0.79	0	7,16,16	0.79	0	
6	SO4	J	404	-	4,4,4	0.31	0	6,6,6	0.22	0	
7	GOL	Н	406	-	$5,\!5,\!5$	0.53	0	$5,\!5,\!5$	0.29	0	
7	GOL	L	406	-	$5,\!5,\!5$	0.24	0	5,5,5	2.36	2 (40%)	
7	GOL	В	404	-	$5,\!5,\!5$	0.57	0	$5,\!5,\!5$	0.55	0	
7	GOL	Н	405	-	5, 5, 5	0.52	0	5,5,5	0.22	0	
5	BTB	G	403	-	13,13,13	1.06	2 (15%)	7,16,16	1.14	0	



Mal	Turne	Chain	Dec	Timle	Bond lengths		Bond angles			
WIOI	туре	Unain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	D	403	-	$5,\!5,\!5$	0.52	0	$5,\!5,\!5$	0.27	0
7	GOL	F	405	-	$5,\!5,\!5$	0.57	0	$5,\!5,\!5$	0.45	0
4	NAI	Ι	403	-	42,48,48	2.07	9 (21%)	47,73,73	1.93	11 (23%)
3	OXM	Ι	402	-	$5,\!5,\!5$	2.66	2 (40%)	4,6,6	1.14	0
4	NAI	Н	402	-	42,48,48	2.17	12 (28%)	47,73,73	2.35	20 (42%)
6	SO4	С	407	-	4,4,4	0.16	0	$6,\!6,\!6$	0.39	0
7	GOL	С	405	-	$5,\!5,\!5$	0.54	0	$5,\!5,\!5$	0.33	0
3	OXM	Н	401	-	$5,\!5,\!5$	2.63	3 (60%)	4,6,6	1.06	0
7	GOL	Н	404	-	$5,\!5,\!5$	0.47	0	$5,\!5,\!5$	0.55	0
4	NAI	J	402	-	42,48,48	2.14	12 (28%)	47,73,73	2.02	17 (36%)
8	PEG	Н	407	-	$6,\!6,\!6$	0.13	0	$5,\!5,\!5$	0.10	0
6	SO4	С	406	-	4,4,4	0.13	0	6,6,6	0.46	0
6	SO4	В	406	-	4,4,4	0.14	0	6,6,6	0.46	0
3	OXM	L	401	-	$5,\!5,\!5$	2.80	3 (60%)	4,6,6	1.22	0
8	PEG	В	408	-	$6,\!6,\!6$	0.22	0	$5,\!5,\!5$	0.10	0
8	PEG	J	407	-	$6,\!6,\!6$	0.16	0	$5,\!5,\!5$	0.12	0
4	NAI	F	403	-	42,48,48	2.05	11 (26%)	47,73,73	2.11	15 (31%)
8	PEG	D	407	-	$6,\!6,\!6$	0.19	0	$5,\!5,\!5$	0.04	0
3	OXM	А	402	-	$5,\!5,\!5$	2.81	2 (40%)	4,6,6	1.13	0
8	PEG	D	406	-	6,6,6	0.16	0	$5,\!5,\!5$	0.11	0
7	GOL	Н	403	-	$5,\!5,\!5$	0.54	0	$5,\!5,\!5$	0.27	0
6	SO4	L	408	-	4,4,4	0.20	0	6,6,6	0.32	0
2	SFX	А	401	-	$23,\!23,\!23$	1.11	2 (8%)	30,31,31	1.02	2(6%)
6	SO4	L	407	-	4,4,4	0.15	0	6,6,6	0.29	0
7	GOL	G	405	-	$5,\!5,\!5$	0.57	0	$5,\!5,\!5$	0.26	0
5	BTB	К	403	-	$13,\!13,\!13$	0.81	0	7,16,16	1.08	1 (14%)
7	GOL	В	405	-	$5,\!5,\!5$	0.39	0	$5,\!5,\!5$	0.63	0
6	SO4	А	405	-	4,4,4	0.18	0	6,6,6	0.23	0
4	NAI	G	402	-	42,48,48	2.05	10 (23%)	47,73,73	2.17	20 (42%)
3	OXM	K	401	-	$5,\!5,\!5$	2.78	3 (60%)	4,6,6	1.93	1 (25%)
5	BTB	F	404	-	13,13,13	0.72	0	7,16,16	0.69	0
4	NAI	K	402	-	42,48,48	2.02	8 (19%)	47,73,73	2.08	15 (31%)
7	GOL	K	404	-	$5,\!5,\!5$	0.55	0	5,5,5	0.21	0
7	GOL	G	404	-	$5,\!5,\!5$	0.55	0	$5,\!5,\!5$	0.21	0
4	NAI	В	403	-	42,48,48	2.07	9 (21%)	47,73,73	2.15	13 (27%)
7	GOL	Ι	404	-	$5,\!5,\!5$	0.60	0	5,5,5	0.55	0
7	GOL	L	404	-	$5,\!5,\!5$	0.49	0	$5,\!5,\!5$	0.33	0
2	SFX	Ι	401	_	23,23,23	1.02	1 (4%)	30,31,31	1.67	4 (13%)
6	SO4	G	406	-	4,4,4	0.20	0	6,6,6	0.37	0



Mal	Turne	Chain	Dec	Tiple	B	ond leng	gths	Bond angles		
	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
5	BTB	А	404	-	13,13,13	0.88	1 (7%)	7,16,16	1.14	0
3	OXM	D	401	-	5,5,5	2.67	3 (60%)	4,6,6	1.28	1 (25%)
8	PEG	Е	403	-	6,6,6	0.12	0	5,5,5	0.12	0
3	OXM	F	402	-	5,5,5	2.55	2 (40%)	4,6,6	1.53	1 (25%)
3	OXM	В	402	-	5,5,5	2.61	2 (40%)	4,6,6	1.47	1 (25%)
5	BTB	С	404	-	13,13,13	0.98	1 (7%)	7,16,16	1.36	1 (14%)
3	OXM	J	401	-	5,5,5	2.55	2 (40%)	4,6,6	1.83	2(50%)
6	SO4	D	405	-	4,4,4	0.22	0	6,6,6	0.38	0
2	SFX	F	401	-	23,23,23	1.21	1 (4%)	30,31,31	2.15	4 (13%)
4	NAI	А	403	-	42,48,48	2.10	7 (16%)	47,73,73	2.21	19 (40%)
6	SO4	J	405	-	4,4,4	0.21	0	6,6,6	0.28	0
3	OXM	Е	401	-	5,5,5	2.85	3 (60%)	4,6,6	1.18	0
7	GOL	J	403	-	5,5,5	0.63	0	5,5,5	0.43	0
6	SO4	В	407	-	4,4,4	0.12	0	6,6,6	0.32	0
8	PEG	J	406	-	6,6,6	0.20	0	$5,\!5,\!5$	0.06	0
4	NAI	Е	402	-	42,48,48	1.90	8 (19%)	47,73,73	2.68	19 (40%)
6	SO4	D	404	-	4,4,4	0.24	0	6,6,6	0.10	0
7	GOL	K	405	-	5,5,5	0.48	0	5,5,5	0.40	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	SFX	С	401	-	-	9/18/18/18	0/2/2/2
2	SFX	В	401	-	-	8/18/18/18	0/2/2/2
3	OXM	G	401	-	-	0/3/4/4	-
4	NAI	D	402	-	-	5/25/72/72	0/5/5/5
7	GOL	L	405	-	-	0/4/4/4	-
7	GOL	F	406	-	-	2/4/4/4	-
4	NAI	L	402	-	-	13/25/72/72	0/5/5/5
4	NAI	С	403	-	-	3/25/72/72	0/5/5/5
3	OXM	С	402	-	-	0/3/4/4	-
5	BTB	L	403	-	-	8/21/21/21	-
7	GOL	Н	406	-	-	0/4/4/4	-
7	GOL	Ĺ	406	-	-	0/4/4/4	-
8	PEG	В	408	-	-	2/4/4/4	-



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	В	404	-	-	2/4/4/4	-
7	GOL	Н	405	-	-	2/4/4/4	-
5	BTB	G	403	-	-	9/21/21/21	-
7	GOL	D	403	-	-	0/4/4/4	-
7	GOL	F	405	-	-	2/4/4/4	-
4	NAI	Ι	403	-	-	5/25/72/72	0/5/5/5
3	OXM	Ι	402	-	-	3/3/4/4	-
4	NAI	Н	402	-	-	4/25/72/72	0/5/5/5
7	GOL	С	405	-	-	4/4/4/4	-
7	GOL	Н	404	-	-	$\frac{4}{4}/\frac{4}{4}$	-
3	OXM	Н	401	-	-	0/3/4/4	-
4	NAI	J	402	-	-	4/25/72/72	0/5/5/5
8	PEG	Н	407	-	-	3/4/4/4	-
3	OXM	L	401	-	-	0/3/4/4	-
8	PEG	J	407	-	-	2/4/4/4	-
4	NAI	F	403	-	-	3/25/72/72	0/5/5/5
8	PEG	D	407	-	-	3/4/4/4	-
3	OXM	А	402	-	-	0/3/4/4	-
8	PEG	D	406	-	-	1/4/4/4	-
7	GOL	Н	403	-	-	4/4/4/4	-
2	SFX	А	401	-	-	9/18/18/18	0/2/2/2
7	GOL	G	405	-	-	3/4/4/4	-
5	BTB	K	403	-	-	7/21/21/21	-
7	GOL	В	405	-	-	0/4/4/4	-
4	NAI	G	402	-	-	7/25/72/72	0/5/5/5
3	OXM	K	401	-	-	0/3/4/4	-
5	BTB	F	404	-	-	8/21/21/21	-
4	NAI	K	402	-	-	6/25/72/72	0/5/5/5
7	GOL	K	404	-	-	2/4/4/4	-
7	GOL	G	404	-	-	4/4/4/4	-
4	NAI	В	403	-	-	7/25/72/72	0/5/5/5
7	GOL	Ι	404	-	-	2/4/4/4	-
7	GOL	L	404	-	-	4/4/4/4	-
2	SFX	I	401	_	-	5/18/18/18	0/2/2/2
5	BTB	A	404		-	7/21/21/21	-
3	OXM	D	401	-	-	0/3/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PEG	Е	403	-	-	0/4/4/4	-
3	OXM	F	402	-	-	0/3/4/4	-
3	OXM	В	402	-	-	1/3/4/4	-
5	BTB	С	404	-	-	9/21/21/21	-
3	OXM	J	401	-	-	0/3/4/4	-
2	SFX	F	401	-	-	11/18/18/18	0/2/2/2
4	NAI	А	403	-	-	6/25/72/72	0/5/5/5
3	OXM	Е	401	-	-	0/3/4/4	-
7	GOL	J	403	-	-	4/4/4/4	-
8	PEG	J	406	-	-	3/4/4/4	-
4	NAI	E	402	-	-	7/25/72/72	0/5/5/5
7	GOL	K	405	-	-	2/4/4/4	-

All (156) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(Å)	Ideal(Å)
4	А	403	NAI	C2A-N3A	7.46	1.44	1.32
4	В	403	NAI	C2A-N3A	7.36	1.44	1.32
4	Κ	402	NAI	C2A-N3A	7.36	1.44	1.32
4	Н	402	NAI	PA-O1A	7.34	1.76	1.50
4	J	402	NAI	PA-O1A	7.30	1.76	1.50
4	Ι	403	NAI	C2A-N3A	7.24	1.43	1.32
4	L	402	NAI	PA-O1A	7.09	1.76	1.50
4	G	402	NAI	C2A-N3A	6.73	1.43	1.32
4	Н	402	NAI	C2A-N3A	6.72	1.42	1.32
4	Е	402	NAI	C2A-N3A	6.65	1.42	1.32
4	D	402	NAI	PA-O1A	6.61	1.74	1.50
4	F	403	NAI	PA-O1A	6.61	1.74	1.50
4	С	403	NAI	C2A-N3A	6.51	1.42	1.32
4	L	402	NAI	C2A-N3A	6.43	1.42	1.32
4	D	402	NAI	C2A-N3A	6.35	1.42	1.32
4	J	402	NAI	C2A-N3A	6.24	1.42	1.32
4	F	403	NAI	C2A-N3A	6.22	1.42	1.32
4	Ι	403	NAI	PA-O1A	5.99	1.72	1.50
4	G	402	NAI	PA-O1A	5.88	1.71	1.50
4	А	403	NAI	PA-O1A	5.83	1.71	1.50
4	Κ	402	NAI	PA-O1A	5.68	1.71	1.50
4	С	403	NAI	PA-O1A	5.66	1.71	1.50
4	В	403	NAI	PA-O1A	5.29	1.69	1.50
3	Κ	401	OXM	C1-N1	5.07	1.46	1.33
3	А	402	OXM	C1-N1	5.07	1.46	1.33



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	SFX	O5-C3	-4.89	1.40	1.44
2	В	401	SFX	O5-C3	-4.75	1.40	1.44
3	Ι	402	OXM	C1-N1	4.74	1.46	1.33
4	Е	402	NAI	PA-O1A	4.70	1.67	1.50
3	L	401	OXM	C1-N1	4.69	1.45	1.33
3	Е	401	OXM	C1-N1	4.65	1.45	1.33
4	L	402	NAI	PA-O5B	4.54	1.77	1.59
3	D	401	OXM	C1-N1	4.52	1.45	1.33
3	В	402	OXM	C1-N1	4.52	1.45	1.33
3	С	402	OXM	C1-N1	4.42	1.45	1.33
3	J	401	OXM	C1-N1	4.36	1.45	1.33
3	F	402	OXM	C1-N1	4.36	1.45	1.33
4	А	403	NAI	PN-O1N	4.30	1.75	1.55
4	Е	402	NAI	PN-O1N	4.30	1.75	1.55
3	Н	401	OXM	C1-N1	4.29	1.44	1.33
3	С	402	OXM	C1-C2	-4.20	1.50	1.55
3	G	401	OXM	C1-N1	4.12	1.44	1.33
4	K	402	NAI	PN-O1N	3.92	1.73	1.55
4	В	403	NAI	PN-O1N	3.89	1.73	1.55
4	J	402	NAI	PN-O1N	3.78	1.73	1.55
4	G	402	NAI	PN-O1N	3.77	1.73	1.55
2	А	401	SFX	O5-C3	-3.75	1.41	1.44
4	Ι	403	NAI	PN-O5D	3.74	1.74	1.59
4	Н	402	NAI	PN-O1N	3.73	1.72	1.55
4	В	403	NAI	C4A-N3A	3.69	1.40	1.35
4	L	402	NAI	C6A-N6A	3.68	1.47	1.34
4	J	402	NAI	PA-O5B	3.57	1.73	1.59
4	D	402	NAI	PN-O1N	3.56	1.72	1.55
4	В	403	NAI	PN-O5D	3.55	1.73	1.59
4	С	403	NAI	PN-O5D	3.52	1.73	1.59
4	F	403	NAI	PN-O1N	3.52	1.71	1.55
2	C	401	SFX	O5-C3	-3.50	1.41	1.44
4	D	402	NAI	C6A-N6A	3.49	1.46	1.34
4	F	403	NAI	PN-O5D	3.46	1.73	1.59
4	G	402	NAI	PN-O5D	3.42	1.73	1.59
4	I	403	NAI	PN-01N	3.41	1.71	1.55
4	A	403	NAI	C6A-N6A	3.37	1.46	1.34
3	G	401	OXM	C1-C2	-3.36	1.51	1.55
4	K	402	NAL	PA-O5B	3.35	1.72	1.59
4	A	403	NAI	PA-O5B	3.34	1.72	1.59
4	C	403	NAI	PN-01N	3.33	1.70	1.55
4	L	402	NAI	PN-O1N	3.27	1.70	1.55



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	402	NAI	PN-O5D	3.25	1.72	1.59
4	K	402	NAI	C5A-C4A	-3.22	1.32	1.40
3	Е	401	OXM	C1-C2	-3.17	1.51	1.55
4	Н	402	NAI	PA-O5B	3.11	1.71	1.59
4	В	403	NAI	PA-O5B	3.11	1.71	1.59
2	Ι	401	SFX	O5-C3	-3.11	1.41	1.44
4	С	403	NAI	PA-O5B	3.09	1.71	1.59
4	J	402	NAI	C6A-N6A	3.08	1.45	1.34
4	Н	402	NAI	PN-O5D	3.08	1.71	1.59
4	F	403	NAI	C5A-C4A	-3.06	1.32	1.40
4	J	402	NAI	C4A-N3A	3.03	1.39	1.35
4	Н	402	NAI	O4B-C1B	3.03	1.45	1.41
4	Н	402	NAI	C6A-N6A	3.00	1.45	1.34
4	D	402	NAI	PA-O5B	2.98	1.71	1.59
4	F	403	NAI	PA-O5B	2.95	1.71	1.59
4	G	402	NAI	C6A-N6A	2.95	1.44	1.34
4	D	402	NAI	C5A-C4A	-2.91	1.33	1.40
4	Ι	403	NAI	PA-O5B	2.90	1.71	1.59
4	С	403	NAI	C5A-C4A	-2.90	1.33	1.40
4	L	402	NAI	PN-O5D	2.86	1.70	1.59
4	E	402	NAI	C5A-C4A	-2.85	1.33	1.40
4	G	402	NAI	C5A-C4A	-2.83	1.33	1.40
4	L	402	NAI	C4A-N3A	2.80	1.39	1.35
4	E	402	NAI	PN-O5D	2.79	1.70	1.59
4	Ι	403	NAI	C5A-C4A	-2.74	1.33	1.40
4	A	403	NAI	C5A-C4A	-2.73	1.33	1.40
4	J	402	NAI	C5A-C4A	-2.71	1.33	1.40
4	Ι	403	NAI	C6A-N6A	2.68	1.43	1.34
4	E	402	NAI	C6A-N6A	2.68	1.43	1.34
4	G	402	NAI	C4A-N3A	2.66	1.39	1.35
4	A	403	NAI	PN-O5D	2.66	1.70	1.59
4	F	403	NAI	C6N-N1N	2.65	1.43	1.37
4	С	403	NAI	C6A-N6A	2.62	1.43	1.34
4	I	403	NAI	C4A-N3A	2.61	1.39	1.35
4	В	403	NAI	C5A-C4A	-2.61	1.34	1.40
4	L	402	NAI	C5A-C4A	-2.61	1.34	1.40
4		402	NAI	C6N-N1N	2.60	1.43	1.37
4	D	402	NAI	C4A-N3A	2.56	1.39	1.35
3	F	402	OXM	C1-C2	-2.56	1.52	1.55
3	L	401	OXM	C1-C2	-2.55	1.52	1.55
3	D	401	OXM	C1-C2	-2.52	1.52	1.55
3	H	401	OXM	O1-C1	-2.52	1.18	1.24



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Н	402	NAI	C5A-C4A	-2.50	1.34	1.40
4	J	402	NAI	PN-O5D	2.46	1.69	1.59
3	J	401	OXM	C1-C2	-2.44	1.52	1.55
4	Κ	402	NAI	PN-O5D	2.42	1.69	1.59
4	F	403	NAI	C2A-N1A	-2.42	1.29	1.33
4	Н	402	NAI	C4A-N3A	2.41	1.39	1.35
4	В	403	NAI	O4B-C1B	2.40	1.44	1.41
4	Κ	402	NAI	C6A-N6A	2.39	1.42	1.34
4	В	403	NAI	C6A-N6A	2.38	1.42	1.34
3	А	402	OXM	C1-C2	-2.36	1.52	1.55
5	А	404	BTB	C5-N	-2.34	1.44	1.48
3	Ι	402	OXM	O2-C2	2.34	1.28	1.22
3	L	401	OXM	O1-C1	-2.30	1.19	1.24
4	J	402	NAI	PN-O2N	2.28	1.59	1.50
4	D	402	NAI	C6N-N1N	2.28	1.43	1.37
4	Κ	402	NAI	C4A-N3A	2.28	1.38	1.35
4	С	403	NAI	C2A-N1A	-2.27	1.29	1.33
4	F	403	NAI	C6A-N6A	2.26	1.42	1.34
4	F	403	NAI	O4D-C4D	-2.25	1.40	1.45
4	Е	402	NAI	C2A-N1A	-2.25	1.29	1.33
3	С	402	OXM	O1-C1	-2.24	1.19	1.24
3	G	401	OXM	O1-C1	-2.22	1.19	1.24
4	Н	402	NAI	O4D-C4D	-2.22	1.40	1.45
3	К	401	OXM	O1-C1	-2.19	1.19	1.24
4	J	402	NAI	C6N-N1N	2.19	1.42	1.37
4	L	402	NAI	C2D-C3D	-2.18	1.47	1.53
5	С	404	BTB	C2-N	-2.18	1.44	1.48
2	С	401	SFX	C12-C9	2.16	1.54	1.49
4	Ι	403	NAI	C2A-N1A	-2.15	1.29	1.33
4	G	402	NAI	PA-O5B	2.14	1.68	1.59
3	Κ	401	OXM	C1-C2	-2.12	1.52	1.55
3	Н	401	OXM	C1-C2	-2.12	1.52	1.55
4	J	402	NAI	C2A-N1A	-2.11	1.30	1.33
4	G	402	NAI	PN-O2N	2.11	1.58	1.50
5	G	403	BTB	C5-N	-2.11	1.44	1.48
4	G	402	NAI	C6N-N1N	2.11	1.42	1.37
4	E	402	NAI	C4A-N3A	2.10	1.38	1.35
5	G	403	BTB	C2-N	-2.10	1.44	1.48
4	С	403	NAI	C4A-N3A	2.09	1.38	1.35
3	Е	401	OXM	O1-C1	-2.09	1.19	1.24
2	A	401	SFX	C12-C9	2.08	1.54	1.49
4	F	403	NAI	C5A-N7A	-2.08	1.32	1.39



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
4	Н	402	NAI	C5A-N7A	-2.06	1.32	1.39
3	D	401	OXM	O1-C1	-2.05	1.19	1.24
4	J	402	NAI	C8A-N7A	2.04	1.38	1.34
3	В	402	OXM	O1-C1	-2.03	1.19	1.24
4	Н	402	NAI	C6N-N1N	2.00	1.42	1.37

All (223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	F	401	SFX	C6-O5-C3	-9.78	112.10	118.62
4	L	402	NAI	PN-O3-PA	-9.78	99.27	132.83
4	Е	402	NAI	PN-O3-PA	-8.91	102.25	132.83
4	L	402	NAI	O3B-C3B-C4B	8.19	134.73	111.05
4	А	403	NAI	PN-O3-PA	-7.47	107.18	132.83
2	Ι	401	SFX	C6-O5-C3	6.47	122.93	118.62
4	D	402	NAI	O3B-C3B-C4B	6.45	129.69	111.05
4	D	402	NAI	O4B-C1B-C2B	-6.42	97.55	106.93
4	D	402	NAI	PN-O3-PA	-6.00	112.24	132.83
4	Е	402	NAI	C2D-C1D-N1N	5.91	128.10	113.30
4	С	403	NAI	PN-O3-PA	-5.76	113.06	132.83
4	В	403	NAI	PN-O3-PA	-5.68	113.34	132.83
4	L	402	NAI	N3A-C2A-N1A	-5.63	119.88	128.68
4	D	402	NAI	N3A-C2A-N1A	-5.62	119.89	128.68
4	А	403	NAI	C3B-C2B-C1B	-5.59	92.56	100.98
4	Н	402	NAI	PN-O3-PA	-5.58	113.67	132.83
4	K	402	NAI	PN-O3-PA	-5.53	113.87	132.83
4	L	402	NAI	O2A-PA-O1A	-5.44	85.34	112.24
4	Ι	403	NAI	PN-O3-PA	-5.42	114.22	132.83
4	С	403	NAI	O4B-C4B-C3B	5.31	115.63	105.11
4	F	403	NAI	PN-O3-PA	-5.15	115.16	132.83
4	L	402	NAI	O1N-PN-O5D	5.14	131.61	107.75
4	G	402	NAI	O3B-C3B-C4B	5.14	125.90	111.05
4	F	403	NAI	C3D-C2D-C1D	-5.11	91.72	101.43
4	J	402	NAI	PN-O3-PA	-4.95	115.82	132.83
4	Е	402	NAI	O4D-C1D-N1N	-4.93	98.41	108.06
4	В	403	NAI	N3A-C2A-N1A	-4.88	121.06	128.68
4	K	402	NAI	N3A-C2A-N1A	-4.68	121.36	128.68
4	Ι	403	NAI	N3A-C2A-N1A	-4.67	121.38	128.68
4	Н	402	NAI	O3B-C3B-C4B	4.61	124.36	111.05
4	G	402	NAI	PN-O3-PA	-4.59	117.07	132.83
4	В	403	NAI	C3B-C2B-C1B	-4.54	94.15	100.98
4	Е	402	NAI	O3B-C3B-C4B	4.49	124.04	111.05



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	С	403	NAI	N3A-C2A-N1A	-4.43	121.76	128.68
4	J	402	NAI	N3A-C2A-N1A	-4.41	121.78	128.68
4	Н	402	NAI	N3A-C2A-N1A	-4.36	121.87	128.68
4	F	403	NAI	C3B-C2B-C1B	-4.31	94.49	100.98
4	F	403	NAI	N3A-C2A-N1A	-4.18	122.14	128.68
4	В	403	NAI	O2A-PA-O5B	-4.18	88.34	107.75
4	D	402	NAI	C2B-C3B-C4B	-4.16	94.56	102.64
4	G	402	NAI	N3A-C2A-N1A	-4.15	122.19	128.68
4	С	403	NAI	C2B-C3B-C4B	-4.15	94.58	102.64
4	J	402	NAI	C3B-C2B-C1B	-4.09	94.83	100.98
4	Ι	403	NAI	C3D-C2D-C1D	-4.09	93.67	101.43
4	Е	402	NAI	O4D-C4D-C5D	4.08	122.81	109.37
4	В	403	NAI	O5B-PA-O1A	4.08	125.01	109.07
2	В	401	SFX	C2-C3-C16	-4.04	105.31	112.62
4	Е	402	NAI	O5B-PA-O1A	4.04	124.84	109.07
4	Н	402	NAI	O4B-C1B-C2B	-3.96	101.14	106.93
4	D	402	NAI	O4B-C4B-C3B	3.94	112.91	105.11
4	В	403	NAI	O4B-C1B-C2B	-3.88	101.25	106.93
4	Κ	402	NAI	O3B-C3B-C4B	3.82	122.10	111.05
4	С	403	NAI	O3B-C3B-C4B	3.78	121.98	111.05
4	С	403	NAI	C5B-C4B-C3B	-3.69	101.37	115.18
4	Κ	402	NAI	C2D-C1D-N1N	3.65	122.46	113.30
4	Κ	402	NAI	PN-O5D-C5D	-3.58	100.70	121.68
4	Ι	403	NAI	C2D-C1D-N1N	3.57	122.25	113.30
4	G	402	NAI	O3B-C3B-C2B	-3.55	100.33	111.82
4	Н	402	NAI	C3B-C2B-C1B	-3.51	95.69	100.98
4	Ε	402	NAI	O4B-C1B-C2B	-3.49	101.83	106.93
4	Κ	402	NAI	O4D-C1D-N1N	-3.47	101.27	108.06
4	L	402	NAI	O4B-C4B-C3B	3.46	111.97	105.11
4	Н	402	NAI	C5D-C4D-C3D	-3.46	102.23	115.18
4	С	403	NAI	PA-O5B-C5B	-3.44	101.48	121.68
4	Е	402	NAI	N3A-C2A-N1A	-3.44	123.30	128.68
4	G	402	NAI	C3N-C2N-N1N	-3.43	118.20	123.10
4	J	402	NAI	PN-O5D-C5D	-3.42	101.64	121.68
4	Н	402	NAI	C3D-C2D-C1D	-3.39	94.98	101.43
4	С	403	NAI	C5A-C6A-N6A	3.39	125.50	120.35
4	Е	402	NAI	O1N-PN-O2N	-3.37	95.59	112.24
4	J	402	NAI	O1N-PN-O5D	3.35	123.32	107.75
4	C	403	NAI	O4B-C1B-C2B	-3.33	$102.0\overline{5}$	106.93
4	А	403	NAI	N3A-C2A-N1A	-3.30	123.51	128.68
4	L	402	NAI	C5B-C4B-C3B	-3.30	102.81	115.18
4	D	402	NAI	O1N-PN-O5D	3.30	123.06	107.75



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	401	SFX	O5-C3-C2	3.29	110.44	105.18
4	Н	402	NAI	O3D-C3D-C4D	3.27	120.50	111.05
7	L	406	GOL	O1-C1-C2	-3.27	94.52	110.20
4	Н	402	NAI	C2D-C1D-N1N	3.26	121.47	113.30
4	Е	402	NAI	C3B-C2B-C1B	-3.24	96.10	100.98
4	F	403	NAI	O3B-C3B-C4B	3.22	120.37	111.05
4	Κ	402	NAI	O4B-C1B-C2B	-3.22	102.22	106.93
4	В	403	NAI	PN-O5D-C5D	-3.22	102.82	121.68
4	А	403	NAI	C5A-C6A-N1A	-3.20	113.11	120.35
4	В	403	NAI	C2B-C3B-C4B	3.18	108.82	102.64
4	С	403	NAI	PN-O5D-C5D	-3.17	103.07	121.68
4	Н	402	NAI	O4D-C4D-C5D	3.17	119.81	109.37
4	Κ	402	NAI	PA-O5B-C5B	-3.16	103.16	121.68
4	F	403	NAI	C2D-C3D-C4D	3.15	108.76	102.64
4	F	403	NAI	C4D-O4D-C1D	-3.14	102.54	109.47
4	L	402	NAI	C2A-N1A-C6A	3.11	124.07	118.75
3	Κ	401	OXM	O3-C2-C1	3.11	121.03	113.84
4	D	402	NAI	O2A-PA-O1A	-3.10	96.91	112.24
4	G	402	NAI	C4D-O4D-C1D	-3.10	102.64	109.47
4	L	402	NAI	O4D-C4D-C5D	-3.07	99.27	109.37
4	Ι	403	NAI	PN-O5D-C5D	-3.04	103.85	121.68
4	А	403	NAI	O1N-PN-O5D	3.04	121.84	107.75
4	Ε	402	NAI	O3D-C3D-C4D	3.02	119.78	111.05
4	Н	402	NAI	O4D-C1D-N1N	-3.01	102.16	108.06
7	L	406	GOL	O3-C3-C2	-3.01	95.76	110.20
4	В	403	NAI	O4B-C4B-C3B	-2.97	99.25	105.11
4	L	402	NAI	O3B-C3B-C2B	-2.97	102.23	111.82
4	L	402	NAI	C5D-C4D-C3D	2.96	126.28	115.18
4	Н	402	NAI	C5A-C6A-N6A	2.95	124.84	120.35
4	L	402	NAI	O2D-C2D-C3D	-2.94	102.31	111.82
4	F	403	NAI	C3N-C2N-N1N	-2.94	118.90	123.10
4	G	402	NAI	C3D-C2D-C1D	-2.94	95.84	101.43
4	D	402	NAI	PN-O5D-C5D	-2.93	104.48	121.68
4	L	402	NAI	O5D-C5D-C4D	-2.93	98.92	108.99
4	J	402	NAI	O2A-PA-O1A	-2.93	97.77	112.24
4	Ι	403	NAI	$O4B-\overline{C1B}-C2B$	-2.90	$1\overline{02.69}$	106.93
4	Ε	402	NAI	C3D-C2D-C1D	-2.89	95.93	101.43
4	K	402	NAI	C3D-C2D-C1D	-2.89	95.93	101.43
2	B	401	SFX	C6-O5-C3	2.89	$120.5\overline{5}$	118.62
4	А	403	NAI	PN-O5D-C5D	-2.88	104.77	121.68
4	Ε	402	NAI	C3N-C2N-N1N	-2.88	118.98	123.10
4	G	402	NAI	PN-O5D-C5D	-2.87	104.85	121.68



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	Ι	403	NAI	O4D-C1D-N1N	-2.87	102.45	108.06
4	Е	402	NAI	PN-O5D-C5D	-2.85	104.95	121.68
4	Κ	402	NAI	O5B-C5B-C4B	-2.85	99.19	108.99
4	G	402	NAI	C3N-C7N-N7N	2.83	122.69	117.67
3	J	401	OXM	O3-C2-C1	2.81	120.33	113.84
4	G	402	NAI	C3B-C2B-C1B	-2.80	96.76	100.98
4	В	403	NAI	O5B-C5B-C4B	-2.80	99.36	108.99
4	Κ	402	NAI	C5B-C4B-C3B	-2.77	104.79	115.18
4	Ι	403	NAI	O4D-C4D-C5D	2.77	118.49	109.37
4	G	402	NAI	C5B-C4B-C3B	-2.76	104.85	115.18
2	Ι	401	SFX	O5-C3-C16	2.75	117.15	111.92
4	L	402	NAI	O2B-C2B-C1B	-2.74	100.73	110.85
4	Н	402	NAI	PA-O5B-C5B	-2.74	105.62	121.68
4	А	403	NAI	O2A-PA-O1A	-2.72	98.81	112.24
4	Н	402	NAI	O4D-C1D-C2D	-2.70	100.76	106.64
4	А	403	NAI	C2D-C1D-N1N	2.66	119.98	113.30
4	G	402	NAI	O5B-C5B-C4B	-2.66	99.83	108.99
4	L	402	NAI	O1N-PN-O2N	-2.66	99.10	112.24
2	Ι	401	SFX	C2-C3-C16	-2.65	107.82	112.62
4	Н	402	NAI	O3D-C3D-C2D	-2.64	103.28	111.82
4	F	403	NAI	O5D-C5D-C4D	-2.64	99.91	108.99
4	G	402	NAI	O2B-C2B-C1B	-2.64	101.12	110.85
4	D	402	NAI	C2A-N1A-C6A	2.63	123.25	118.75
4	Н	402	NAI	O3B-C3B-C2B	-2.62	103.36	111.82
4	G	402	NAI	O5D-C5D-C4D	-2.61	100.01	108.99
4	Е	402	NAI	C5D-C4D-C3D	-2.60	105.43	115.18
4	F	403	NAI	PN-O5D-C5D	-2.60	106.43	121.68
2	В	401	SFX	F13-C12-C9	-2.58	107.27	112.93
2	А	401	SFX	C2-C3-C16	-2.57	107.97	112.62
4	К	402	NAI	O2D-C2D-C1D	-2.57	101.43	110.02
4	F	403	NAI	O5B-C5B-C4B	-2.57	100.15	108.99
4	L	402	NAI	C3B-C2B-C1B	-2.56	97.12	100.98
4	С	403	NAI	O7N-C7N-N7N	-2.55	116.91	122.88
4	J	402	NAI	C3D-C2D-C1D	-2.54	96.60	101.43
2	F	401	SFX	C2-C1-N4	-2.53	107.61	111.79
4	D	402	NAI	PA-O5B-C5B	-2.53	106.87	121.68
4	Е	402	NAI	C5B-C4B-C3B	-2.52	105.73	115.18
4	J	402	NAI	C2A-N1A-C6A	2.48	123.00	118.75
4	F	403	NAI	C3N-C7N-N7N	2.45	122.02	117.67
4	Е	402	NAI	PA-O5B-C5B	-2.45	107.33	121.68
4	J	402	NAI	03B-C3B-C4B	2.44	118.09	111.05
4	D	402	NAI	O5B-C5B-C4B	-2.44	100.61	108.99



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	F	401	SFX	O5-C3-C2	2.44	109.07	105.18
4	Е	402	NAI	C3N-C7N-N7N	2.43	121.99	117.67
4	А	403	NAI	C5A-C6A-N6A	2.42	124.04	120.35
4	А	403	NAI	O5B-C5B-C4B	-2.42	100.66	108.99
4	А	403	NAI	O4B-C1B-C2B	2.42	110.46	106.93
4	Ι	403	NAI	C5D-C4D-C3D	-2.39	106.22	115.18
4	J	402	NAI	C5B-C4B-C3B	-2.39	106.23	115.18
2	А	401	SFX	O5-C3-C2	2.38	108.98	105.18
2	Ι	401	SFX	F15-C12-C9	-2.38	107.71	112.93
4	G	402	NAI	O1N-PN-O5D	2.37	118.74	107.75
3	F	402	OXM	O3-C2-C1	2.36	119.28	113.84
4	В	403	NAI	C4A-C5A-N7A	2.36	111.85	109.40
4	Ι	403	NAI	C5B-C4B-C3B	-2.35	106.36	115.18
4	G	402	NAI	O7N-C7N-C3N	-2.34	116.50	120.90
4	А	403	NAI	O4D-C4D-C5D	2.32	117.01	109.37
3	G	401	OXM	O3-C2-C1	2.31	119.19	113.84
4	F	403	NAI	O2D-C2D-C1D	2.31	117.74	110.02
4	J	402	NAI	O5B-PA-O1A	2.31	118.08	109.07
4	J	402	NAI	C5A-C6A-N6A	2.31	123.86	120.35
3	В	402	OXM	O3-C2-C1	2.31	119.17	113.84
4	Н	402	NAI	PN-O5D-C5D	-2.30	108.20	121.68
3	J	401	OXM	O2-C2-C1	-2.30	116.95	122.06
4	Ι	403	NAI	C1D-N1N-C6N	-2.28	115.91	120.83
4	А	403	NAI	O7N-C7N-N7N	-2.27	117.57	122.88
4	А	403	NAI	C3N-C7N-N7N	2.27	121.70	117.67
4	G	402	NAI	PA-O5B-C5B	-2.25	108.49	121.68
4	J	402	NAI	O2D-C2D-C1D	2.25	117.54	110.02
4	В	403	NAI	C2D-C1D-N1N	2.24	118.93	113.30
4	Н	402	NAI	C1D-N1N-C6N	-2.22	116.04	120.83
3	С	402	OXM	O3-C2-C1	2.22	118.97	113.84
4	K	402	NAI	C3N-C2N-N1N	-2.22	119.93	123.10
4	F	403	NAI	O1N-PN-O5D	2.21	118.03	107.75
4	J	402	NAI	C1B-N9A-C4A	-2.21	122.76	126.64
4	J	402	NAI	C3N-C2N-N1N	-2.21	119.95	123.10
4	J	402	NAI	O4B-C4B-C3B	2.20	109.48	105.11
4	A	403	NAI	C2A-N1A-C6A	2.19	122.50	118.75
4	С	403	NAI	C1D-N1N-C6N	-2.18	116.13	120.83
4	J	402	NAI	O7N-C7N-N7N	-2.18	117.78	122.88
4	Е	402	NAI	O5D-PN-O2N	-2.15	100.68	109.07
4	A	403	NAI	O4B-C4B-C5B	-2.14	102.33	109.37
4	K	402	NAI	O3D-C3D-C4D	2.14	117.23	111.05
4	С	403	NAI	C2A-N1A-C6A	2.13	122.40	118.75



Mol	Chain	\mathbf{Res}	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
4	L	402	NAI	O2A-PA-O5B	-2.12	97.90	107.75
4	Н	402	NAI	C2A-N1A-C6A	2.12	122.38	118.75
4	D	402	NAI	C4D-O4D-C1D	-2.11	104.82	109.47
5	Κ	403	BTB	O1-C1-C2	-2.09	105.72	111.44
4	С	403	NAI	C3D-C2D-C1D	-2.09	97.46	101.43
2	F	401	SFX	F14-C12-C9	-2.08	108.35	112.93
4	А	403	NAI	O4B-C4B-C3B	2.08	109.23	105.11
4	Κ	402	NAI	C3B-C2B-C1B	-2.07	97.86	100.98
4	А	403	NAI	C1D-N1N-C6N	-2.07	116.37	120.83
4	G	402	NAI	C1D-N1N-C6N	-2.06	116.38	120.83
4	С	403	NAI	O2B-C2B-C3B	-2.06	105.16	111.82
4	Н	402	NAI	C5A-C6A-N1A	-2.06	115.69	120.35
3	D	401	OXM	O3-C2-C1	2.06	118.60	113.84
4	В	403	NAI	C5B-C4B-C3B	2.03	122.80	115.18
4	D	402	NAI	C5B-C4B-C3B	-2.03	107.57	115.18
4	L	402	NAI	C5A-C6A-N1A	-2.03	115.76	120.35
5	С	404	BTB	O6-C6-C5	-2.03	102.79	111.19
4	G	402	NAI	O3D-C3D-C4D	2.02	116.89	111.05
4	А	403	NAI	N6A-C6A-N1A	2.02	122.76	118.57
4	F	403	NAI	C5B-C4B-C3B	-2.01	107.64	115.18
4	G	402	NAI	O2A-PA-O5B	2.00	117.05	107.75
4	D	402	NAI	C3N-C2N-N1N	-2.00	120.24	123.10

There are no chirality outliers.

All (219) torsion outliers are listed below	w:
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Mol	Chain	Res	Type	Atoms
2	А	401	SFX	C2-C3-O5-C6
2	А	401	SFX	C16-C3-O5-C6
2	А	401	SFX	C1-C2-C3-O5
2	А	401	SFX	C1-C2-C3-C16
2	А	401	SFX	C17-C16-C3-C2
2	А	401	SFX	C21-C16-C3-C2
2	А	401	SFX	N4-C1-C2-C3
2	В	401	SFX	C17-C16-C3-C2
2	В	401	SFX	C21-C16-C3-C2
2	С	401	SFX	C2-C3-O5-C6
2	С	401	SFX	C1-C2-C3-O5
2	С	401	SFX	C1-C2-C3-C16
2	С	401	SFX	C17-C16-C3-C2
2	С	401	SFX	C21-C16-C3-C2
2	С	401	SFX	N4-C1-C2-C3



Mol	Chain	Res	Type	Atoms
2	F	401	SFX	C2-C3-O5-C6
2	F	401	SFX	C16-C3-O5-C6
2	F	401	SFX	C1-C2-C3-O5
2	F	401	SFX	C1-C2-C3-C16
2	F	401	SFX	C2-C1-N4-C22
2	Ι	401	SFX	C16-C3-O5-C6
2	Ι	401	SFX	C1-C2-C3-C16
2	Ι	401	SFX	N4-C1-C2-C3
3	Ι	402	OXM	N1-C1-C2-O3
4	В	403	NAI	C5B-O5B-PA-O1A
4	Е	402	NAI	C5D-O5D-PN-O3
4	Е	402	NAI	C5D-O5D-PN-O2N
4	G	402	NAI	C5B-O5B-PA-O3
4	J	402	NAI	C5B-O5B-PA-O3
4	K	402	NAI	C5B-O5B-PA-O3
4	L	402	NAI	C5B-O5B-PA-O3
4	L	402	NAI	C5D-O5D-PN-O2N
5	А	404	BTB	O1-C1-C2-C3
5	А	404	BTB	O1-C1-C2-C4
5	А	404	BTB	O1-C1-C2-N
5	А	404	BTB	C3-C2-C4-O4
5	С	404	BTB	O1-C1-C2-C3
5	С	404	BTB	O1-C1-C2-C4
5	С	404	BTB	O1-C1-C2-N
5	С	404	BTB	C1-C2-C4-O4
5	С	404	BTB	C3-C2-C4-O4
5	С	404	BTB	N-C2-C4-O4
5	F	404	BTB	O1-C1-C2-C3
5	F	404	BTB	O1-C1-C2-C4
5	F	404	BTB	O1-C1-C2-N
5	G	403	BTB	C1-C2-C4-O4
5	G	403	BTB	C3-C2-C4-O4
5	G	403	BTB	N-C2-C4-O4
5	G	403	BTB	C1-C2-N-C5
5	G	403	BTB	C1-C2-N-C7
5	G	403	BTB	C3-C2-N-C5
5	G	403	BTB	C3-C2-N-C7
5	G	403	BTB	C4-C2-N-C5
5	G	403	BTB	C4-C2-N-C7
5	Κ	403	BTB	O1-C1-C2-C3
5	Κ	403	BTB	C1-C2-C3-O3
5	K	403	BTB	C4-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	K	403	BTB	N-C2-C3-O3
5	L	403	BTB	O1-C1-C2-C3
5	L	403	BTB	O1-C1-C2-C4
5	L	403	BTB	O1-C1-C2-N
5	L	403	BTB	C3-C2-C4-O4
5	L	403	BTB	N-C2-C4-O4
7	В	404	GOL	C1-C2-C3-O3
7	С	405	GOL	O1-C1-C2-C3
7	F	405	GOL	C1-C2-C3-O3
7	G	404	GOL	O1-C1-C2-O2
7	G	404	GOL	O1-C1-C2-C3
7	G	404	GOL	C1-C2-C3-O3
7	G	405	GOL	C1-C2-C3-O3
7	Н	403	GOL	O1-C1-C2-C3
7	Н	403	GOL	C1-C2-C3-O3
7	Н	404	GOL	O1-C1-C2-O2
7	Н	404	GOL	O1-C1-C2-C3
7	Н	404	GOL	C1-C2-C3-O3
7	J	403	GOL	O1-C1-C2-C3
7	J	403	GOL	C1-C2-C3-O3
7	L	404	GOL	O1-C1-C2-C3
4	В	403	NAI	C3B-C4B-C5B-O5B
4	L	402	NAI	O4D-C4D-C5D-O5D
2	В	401	SFX	C11-C6-O5-C3
8	Н	407	PEG	C1-C2-O2-C3
8	J	407	PEG	C4-C3-O2-C2
2	В	401	SFX	C7-C6-O5-C3
8	В	408	PEG	O1-C1-C2-O2
8	J	406	PEG	O2-C3-C4-O4
5	F	404	BTB	N-C5-C6-O6
7	G	405	GOL	O2-C2-C3-O3
7	J	403	GOL	O2-C2-C3-O3
7	Κ	404	GOL	O1-C1-C2-O2
8	J	407	PEG	O2-C3-C4-O4
2	А	401	SFX	C7-C6-O5-C3
4	E	402	NAI	C2D-C1D-N1N-C2N
4	L	402	NAI	C2D-C1D-N1N-C2N
4	L	402	NAI	C2D-C1D-N1N-C6N
2	Ι	401	SFX	C2-C1-N4-C22
7	C	405	GOL	C1-C2-C3-O3
7	Н	405	GOL	O1-C1-C2-C3
7	Ι	404	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
7	K	404	GOL	O1-C1-C2-C3
7	K	405	GOL	C1-C2-C3-O3
7	L	404	GOL	C1-C2-C3-O3
5	С	404	BTB	N-C5-C6-O6
4	Е	402	NAI	C2D-C1D-N1N-C6N
5	K	403	BTB	N-C7-C8-O8
5	L	403	BTB	N-C5-C6-O6
5	L	403	BTB	N-C7-C8-O8
7	G	404	GOL	O2-C2-C3-O3
7	Н	403	GOL	O1-C1-C2-O2
7	Н	404	GOL	O2-C2-C3-O3
7	J	403	GOL	O1-C1-C2-O2
7	L	404	GOL	O1-C1-C2-O2
4	В	403	NAI	O4B-C4B-C5B-O5B
2	А	401	SFX	C11-C6-O5-C3
5	F	404	BTB	N-C7-C8-O8
8	Н	407	PEG	O1-C1-C2-O2
4	D	402	NAI	C2D-C1D-N1N-C2N
4	Ι	403	NAI	C2D-C1D-N1N-C2N
4	K	402	NAI	C2D-C1D-N1N-C2N
2	С	401	SFX	C11-C6-O5-C3
7	В	404	GOL	O2-C2-C3-O3
7	С	405	GOL	O2-C2-C3-O3
7	F	405	GOL	O2-C2-C3-O3
7	Ι	404	GOL	O1-C1-C2-O2
2	Ι	401	SFX	C1-C2-C3-O5
2	С	401	SFX	C7-C6-O5-C3
2	С	401	SFX	C2-C1-N4-C22
5	А	404	BTB	N-C7-C8-O8
2	В	401	SFX	C17-C16-C3-O5
2	В	401	SFX	C21-C16-C3-O5
7	C	405	GOL	O1-C1-C2-O2
2	F	401	SFX	C11-C6-O5-C3
2	F	401	SFX	C7-C6-O5-C3
4	A	403	NAI	C2D-C1D-N1N-C2N
8	J	406	PEG	C1-C2-O2-C3
5	С	404	BTB	N-C7-C8-O8
8	D	406	PEG	C1-C2-O2-C3
4	G	$40\overline{2}$	NAI	C2D-C1D-N1N-C2N
4	E	402	NAI	O4D-C1D-N1N-C2N
4	Ι	403	NAI	O4D-C1D-N1N-C2N
4	L	402	NAI	C5D-O5D-PN-O3



Mol	Chain	Res	Type	Atoms
7	F	406	GOL	O2-C2-C3-O3
7	G	405	GOL	O1-C1-C2-O2
7	Н	403	GOL	O2-C2-C3-O3
7	K	405	GOL	O2-C2-C3-O3
4	L	402	NAI	PA-O3-PN-O1N
7	F	406	GOL	C1-C2-C3-O3
4	D	402	NAI	O4D-C1D-N1N-C2N
4	Е	402	NAI	O4D-C1D-N1N-C6N
4	K	402	NAI	O4D-C1D-N1N-C2N
4	L	402	NAI	O4D-C1D-N1N-C2N
4	L	402	NAI	O4D-C1D-N1N-C6N
4	В	403	NAI	C2D-C1D-N1N-C2N
4	G	402	NAI	C5B-O5B-PA-O2A
4	L	402	NAI	C5B-O5B-PA-O2A
8	Н	407	PEG	O2-C3-C4-O4
2	В	401	SFX	N4-C1-C2-C3
5	А	404	BTB	C1-C2-C4-O4
5	L	403	BTB	C1-C2-C4-O4
2	F	401	SFX	C17-C16-C3-O5
4	D	402	NAI	C2D-C1D-N1N-C6N
4	Ι	403	NAI	C2D-C1D-N1N-C6N
4	K	402	NAI	C2D-C1D-N1N-C6N
5	А	404	BTB	N-C2-C3-O3
5	С	404	BTB	N-C2-C3-O3
5	F	404	BTB	C1-C2-N-C7
5	F	404	BTB	C3-C2-N-C5
5	F	404	BTB	C4-C2-N-C5
5	K	403	BTB	O1-C1-C2-N
7	Н	405	GOL	O1-C1-C2-O2
7	L	404	GOL	O2-C2-C3-O3
4	А	403	NAI	O4D-C1D-N1N-C2N
4	В	403	NAI	O4D-C1D-N1N-C2N
8	J	406	PEG	C4-C3-O2-C2
4	С	403	NAI	O4B-C4B-C5B-O5B
8	В	408	PEG	C4-C3-O2-C2
4	Н	402	NAI	C2D-C1D-N1N-C2N
2	F	401	SFX	C17-C16-C3-C2
2	F	401	SFX	C21-C16-C3-C2
2	F	401	SFX	C21-C16-C3-O5
4	G	402	NAI	O4D-C1D-N1N-C2N
4	Н	402	NAI	O4D-C1D-N1N-C2N
2	В	401	SFX	C2-C1-N4-C22

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Mol	Chain	Res	Type	Atoms	
4	С	403	NAI	O4D-C1D-N1N-C2N	
4	J	402	NAI	O4D-C1D-N1N-C2N	
8	D	407	PEG	O2-C3-C4-O4	
4	G	402	NAI	O4B-C4B-C5B-O5B	
4	F	403	NAI	O4D-C1D-N1N-C2N	
4	С	403	NAI	C2D-C1D-N1N-C2N	
4	J	402	NAI	O4B-C4B-C5B-O5B	
3	В	402	OXM	N1-C1-C2-O2	
3	Ι	402	OXM	N1-C1-C2-O2	
4	Ι	403	NAI	O4D-C1D-N1N-C6N	
4	А	403	NAI	C2D-C1D-N1N-C6N	
4	Н	402	NAI	C2D-C1D-N1N-C6N	
8	D	407	PEG	C4-C3-O2-C2	
3	Ι	402	OXM	O1-C1-C2-O2	
4	D	402	NAI	O4D-C1D-N1N-C6N	
4	K	402	NAI	O4D-C1D-N1N-C6N	
4	В	403	NAI	C2D-C1D-N1N-C6N	
4	F	403	NAI	C2D-C1D-N1N-C2N	
4	J	402	NAI	C2D-C1D-N1N-C2N	
8	D	407	PEG	C1-C2-O2-C3	
4	G	402	NAI	C2D-C1D-N1N-C6N	
4	А	403	NAI	O4D-C1D-N1N-C6N	
4	G	402	NAI	O4D-C1D-N1N-C6N	
4	А	403	NAI	O4B-C4B-C5B-O5B	
4	В	403	NAI	O4D-C1D-N1N-C6N	
4	А	403	NAI	C5B-O5B-PA-O3	
4	D	402	NAI	O4B-C4B-C5B-O5B	
4	Е	402	NAI	O4B-C4B-C5B-O5B	
4	F	403	NAI	O4B-C4B-C5B-O5B	
4	Ι	403	NAI	O4B-C4B-C5B-O5B	
4	L	402	NAI	O4B-C4B-C5B-O5B	
4	L	402	NAI	C2N-C3N-C7N-N7N	
4	Н	402	NAI	O4B-C4B-C5B-O5B	
4	К	402	NAI	O4B-C4B-C5B-O5B	
5	K	403	BTB	O1-C1-C2-C4	
4	L	402	NAI	C3D-C4D-C5D-O5D	

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There are no ring outliers.

42 monomers are involved in 125 short contacts:

2 C 401 SFX 4 0	Mol	Chain	Res	Type	Clashes	Symm-Clashes
	2	С	401	SFX	4	0



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	401	SFX	12	0
4	D	402	NAI	3	0
4	L	402	NAI	12	0
4	С	403	NAI	3	0
5	L	403	BTB	4	0
7	L	406	GOL	2	0
7	В	404	GOL	1	0
5	G	403	BTB	2	0
7	F	405	GOL	1	0
4	Ι	403	NAI	2	0
3	Ι	402	OXM	1	0
4	Н	402	NAI	3	0
7	Н	404	GOL	1	0
4	J	402	NAI	2	0
8	Н	407	PEG	1	0
3	L	401	OXM	4	0
8	J	407	PEG	1	0
4	F	403	NAI	2	0
3	А	402	OXM	2	0
2	А	401	SFX	8	0
5	K	403	BTB	1	0
4	G	402	NAI	1	0
3	K	401	OXM	1	0
5	F	404	BTB	5	0
4	K	402	NAI	2	0
4	В	403	NAI	6	0
7	Ι	404	GOL	1	0
7	L	404	GOL	1	0
2	Ι	401	SFX	7	0
5	A	404	BTB	2	0
3	D	401	OXM	1	0
8	E	403	PEG	1	0
3	F	402	OXM	4	0
3	В	402	OXM	1	0
5	С	404	BTB	4	0
3	J	401	OXM	1	0
2	F	401	SFX	11	0
4	A	403	NAI	5	0
8	J	406	PEG	2	0
4	E	402	NAI	1	0
7	K	405	GOL	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,



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
















































































































5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	# RSRZ >	>2	$OWAB(Å^2)$	Q < 0.9
1	А	333/349~(95%)	0.90	18 (5%) 32	34	29, 40, 62, 78	1 (0%)
1	В	333/349~(95%)	0.79	10 (3%) 52	54	29, 39, 61, 83	0
1	С	334/349~(95%)	0.80	18 (5%) 32	34	17, 36, 60, 85	2 (0%)
1	D	332/349~(95%)	0.84	20 (6%) 29	30	26, 39, 57, 77	2(0%)
1	Ε	332/349~(95%)	0.93	25 (7%) 22	23	29, 40, 65, 86	0
1	F	334/349~(95%)	0.89	20 (5%) 29	30	28, 38, 59, 78	0
1	G	333/349~(95%)	0.84	6 (1%) 67	69	29, 39, 58, 72	0
1	Н	334/349~(95%)	0.97	16 (4%) 36	38	20, 43, 61, 80	2(0%)
1	Ι	333/349~(95%)	0.78	12 (3%) 46	48	27, 37, 57, 82	0
1	J	332/349~(95%)	0.96	13 (3%) 44	45	32, 43, 59, 78	2(0%)
1	Κ	334/349~(95%)	1.07	27 (8%) 19	21	30, 43, 69, 83	0
1	L	334/349~(95%)	1.39	61 (18%) 4	4	35, 50, 73, 91	4 (1%)
All	All	3998/4188~(95%)	0.93	246 (6%) 28	28	17, 41, 64, 91	13 (0%)

All (246) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	16	ALA	5.3
1	С	16	ALA	4.8
1	D	227	TRP	4.6
1	L	227	TRP	4.4
1	J	227	TRP	4.4
1	Н	227	TRP	4.4
1	G	227	TRP	4.1
1	L	150	LEU	4.0
1	F	227	TRP	4.0
1	L	120	ILE	3.9
1	Е	119	PHE	3.9



Mol	Chain	Res	Type	RSRZ
1	K	333	LEU	3.8
1	L	333	LEU	3.8
1	L	324	TRP	3.8
1	А	1	ALA	3.8
1	Ι	119	PHE	3.7
1	K	16	ALA	3.7
1	Е	2	THR	3.6
1	D	119	PHE	3.6
1	L	17	THR	3.5
1	С	19	PRO	3.5
1	J	18	VAL	3.5
1	L	287	VAL	3.3
1	J	332	ASP	3.3
1	Н	119	PHE	3.2
1	D	330	LEU	3.2
1	K	1	ALA	3.2
1	K	235	VAL	3.2
1	В	119	PHE	3.2
1	В	1	ALA	3.2
1	Е	16	ALA	3.2
1	А	3	LEU	3.1
1	D	1	ALA	3.1
1	L	320	ALA	3.1
1	D	17	THR	3.1
1	D	14	GLU	3.1
1	G	323	LEU	3.0
1	L	330	LEU	3.0
1	L	282	GLY	3.0
1	С	18	VAL	3.0
1	K	146	VAL	2.9
1	L	18	VAL	2.9
1	D	16	ALA	2.9
1	В	222	ASN	2.9
1	L	322	THR	2.9
1	E	11	VAL	2.9
1	J	331	LYS	2.9
1	В	17	THR	2.9
1	С	227	TRP	2.8
1	L	123	GLN	2.8
1	L	315	GLN	2.8
1	A	18	VAL	2.8
1	С	120	ILE	2.8



Mol	Chain	Res	Type	RSRZ
1	Е	27	GLY	2.8
1	J	17	THR	2.8
1	K	18	VAL	2.8
1	L	288	PHE	2.7
1	А	20	ASN	2.7
1	F	18	VAL	2.7
1	D	282	GLY	2.7
1	F	17	THR	2.7
1	K	332	ASP	2.7
1	L	313	VAL	2.7
1	В	227	TRP	2.7
1	E	227	TRP	2.7
1	А	177	LYS	2.7
1	L	110	VAL	2.7
1	L	198	VAL	2.7
1	С	17	THR	2.7
1	L	148	TRP	2.7
1	Ι	213	GLU	2.7
1	L	317	LYS	2.6
1	L	328	LYS	2.6
1	Ι	3	LEU	2.6
1	K	323	LEU	2.6
1	L	109	LEU	2.6
1	Е	60	GLY	2.6
1	Ε	303	VAL	2.6
1	Κ	17	THR	2.6
1	K	269	ARG	2.6
1	С	333	LEU	2.6
1	L	208	GLY	2.6
1	А	257	ALA	2.6
1	D	324	TRP	2.6
1	Н	152	GLY	2.5
1	С	269[A]	ARG	2.5
1	L	327	GLN	2.5
1	L	316	LEU	2.5
1	G	177	LYS	2.5
1	F	303	VAL	2.5
1	K	241	VAL	2.5
1	L	277	VAL	2.5
1	K	119	PHE	2.5
1	L	283	ILE	2.5
1	L	114	VAL	2.5



Mol	Chain	Res	Type	RSRZ
1	Е	120	ILE	2.5
1	L	326	ILE	2.5
1	Е	93	VAL	2.5
1	Ι	2	THR	2.5
1	L	275	THR	2.5
1	L	237	SER	2.4
1	Е	8	ILE	2.4
1	Е	3	LEU	2.4
1	F	174	MET	2.4
1	С	175	ALA	2.4
1	F	285	ASN	2.4
1	В	125	VAL	2.4
1	Е	85	VAL	2.4
1	В	282	GLY	2.4
1	С	124	ILE	2.4
1	С	332	ASP	2.4
1	Н	333	LEU	2.4
1	В	2	THR	2.4
1	Е	125	VAL	2.4
1	Н	18	VAL	2.4
1	Ι	273	VAL	2.4
1	L	31	VAL	2.4
1	L	122	PRO	2.4
1	Н	332	ASP	2.4
1	L	284	GLU	2.3
1	Е	333	LEU	2.3
1	Ι	16	ALA	2.3
1	Ι	17	THR	2.3
1	K	2	THR	2.3
1	A	19	PRO	2.3
1	J	303	VAL	2.3
1	K	303	VAL	2.3
1	L	127	TYR	2.3
1	K	120	ILE	2.3
1	F	53	VAL	2.3
1	L	146	VAL	2.3
1	Е	311	ASP	2.3
1	F	311	ASP	2.3
1	C	15	GLU	2.3
1	A	170	PHE	2.3
1	Н	331	LYS	2.3
1	L	145	TYR	2.3



Mol	Chain	Res	Type	RSRZ
1	F	222	ASN	2.3
1	L	222	ASN	2.3
1	K	214	LEU	2.3
1	K	216	PRO	2.3
1	А	277	VAL	2.3
1	С	334	GLU	2.3
1	Н	125	VAL	2.3
1	F	219	GLY	2.3
1	K	227	TRP	2.3
1	F	309	LYS	2.3
1	А	333	LEU	2.3
1	L	107	LEU	2.3
1	А	314	ALA	2.3
1	Ι	314	ALA	2.3
1	J	95	THR	2.3
1	J	185	CYS	2.2
1	К	19	PRO	2.2
1	А	227	TRP	2.2
1	K	170	PHE	2.2
1	L	117	PHE	2.2
1	Е	180	ILE	2.2
1	L	159	ILE	2.2
1	Н	174	MET	2.2
1	L	111	GLN	2.2
1	Е	17	THR	2.2
1	В	16	ALA	2.2
1	F	45	ALA	2.2
1	Κ	237	SER	2.2
1	L	224	SER	2.2
1	E	19	PRO	2.2
1	Ι	303	VAL	2.2
1	L	20	ASN	2.2
1	L	119	PHE	2.2
1	D	315	GLN	2.2
1	L	86	THR	2.2
1	D	325	ASP	2.2
1	Е	10	PRO	2.2
1	А	11	VAL	2.2
1	J	21	ASN	2.2
1	A	17	THR	2.2
1	D	320	ALA	2.2
1	Е	38	SER	2.2



Mol	Chain	Res	Type	RSRZ
1	F	314	ALA	2.2
1	L	274	SER	2.2
1	F	331	LYS	2.2
1	L	332	ASP	2.2
1	Н	185	CYS	2.2
1	L	21	ASN	2.2
1	D	18	VAL	2.2
1	А	295	LEU	2.1
1	Н	330	LEU	2.1
1	L	260	ILE	2.1
1	F	328	LYS	2.1
1	G	17	THR	2.1
1	D	148	TRP	2.1
1	H	324	TRP	2.1
1	L	314	ALA	2.1
1	Κ	10	PRO	2.1
1	K	282	GLY	2.1
1	Н	222	ASN	2.1
1	Κ	226	ASN	2.1
1	J	98	VAL	2.1
1	L	140	VAL	2.1
1	K	225	GLU	2.1
1	В	214	LEU	2.1
1	С	214	LEU	2.1
1	L	143	LEU	2.1
1	L	190	LEU	2.1
1	D	224	SER	2.1
1	D	19	PRO	2.1
1	Е	324	TRP	2.1
1	K	324	TRP	2.1
1	J	158	VAL	2.1
1	L	98	VAL	2.1
1	D	323	LEU	2.1
1	A	2	THR	2.1
1	F	283	ILE	2.1
1	Н	311	ASP	2.1
1	L	321	ASP	2.1
1	Ι	10	PRO	2.1
1	J	174	MET	2.1
1	Н	285	ASN	2.1
1	I	21	ASN	2.1
1	G	14	GLU	2.1



Mol	Chain	Res	Type	RSRZ
1	Ι	13	GLU	2.1
1	Κ	185	CYS	2.1
1	А	325	ASP	2.1
1	Е	332	ASP	2.1
1	С	224	SER	2.1
1	F	173	LEU	2.1
1	D	326	ILE	2.1
1	L	19	PRO	2.0
1	L	307	LYS	2.0
1	D	116	VAL	2.0
1	F	185	CYS	2.0
1	F	230	VAL	2.0
1	С	223	ASP	2.0
1	С	321	ASP	2.0
1	L	319	SER	2.0
1	С	3	LEU	2.0
1	Е	150	LEU	2.0
1	L	294	ILE	2.0
1	А	191	GLY	2.0
1	Н	164	ASN	2.0
1	D	175	ALA	2.0
1	Е	12	ALA	2.0
1	F	287	VAL	2.0
1	G	110	VAL	2.0
1	J	85	VAL	2.0

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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	$B-factors(A^2)$	Q<0.9
2	SFX	В	401	22/22	0.62	0.26	37,46,52,57	22
2	SFX	С	401	22/22	0.62	0.24	46,52,60,66	22
5	BTB	G	403	14/14	0.63	0.21	42,48,56,56	0
5	BTB	А	404	14/14	0.65	0.21	45,48,52,53	14
2	SFX	А	401	22/22	0.65	0.24	46,50,53,54	22
2	SFX	Ι	401	22/22	0.66	0.25	43,52,60,65	22
5	BTB	K	403	14/14	0.67	0.18	43,53,58,61	14
5	BTB	F	404	14/14	0.70	0.17	51,54,62,62	0
5	BTB	L	403	14/14	0.71	0.15	57,62,65,68	0
7	GOL	G	404	6/6	0.71	0.17	61,64,66,68	0
8	PEG	J	407	7/7	0.71	0.16	47,55,64,67	0
2	SFX	F	401	22/22	0.72	0.20	42,51,61,67	22
5	BTB	С	404	14/14	0.73	0.17	37,44,47,48	14
7	GOL	F	406	6/6	0.74	0.15	49,52,55,58	0
8	PEG	D	406	7/7	0.75	0.17	57,61,64,67	0
8	PEG	Н	407	7/7	0.77	0.15	50,54,59,61	0
7	GOL	L	404	6/6	0.78	0.16	$57,\!58,\!60,\!65$	0
7	GOL	Н	403	6/6	0.78	0.14	57,64,66,69	0
7	GOL	Н	404	6/6	0.79	0.14	55,58,59,64	0
7	GOL	K	405	6/6	0.79	0.13	43,47,49,54	0
8	PEG	J	406	7/7	0.79	0.15	51,55,60,60	0
7	GOL	G	405	6/6	0.79	0.13	51,51,52,53	0
8	PEG	В	408	7/7	0.80	0.15	41,49,56,59	0
7	GOL	K	404	6/6	0.80	0.12	51,57,60,63	0
7	GOL	D	403	6/6	0.80	0.14	47,55,56,57	0
7	GOL	В	405	6/6	0.80	0.18	36,41,44,44	0
7	GOL	L	405	6/6	0.80	0.15	57,61,64,64	0
7	GOL	L	406	6/6	0.81	0.17	37,45,52,52	0
7	GOL	Н	406	6/6	0.81	0.13	43,53,56,57	0
8	PEG	D	407	7/7	0.82	0.14	52,54,57,65	0
7	GOL	В	404	6/6	0.82	0.13	39,46,49,58	0
7	GOL	J	403	6/6	0.82	0.15	48,50,52,54	0
7	GOL	Н	405	6/6	0.82	0.13	$50,\!55,\!60,\!62$	0
7	GOL	F	405	6/6	0.83	0.15	44,48,48,48	0
7	GOL	С	405	6/6	0.83	0.14	45,46,47,61	0
7	GOL	Ι	404	6/6	0.83	0.15	40,42,45,47	0
3	OXM	С	402	6/6	0.84	0.15	31,35,42,42	0
8	PEG	Е	403	7/7	0.85	0.13	43,48,52,60	0
3	OXM	K	401	6/6	0.85	0.13	39,40,48,48	0
3	OXM	L	401	6/6	0.86	0.14	43,45,53,53	0
3	OXM	E	401	6/6	0.87	0.11	32,35,40,40	0
3	OXM	Ι	402	6/6	0.87	0.11	29,31,36,36	0
3	OXM	А	402	6/6	0.87	0.13	33,37,42,42	0



onti	nued from	m previoi	is page					
lol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
3	OXM	F	402	6/6	0.88	0.12	30,36,37,43	0
3	OXM	G	401	6/6	0.89	0.10	32,36,41,41	0
3	OXM	J	401	6/6	0.89	0.10	34,36,42,42	0
3	OXM	В	402	6/6	0.90	0.11	35,37,44,44	0
4	NAI	Н	402	44/44	0.91	0.10	27,35,44,50	0
4	NAI	J	402	44/44	0.91	0.10	30,36,46,52	0
4	NAI	K	402	44/44	0.91	0.10	28,36,45,48	0
4	NAI	L	402	44/44	0.91	0.10	$31,\!39,\!51,\!55$	0
3	OXM	D	401	6/6	0.91	0.11	36,38,43,43	0
4	NAI	D	402	44/44	0.91	0.10	27,35,44,48	0
4	NAI	С	403	44/44	0.92	0.09	24,31,39,44	0
6	SO4	В	406	5/5	0.92	0.10	34,38,42,43	0
3	OXM	Н	401	6/6	0.92	0.09	32,40,48,48	0
4	NAI	Е	402	44/44	0.92	0.10	22,34,42,46	0
4	NAI	А	403	44/44	0.93	0.09	28,35,44,47	0
4	NAI	F	403	44/44	0.93	0.09	25,32,40,42	0
4	NAI	G	402	44/44	0.93	0.09	27,34,42,50	0
4	NAI	В	403	44/44	0.93	0.09	25,33,42,46	0
6	SO4	L	408	5/5	0.94	0.09	37,40,42,45	0
4	NAI	Ι	403	44/44	0.94	0.09	24,31,43,45	0
6	SO4	D	405	5/5	0.94	0.09	$27,\!32,\!36,\!39$	0
6	SO4	L	407	5/5	0.95	0.08	38,38,45,47	0
6	SO4	D	404	5/5	0.95	0.07	33,37,38,39	0
6	SO4	С	406	5/5	0.95	0.09	31,32,36,39	0
6	SO4	J	404	5/5	0.95	0.07	32,34,39,42	0
6	SO4	В	407	5/5	0.96	0.07	29,37,40,42	0
6	SO4	А	405	5/5	0.96	0.07	35,36,41,45	0
6	SO4	С	407	5/5	0.96	0.07	$30,\!35,\!36,\!37$	0
6	SO4	J	405	5/5	0.96	0.07	37,39,41,42	0
6	SO4	G	406	5/5	0.97	0.06	32,35,41,42	0

C

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.

