

# Full wwPDB X-ray Structure Validation Report (i)

#### Aug 15, 2023 - 04:49 AM EDT

PDB ID	:	1TG6
Title	:	Crystallography and mutagenesis point to an essential role for the N-terminus
		of human mitochondrial ClpP
Authors	:	Kang, S.G.; Maurizi, M.R.; Thompson, M.; Mueser, T.; Ahvazi, B.
Deposited on	:	2004-05-28
Resolution	:	2.10  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 (i)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.10 Å.

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



Motria	Whole archive	Similar resolution
wietric	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain					
1	А	277	52%	11% ••	34%			
1	В	277	48%	16% ••	34%			
1	С	277	46%	18% ••	34%			
1	D	277	53%	10% ••	34%			
1	Е	277	55%	12% ••	29%			
1	F	277	54%	11% ••	32%			
1	G	277	51%	16% ••	30%			



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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	В	1000	-	Х	-	-
4	GOL	В	1001	-	Х	-	-
4	GOL	С	1002	-	Х	-	-
4	GOL	D	1003	-	Х	-	-
4	GOL	Е	1004	-	Х	-	-
4	GOL	F	1005	-	Х	-	-
5	FME	D	1101	-	-	Х	-
5	FME	D	1102	-	-	Х	-
5	FME	D	1103	-	-	Х	-
5	FME	D	1104	-	-	Х	-
5	FME	D	1106	-	-	Х	-



# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11064 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues		A	toms			ZeroOcc	AltConf	Trace
1	А	184	Total	С	Ν	0	S	0 0		0
-		101	1420	906	243	258	13	Ŭ	Ŭ	Ū
1	В	183	Total	С	Ν	0	$\mathbf{S}$	0	0	0
	D	100	1413	901	242	257	13	0	0	0
1	С	192	Total	С	Ν	0	$\mathbf{S}$	0	0	0
	U	105	1413	901	242	257	13	0	0	0
1	П	18/	Total	С	Ν	0	S	0	0	0
	D	104	1420	906	243	258	13	0	0	0
1	F	106	Total	С	Ν	0	S	0	0	0
		190	1514	962	258	281	13	0	0	0
1	Б	197	Total	С	Ν	0	S	0	0	0
	Г	107	1441	917	247	264	13	0	0	0
1	C	104	Total	С	Ν	0	S	0	0	0
	G	194	1496	951	254	278	13		U	U

• Molecule 1 is a protein called Putative ATP-dependent Clp protease proteolytic subunit.

• Molecule 2 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 4 & 2 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 4 & 2 \end{array}$	0	0
2	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 4 & 2 \end{array}$	0	0
2	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 4 & 2 \end{array}$	0	0
2	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 4 & 2 \end{array}$	0	0
2	G	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  4  2 \end{array}$	0	0

• Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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



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

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



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

• Molecule 5 is N-FORMYLMETHIONINE (three-letter code: FME) (formula:  $C_6H_{11}NO_3S$ ).





Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf
5	Л	1	Total	С	Ν	0	S	0	0
0	D	1	10	6	1	2	1	0	0
5	Л	1	Total	С	Ν	Ο	$\mathbf{S}$	0	0
0	D	T	10	6	1	2	1	0	0
5	Л	1	Total	С	Ν	Ο	$\mathbf{S}$	0	0
0	D	1	10	6	1	2	1	0	0
5	П	1	Total	С	Ν	Ο	$\mathbf{S}$	0	0
0	D		10	6	1	2	1	0	0
5	Л	1	Total	С	Ν	Ο	$\mathbf{S}$	0	0
0	D	1	10	6	1	2	1	0	0
5	5 D	1	Total	С	Ν	Ο	$\mathbf{S}$	0	0
0				6	1	2	1	0	0
5	5 D	D 1	Total	С	N	Ō	S	0	0
0	D	1	10	6	1	2	1		0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	77	Total O 77 77	0	0
6	В	90	Total         O           90         90	0	0
6	С	109	Total O 109 109	0	0
6	D	128	Total O 128 128	0	0
6	Е	132	Total         O           132         132	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	126	Total O 126 126	0	0
6	G	111	Total O 111 111	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Putative ATP-dependent Clp protease proteolytic subunit Chain A: 52% 11% 34% GLN GLN GLN GLY GLY GLU ARG • Molecule 1: Putative ATP-dependent Clp protease proteolytic subunit Chain B: 48% 16% 34% METTER TREATING CONTRACTION OF CONTRACTION AND CONTRACTION OF CONTRACTION OF CONTRACTION OF CONTRACTION AND CONTRACTION OF CONTRACTION OF CONTRACTION OF CONTRACTION AND CONTRACTION OF CO SLU SLN SLN SLY SLY SLU PRO GLN SLY SLV SLU VSP VSP SER • Molecule 1: Putative ATP-dependent Clp protease proteolytic subunit Chain C: 46% 18% 34% GLN GLN GLY GLY GLY GLV ALA

Note EDS was not executed.



# • Molecule 1: Putative ATP-dependent Clp protease proteolytic subunit Chain D: 53% 10% 34% GLU GLN GLY GLY GLY GLV GLU ARG • Molecule 1: Putative ATP-dependent Clp protease proteolytic subunit Chain E: 55% 12% 29% GLU GLN GLN GLY GLY GLV GLU ARG K205 GLU GLU VAL VAL GLU GLU PRO PRO PRO PRO PRO SER SER • Molecule 1: Putative ATP-dependent Clp protease proteolytic subunit Chain F: 54% 32% 11% . . GLU GLN GLY GLY GLY GLY GLV ARG • Molecule 1: Putative ATP-dependent Clp protease proteolytic subunit Chain G: 51% 16% 30% GLU GLN GLY GLY GLY GLY GLU ARG ARG

#### H112 H113 H113 H114 H126 H126 H126 H266 H266



# 4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	C 1 2 1	Depositor	
Cell constants	162.57Å 119.00Å 118.65Å	Deperitor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $130.16^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	20.00 - 2.10	Depositor	
% Data completeness	(Not available) (20.00-2.10)	Depositor	
(in resolution range)	(1000 available) (20.00-2.10)	Depositor	
$\mathrm{R}_{merge}$	(Not available)	Depositor	
$R_{sym}$	(Not available)	Depositor	
Refinement program	CNS 0.9	Depositor	
$R, R_{free}$	0.224 , $0.262$	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	11064	wwPDB-VP	
Average B, all atoms $(Å^2)$	28.0	wwPDB-VP	



# 5 Model quality (i)

# 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FME, EDO, DIO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Chain	Bo	ond lengths	Bond angles		
WIOI	Unain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.53	2/1447~(0.1%)	1.19	10/1959~(0.5%)	
1	В	0.53	3/1439~(0.2%)	0.89	10/1947~(0.5%)	
1	С	0.39	0/1439	0.78	5/1947~(0.3%)	
1	D	0.52	2/1447~(0.1%)	1.15	14/1959~(0.7%)	
1	Ε	0.62	6/1542~(0.4%)	0.95	12/2088~(0.6%)	
1	F	1.14	4/1468~(0.3%)	1.24	17/1987~(0.9%)	
1	G	0.53	1/1524~(0.1%)	0.74	4/2065~(0.2%)	
All	All	0.65	18/10306~(0.2%)	1.01	72/13952~(0.5%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	1
1	В	0	1
1	Ε	0	2
1	F	0	3
1	G	0	3
All	All	0	10

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	6	VAL	C-N	-31.14	0.62	1.34
1	F	7	VAL	N-CA	-23.52	0.99	1.46
1	G	6	VAL	C-N	-13.38	1.03	1.34
1	В	17	TYR	C-N	11.32	1.60	1.34
1	Е	17	TYR	C-N	9.72	1.56	1.34
1	А	6	VAL	C-N	9.57	1.56	1.34



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	Ε	6	VAL	C-N	-8.06	1.15	1.34
1	F	3	ILE	C-N	6.97	1.47	1.34
1	Е	5	ILE	N-CA	-6.58	1.33	1.46
1	Е	4	PRO	N-CA	6.11	1.57	1.47
1	А	4	PRO	N-CA	5.93	1.57	1.47
1	D	4	PRO	N-CA	5.47	1.56	1.47
1	Е	1	PRO	C-N	-5.33	1.21	1.34
1	Е	3	ILE	C-N	5.26	1.44	1.34
1	D	2	LEU	C-N	-5.21	1.22	1.34
1	F	4	PRO	CA-C	-5.17	1.42	1.52
1	В	6	VAL	C-N	-5.16	1.22	1.34
1	В	5	ILE	C-N	-5.05	1.22	1.34

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	F	6	VAL	O-C-N	-28.91	76.45	122.70
1	А	17	TYR	CB-CG-CD2	-24.05	106.57	121.00
1	А	17	TYR	CB-CG-CD1	23.23	134.94	121.00
1	D	17	TYR	CB-CG-CD1	-17.59	110.45	121.00
1	D	17	TYR	CB-CG-CD2	16.41	130.84	121.00
1	F	6	VAL	CA-C-N	15.61	151.55	117.20
1	Е	6	VAL	O-C-N	-15.50	97.90	122.70
1	D	6	VAL	O-C-N	14.60	146.06	122.70
1	А	6	VAL	CA-C-N	-13.64	87.18	117.20
1	D	6	VAL	CA-C-N	-13.60	87.29	117.20
1	В	6	VAL	CA-C-N	-13.43	87.65	117.20
1	А	6	VAL	C-N-CA	-13.22	88.64	121.70
1	А	6	VAL	O-C-N	12.87	143.29	122.70
1	F	7	VAL	N-CA-C	12.32	144.26	111.00
1	В	6	VAL	C-N-CA	-11.79	92.23	121.70
1	Е	4	PRO	CA-N-CD	-11.52	95.37	111.50
1	D	3	ILE	N-CA-C	11.50	142.05	111.00
1	F	3	ILE	N-CA-C	11.22	141.28	111.00
1	D	3	ILE	CA-C-N	10.92	147.68	117.10
1	D	6	VAL	C-N-CA	-10.84	94.61	121.70
1	F	1	PRO	C-N-CA	10.80	148.70	121.70
1	Е	17	TYR	C-N-CA	10.73	148.53	121.70
1	Е	5	ILE	CA-C-N	-10.09	95.00	117.20
1	В	17	TYR	CA-C-N	-10.07	95.05	117.20
1	D	17	TYR	CB-CA-C	-9.79	90.82	110.40
1	F	4	PRO	CA-N-CD	-9.05	98.83	111.50



Mol	Chain	Res	Type	Atoms Z		$Observed(^{o})$	$Ideal(^{o})$
1	Е	6	VAL	CA-C-N	8.54	135.99	117.20
1	С	17	TYR	C-N-CA	8.33	142.53	121.70
1	В	3	ILE	N-CA-C	8.12	132.93	111.00
1	F	2	LEU	C-N-CA	8.10	141.95	121.70
1	В	6	VAL	O-C-N	8.06	135.60	122.70
1	F	1	PRO	CA-C-N	-7.96	99.70	117.20
1	F	2	LEU	CB-CA-C	7.89	125.19	110.20
1	D	3	ILE	O-C-N	-7.86	106.16	121.10
1	Е	17	TYR	O-C-N	-7.76	110.28	122.70
1	F	6	VAL	C-N-CA	7.71	140.96	121.70
1	А	17	TYR	CA-CB-CG	7.62	127.88	113.40
1	F	1	PRO	CB-CA-C	7.53	130.84	112.00
1	F	2	LEU	CA-C-N	-7.32	101.10	117.20
1	G	5	ILE	N-CA-C	-7.28	91.36	111.00
1	G	18	ASP	N-CA-CB	-7.23	97.59	110.60
1	С	17	TYR	CA-C-N	-6.97	101.87	117.20
1	Е	5	ILE	O-C-N	6.91	133.75	122.70
1	G	1	PRO	O-C-N	6.68	133.39	122.70
1	В	17	TYR	O-C-N	6.66	133.36	122.70
1	D	3	ILE	CA-C-O	-6.66	106.11	120.10
1	А	3	ILE	N-CA-C	6.46	128.44	111.00
1	D	17	TYR	CA-C-N	-6.21	103.53	117.20
1	А	3	ILE	CB-CA-C	-6.16	99.29	111.60
1	F	1	PRO	O-C-N	6.07	132.40	122.70
1	D	4	PRO	CA-N-CD	-5.97	103.14	111.50
1	Е	4	PRO	N-CA-C	5.94	127.53	112.10
1	Е	4	PRO	C-N-CA	-5.83	107.12	121.70
1	В	18	ASP	N-CA-CB	-5.82	100.12	110.60
1	В	2	LEU	C-N-CA	5.78	136.16	121.70
1	F	4	PRO	C-N-CA	-5.78	107.24	121.70
1	D	17	TYR	C-N-CA	5.77	136.13	121.70
1	Е	4	PRO	N-CD-CG	5.71	111.77	103.20
1	Е	3	ILE	N-CA-C	5.71	126.42	111.00
1	С	185	LEU	CA-CB-CG	5.55	128.06	115.30
1	F	3	ILE	N-CA-CB	-5.53	98.09	110.80
1	D	3	ILE	N-CA-CB	-5.49	98.18	110.80
1	В	17	TYR	CA-C-O	5.47	131.58	120.10
1	В	3	ILE	N-CA-CB	-5.35	98.50	110.80
1	Е	5	ILE	CA-C-O	5.30	131.23	120.10
1	F	4	PRO	N-CA-CB	5.29	109.66	103.30
1	G	5	ILE	C-N-CA	-5.23	108.63	121.70
1	С	2	LEU	N-CA-C	5.20	125.04	111.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	17	TYR	O-C-N	5.18	130.99	122.70
1	F	18	ASP	N-CA-CB	-5.16	101.31	110.60
1	А	18	ASP	CB-CA-C	5.16	120.71	110.40
1	А	3	ILE	CA-C-N	5.11	131.41	117.10

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	6	VAL	Mainchain
1	В	6	VAL	Mainchain
1	Е	17	TYR	Peptide
1	Е	6	VAL	Mainchain
1	F	2	LEU	Peptide
1	F	6	VAL	Mainchain,Peptide
1	G	5	ILE	Mainchain
1	G	6	VAL	Mainchain,Peptide

## 5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1420	0	1465	50	0
1	В	1413	0	1458	60	0
1	С	1413	0	1458	64	0
1	D	1420	0	1463	67	0
1	Е	1514	0	1550	53	0
1	F	1441	0	1479	68	0
1	G	1496	0	1529	105	0
2	А	6	0	8	1	0
2	В	6	0	8	2	0
2	D	6	0	8	1	0
2	Е	6	0	8	2	0
2	F	6	0	8	1	0
2	G	6	0	8	0	0
3	А	4	0	5	1	0
3	В	8	0	10	2	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	С	8	0	10	1	0
3	D	4	0	5	0	0
3	F	4	0	5	0	0
3	G	4	0	5	0	0
4	В	12	0	8	3	0
4	С	6	0	4	0	0
4	D	6	0	4	2	0
4	Ε	6	0	4	0	0
4	F	6	0	4	1	0
5	D	70	0	70	55	0
6	А	77	0	0	3	0
6	В	90	0	0	4	0
6	С	109	0	0	2	0
6	D	128	0	0	6	0
6	Ε	132	0	0	1	0
6	F	126	0	0	3	0
6	G	111	0	0	5	0
All	All	11064	0	10584	407	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 20.

All (407) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom-2	Interatomic	Clash
Atom-1		distance (Å)	overlap (Å)
1:F:17:TYR:CG	1:G:5:ILE:HD11	1.27	1.66
1:G:5:ILE:HG22	1:G:17:TYR:CE2	1.37	1.58
1:F:17:TYR:CD2	1:G:5:ILE:HD11	1.04	1.55
1:F:17:TYR:CE2	1:G:5:ILE:CD1	1.91	1.51
1:F:17:TYR:CD2	1:G:5:ILE:CD1	1.90	1.49
1:G:5:ILE:CG2	1:G:17:TYR:CE2	1.99	1.44
1:A:6:VAL:CG2	1:A:7:VAL:H	1.03	1.39
1:C:17:TYR:CD1	1:D:5:ILE:HG21	1.58	1.37
1:A:2:LEU:H	1:A:2:LEU:CD2	1.36	1.33
1:F:17:TYR:HD2	1:F:18:ASP:CB	1.42	1.32
1:A:6:VAL:HG23	1:A:7:VAL:N	1.15	1.31
1:F:17:TYR:CZ	1:G:5:ILE:CD1	2.13	1.30
1:F:17:TYR:CE1	1:G:5:ILE:HD12	1.66	1.30
1:A:2:LEU:N	1:A:2:LEU:HD23	1.37	1.28
1:F:17:TYR:CE2	1:G:5:ILE:HD11	1.63	1.22
1:E:6:VAL:O	1:E:7:VAL:CG2	1.88	1.21



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:6:VAL:O	1:E:7:VAL:HG23	1.41	1.20
1:F:17:TYR:CD2	1:F:18:ASP:CB	2.24	1.19
1:B:6:VAL:N	1:B:17:TYR:O	1.74	1.18
1:F:17:TYR:CG	1:G:5:ILE:CD1	2.14	1.18
1:F:17:TYR:HD2	1:F:18:ASP:HB3	0.98	1.14
1:D:2:LEU:HG	1:D:20:TYR:HE2	1.04	1.14
1:D:1:PRO:0	1:D:2:LEU:HB2	1.44	1.12
1:F:17:TYR:CD1	1:G:5:ILE:CD1	2.31	1.12
1:A:42:LEU:HD11	1:B:2:LEU:HG	1.15	1.11
1:F:17:TYR:CE2	1:G:5:ILE:HD13	1.66	1.10
1:F:17:TYR:CD2	1:F:18:ASP:HB2	1.87	1.10
1:G:6:VAL:HG12	1:G:7:VAL:N	1.56	1.09
1:C:6:VAL:HG23	1:C:7:VAL:N	1.67	1.08
1:G:5:ILE:HG21	1:G:17:TYR:CZ	1.89	1.07
1:F:17:TYR:CD1	1:G:5:ILE:HD11	1.88	1.06
1:F:17:TYR:CE1	1:G:5:ILE:CD1	2.32	1.06
1:F:17:TYR:CZ	1:G:5:ILE:HD12	1.83	1.05
5:D:1106:FME:HA	1:G:97:SER:OG	1.57	1.05
1:F:17:TYR:CD2	1:F:18:ASP:HB3	1.88	1.05
1:G:6:VAL:CG1	1:G:7:VAL:N	2.14	1.03
1:F:25:ARG:HH22	1:G:7:VAL:HG22	1.23	1.02
1:C:6:VAL:HG23	1:C:7:VAL:H	1.17	1.01
1:D:2:LEU:CG	1:D:20:TYR:HE2	1.72	1.01
1:D:2:LEU:HG	1:D:20:TYR:CE2	1.93	1.01
1:C:17:TYR:HD1	1:D:5:ILE:CG2	1.73	1.01
1:C:97:SER:OG	5:D:1102:FME:HA	1.62	0.99
1:A:6:VAL:CG2	1:A:7:VAL:N	1.77	0.99
1:D:97:SER:OG	5:D:1103:FME:HA	1.63	0.99
1:G:5:ILE:HG21	1:G:17:TYR:CE2	1.92	0.98
1:A:42:LEU:CD1	1:B:2:LEU:HG	1.94	0.98
1:G:88:CYS:HB3	6:G:914:HOH:O	1.63	0.97
1:F:40:ALA:HA	1:F:76:ILE:HD11	1.47	0.97
1:D:5:ILE:HG13	1:D:6:VAL:N	1.80	0.95
1:D:1:PRO:0	1:D:2:LEU:CB	2.08	0.93
1:F:17:TYR:CE2	1:F:18:ASP:HB2	2.03	0.93
1:G:83:ILE:HD11	1:G:87:ILE:HD11	1.48	0.93
1:F:25:ARG:NH2	1:G:7:VAL:CG2	2.32	0.92
1:C:17:TYR:HD1	1:D:5:ILE:HG21	0.78	0.91
1:G:5:ILE:HG22	1:G:17:TYR:CD2	2.04	0.91
1:F:25:ARG:NH2	1:G:7:VAL:HG22	1.88	0.88
1:G:6:VAL:HG13	1:G:7:VAL:HG23	1.56	0.88



	• • • • • •	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:17:TYR:CD1	1:G:5:ILE:HD12	1.99	0.88
1:D:2:LEU:C	1:D:3:ILE:HG13	1.95	0.87
5:D:1105:FME:HG2	1:F:97:SER:OG	1.75	0.87
1:G:5:ILE:HG22	1:G:17:TYR:HE2	1.08	0.87
1:G:2:LEU:C	1:G:2:LEU:HD23	1.96	0.86
1:B:2:LEU:O	1:B:4:PRO:HD3	1.76	0.84
1:E:103:LEU:HD11	1:E:185:LEU:HD21	1.60	0.84
1:G:2:LEU:HD23	1:G:3:ILE:N	1.93	0.83
1:B:17:TYR:CD2	1:B:18:ASP:N	2.47	0.83
6:A:975:HOH:O	1:B:2:LEU:HD21	1.78	0.83
1:G:2:LEU:C	1:G:2:LEU:CD2	2.47	0.83
1:A:97:SER:OG	5:D:1100:FME:HA	1.79	0.82
1:F:17:TYR:CD2	1:F:18:ASP:N	2.48	0.82
1:C:6:VAL:CG2	1:C:7:VAL:N	2.38	0.82
1:C:17:TYR:CD1	1:D:5:ILE:CG2	2.55	0.82
1:E:17:TYR:HB3	1:E:21:SER:HB2	1.60	0.81
1:A:17:TYR:HD1	1:A:18:ASP:H	1.26	0.81
1:B:17:TYR:HD2	1:B:17:TYR:C	1.84	0.81
1:D:2:LEU:CG	1:D:20:TYR:CE2	2.55	0.81
1:A:5:ILE:HD12	1:G:21:SER:OG	1.81	0.80
1:A:2:LEU:CD2	1:A:2:LEU:N	2.11	0.80
1:G:6:VAL:HG12	1:G:7:VAL:HB	1.64	0.79
1:C:42:LEU:HD21	1:D:2:LEU:C	2.03	0.78
1:G:6:VAL:CG1	1:G:7:VAL:HB	2.14	0.78
1:B:42:LEU:HD11	1:C:4:PRO:HD2	1.67	0.77
1:A:2:LEU:H	1:A:2:LEU:HD23	0.62	0.76
1:D:6:VAL:HG13	1:D:17:TYR:O	1.86	0.76
5:D:1106:FME:HE1	1:G:149:LEU:HD13	1.67	0.76
1:C:6:VAL:CG1	1:C:18:ASP:C	2.54	0.76
1:F:25:ARG:HH22	1:G:7:VAL:CG2	1.93	0.75
1:B:17:TYR:CD2	1:B:17:TYR:C	2.58	0.75
1:A:151:ASN:HD22	1:A:161:LEU:HD21	1.52	0.75
1:A:1:PRO:O	1:A:3:ILE:HG23	1.86	0.74
1:B:41:SER:HB2	1:C:32:MET:HE1	1.67	0.74
1:A:83:ILE:HD11	1:A:87:ILE:HD11	1.70	0.73
1:A:167:ALA:HA	1:A:172:ARG:HH12	1.52	0.72
1:F:161:LEU:O	1:F:165:GLU:HG3	1.89	0.72
1:D:68:GLY:H	5:D:1103:FME:C	2.02	0.72
1:G:6:VAL:HG12	1:G:7:VAL:CA	2.20	0.71
1:D:98:MET:HG2	5:D:1103:FME:HB2	1.72	0.71
1:A:6:VAL:HG23	1:A:7:VAL:H	0.57	0.70



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:G:6:VAL:HG12	1:G:7:VAL:CB	2.21	0.70
1:E:42:LEU:HD11	1:F:3:ILE:HG13	1.74	0.69
1:F:5:ILE:HG13	1:F:6:VAL:N	2.07	0.69
1:G:6:VAL:CG1	1:G:7:VAL:CB	2.71	0.69
1:D:3:ILE:O	1:D:4:PRO:C	2.31	0.69
1:F:42:LEU:HD12	1:F:46:GLN:NE2	2.08	0.69
1:G:6:VAL:HG13	1:G:7:VAL:CG2	2.23	0.69
1:A:151:ASN:ND2	1:A:161:LEU:HD21	2.08	0.68
1:A:98:MET:HG2	5:D:1100:FME:HB2	1.76	0.68
2:A:800:DIO:H2'2	1:G:48:LEU:HD21	1.75	0.68
5:D:1104:FME:HE3	1:E:122:HIS:O	1.94	0.68
1:B:149:LEU:HD13	5:D:1101:FME:HE1	1.76	0.68
1:A:42:LEU:HD11	1:B:2:LEU:CG	2.09	0.67
1:B:3:ILE:HG22	1:B:3:ILE:O	1.95	0.66
1:G:1:PRO:HD2	1:G:2:LEU:HD13	1.75	0.66
1:F:40:ALA:CA	1:F:76:ILE:HD11	2.23	0.66
1:C:98:MET:HG2	5:D:1102:FME:HB2	1.76	0.66
1:D:2:LEU:HD11	1:D:20:TYR:OH	1.97	0.65
1:E:6:VAL:O	1:E:7:VAL:CB	2.17	0.65
1:B:98:MET:HG2	5:D:1101:FME:HB2	1.78	0.65
5:D:1104:FME:HA	1:E:97:SER:HB3	1.79	0.65
1:B:122:HIS:O	5:D:1101:FME:HE2	1.97	0.65
1:D:41:SER:HA	2:E:803:DIO:H21	1.78	0.65
1:F:3:ILE:HD13	1:F:18:ASP:OD1	1.97	0.65
1:F:44:ILE:HG13	1:F:76:ILE:HD13	1.78	0.65
1:C:18:ASP:OD1	1:C:21:SER:OG	2.05	0.65
1:G:54:SER:OG	1:G:57:LYS:HG3	1.97	0.64
1:G:55:ASN:HA	1:G:85:ASN:HD22	1.63	0.64
1:F:3:ILE:HD11	1:F:19:ILE:HG22	1.80	0.64
1:C:6:VAL:HG13	1:C:18:ASP:C	2.19	0.63
1:D:2:LEU:CD1	1:D:20:TYR:CE2	2.82	0.63
1:G:5:ILE:HG21	1:G:17:TYR:OH	1.99	0.63
1:F:25:ARG:NH2	1:G:7:VAL:HG23	2.13	0.62
1:C:68:GLY:H	5:D:1102:FME:C	2.10	0.62
1:C:6:VAL:CG1	1:C:19:ILE:N	2.63	0.62
1:C:42:LEU:HD11	1:D:2:LEU:HA	1.82	0.62
1:D:49:PHE:CE2	1:E:6:VAL:HG12	2.35	0.62
1:G:151:ASN:HD22	1:G:161:LEU:HD21	1.65	0.61
1:C:42:LEU:HD21	1:D:2:LEU:CA	2.30	0.61
1:F:156:HIS:HD2	6:F:1008:HOH:O	1.84	0.61
1:D:2:LEU:HD11	1:D:20:TYR:CZ	2.36	0.61



	1.5	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:B:801:DIO:H22	1:C:114:LEU:HD11	1.81	0.61
1:B:17:TYR:HD2	1:B:18:ASP:N	1.94	0.61
1:E:75:ALA:HB1	1:F:92:VAL:HG12	1.83	0.61
1:G:5:ILE:CG2	1:G:17:TYR:CZ	2.54	0.60
1:E:83:ILE:HD11	1:E:87:ILE:HD11	1.82	0.60
1:C:97:SER:HG	5:D:1102:FME:HA	1.62	0.60
1:C:77:TYR:OH	1:C:156:HIS:HE1	1.85	0.60
6:A:975:HOH:O	1:B:2:LEU:HD11	2.02	0.59
1:B:41:SER:HB3	6:B:1061:HOH:O	2.02	0.59
1:D:2:LEU:HD11	1:D:20:TYR:CE2	2.37	0.59
1:A:77:TYR:OH	1:A:156:HIS:HE1	1.85	0.59
1:E:42:LEU:CD1	1:F:3:ILE:HG13	2.32	0.59
1:A:5:ILE:O	1:G:21:SER:HB3	2.02	0.59
1:C:175:SER:OG	1:C:178:GLU:HG3	2.01	0.59
5:D:1105:FME:HG3	1:F:98:MET:HG2	1.85	0.59
1:E:97:SER:OG	1:E:122:HIS:NE2	2.36	0.58
1:F:77:TYR:OH	1:F:156:HIS:HE1	1.84	0.58
1:D:5:ILE:CG1	1:D:6:VAL:N	2.60	0.58
5:D:1104:FME:HA	1:E:97:SER:CB	2.34	0.58
1:A:32:MET:HG2	3:A:900:EDO:O1	2.03	0.58
5:D:1106:FME:HE3	1:G:122:HIS:O	2.03	0.58
1:C:6:VAL:HG11	1:C:18:ASP:C	2.24	0.58
1:B:83:ILE:HD11	1:B:87:ILE:HD11	1.86	0.58
1:B:48:LEU:HD21	2:B:801:DIO:H2'2	1.85	0.57
1:B:97:SER:HB3	5:D:1101:FME:HA	1.87	0.57
1:B:75:ALA:HB1	1:C:92:VAL:HG12	1.85	0.57
1:A:17:TYR:CD1	1:A:18:ASP:N	2.70	0.57
1:A:6:VAL:HG22	1:A:17:TYR:O	2.04	0.57
1:D:77:TYR:OH	1:D:156:HIS:HE1	1.87	0.57
1:A:92:VAL:HG12	1:G:75:ALA:HB1	1.86	0.57
1:G:112:HIS:CD2	6:G:914:HOH:O	2.57	0.57
5:D:1104:FME:HE1	1:E:149:LEU:HD13	1.87	0.56
1:D:2:LEU:CD1	1:D:20:TYR:HE2	2.17	0.56
1:E:92:VAL:HG13	1:E:114:LEU:HD12	1.87	0.56
1:E:115:PRO:HD3	1:E:189:LEU:O	2.05	0.56
1:F:3:ILE:HG12	1:F:4:PRO:N	2.19	0.56
1:G:156:HIS:HD2	6:G:928:HOH:O	1.87	0.56
1:B:22:ARG:HG2	1:B:22:ARG:HH11	1.70	0.56
1:B:181:GLU:HG3	6:B:1056:HOH:O	2.06	0.56
1:B:77:TYR:OH	1:B:156:HIS:HE1	1.88	0.56
1:B:105:ALA:HA	1:B:156:HIS:CD2	2.40	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:6:VAL:HG11	1:C:19:ILE:HA	1.88	0.56
1:G:189:LEU:HG	1:G:202:LEU:CD2	2.36	0.56
1:A:51:GLN:HG3	1:A:85:ASN:OD1	2.06	0.56
1:B:51:GLN:HG3	1:B:85:ASN:OD1	2.06	0.56
1:F:49:PHE:CE2	1:G:6:VAL:HG21	2.41	0.56
1:A:167:ALA:HA	1:A:172:ARG:NH1	2.21	0.55
1:C:30:CYS:HB3	1:C:32:MET:CE	2.37	0.55
1:D:122:HIS:O	5:D:1103:FME:HE2	2.06	0.55
1:D:140:GLU:O	1:D:143:MET:CG	2.54	0.55
1:C:2:LEU:C	1:C:3:ILE:HG13	2.26	0.55
1:C:180:GLN:HA	1:C:185:LEU:HD22	1.87	0.55
1:C:32:MET:HB3	3:C:903:EDO:O2	2.06	0.55
1:E:88:CYS:SG	1:E:112:HIS:CD2	3.00	0.55
1:F:17:TYR:CZ	1:G:5:ILE:HD13	2.11	0.55
1:G:51:GLN:HG3	1:G:85:ASN:HD21	1.71	0.55
1:A:6:VAL:HG23	1:A:7:VAL:CA	2.22	0.55
6:D:1224:HOH:O	1:E:20:TYR:HE1	1.89	0.55
1:A:20:TYR:OH	1:G:42:LEU:HD22	2.08	0.54
1:A:156:HIS:HD2	6:A:906:HOH:O	1.89	0.54
1:F:17:TYR:CG	1:G:5:ILE:CG1	2.90	0.54
1:D:156:HIS:HD2	6:D:1109:HOH:O	1.90	0.54
1:G:77:TYR:OH	1:G:156:HIS:HE1	1.90	0.54
1:D:128:ALA:HA	1:D:138:GLN:OE1	2.07	0.54
1:G:112:HIS:CE1	1:G:187:LYS:HD2	2.43	0.54
1:B:115:PRO:HD3	1:B:189:LEU:O	2.08	0.54
1:D:177:MET:HG3	6:D:1122:HOH:O	2.07	0.54
1:B:160:SER:OG	1:B:163:VAL:HG23	2.08	0.54
1:E:103:LEU:HD11	1:E:185:LEU:CD2	2.35	0.54
1:F:42:LEU:HD12	1:F:46:GLN:HE21	1.72	0.54
1:F:42:LEU:HD11	1:G:4:PRO:HD2	1.90	0.54
1:G:24:LEU:HD13	1:G:24:LEU:O	2.08	0.54
5:D:1104:FME:CE	1:E:122:HIS:O	2.56	0.53
1:B:68:GLY:H	5:D:1101:FME:C	2.20	0.53
1:D:140:GLU:O	1:D:143:MET:HG3	2.08	0.53
5:D:1105:FME:N	1:F:97:SER:OG	2.41	0.53
1:E:4:PRO:C	1:E:5:ILE:HG22	2.28	0.53
1:B:32:MET:HG2	3:B:901:EDO:O2	2.09	0.53
1:B:143:MET:HE1	6:B:1022:HOH:O	2.09	0.53
1:B:22:ARG:NH1	1:B:25:ARG:HD2	2.24	0.52
1:B:154:ALA:HA	1:B:164:ILE:HD11	1.90	0.52
5:D:1104:FME:HG2	1:E:124:PRO:HB3	1.91	0.52



	A de D	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:G:19:ILE:O	1:G:23:LEU:HD13	2.09	0.52
1:C:51:GLN:HG3	1:C:85:ASN:OD1	2.10	0.52
1:A:44:ILE:O	1:A:48:LEU:HD13	2.08	0.52
1:C:42:LEU:CD2	1:D:2:LEU:C	2.75	0.52
1:G:17:TYR:CD2	1:G:18:ASP:N	2.78	0.52
1:B:17:TYR:CG	1:B:18:ASP:N	2.67	0.52
1:E:189:LEU:HD22	1:E:202:LEU:CD2	2.40	0.52
1:D:68:GLY:N	5:D:1103:FME:O	2.39	0.51
1:G:83:ILE:HD12	1:G:85:ASN:OD1	2.10	0.51
5:D:1106:FME:O	1:G:68:GLY:N	2.38	0.51
1:F:25:ARG:HH21	1:G:7:VAL:HG23	1.75	0.51
1:F:143:MET:SD	1:F:147:LYS:HE3	2.50	0.51
1:D:2:LEU:CD2	1:D:20:TYR:CE2	2.93	0.51
1:E:156:HIS:HD2	6:E:1013:HOH:O	1.93	0.51
5:D:1104:FME:C	1:E:68:GLY:H	2.23	0.51
1:E:19:ILE:O	1:E:23:LEU:HD13	2.10	0.51
1:B:114:LEU:HD21	3:B:902:EDO:H21	1.93	0.51
1:C:112:HIS:CE1	1:C:187:LYS:HE3	2.46	0.51
1:D:5:ILE:HA	1:D:18:ASP:HA	1.93	0.50
1:G:42:LEU:O	1:G:46:GLN:HG3	2.12	0.50
1:F:17:TYR:CG	1:F:18:ASP:N	2.78	0.50
1:G:122:HIS:ND1	1:G:171:ASP:OD1	2.30	0.50
1:C:42:LEU:CD2	1:D:2:LEU:O	2.59	0.50
1:D:6:VAL:N	1:D:17:TYR:O	2.44	0.50
1:F:90:TRP:HB3	2:F:804:DIO:H1'2	1.92	0.50
1:G:6:VAL:HG13	1:G:7:VAL:CB	2.40	0.50
1:E:189:LEU:HD22	1:E:202:LEU:HD22	1.93	0.49
5:D:1105:FME:HB3	6:F:1122:HOH:O	2.12	0.49
1:C:123:GLN:C	5:D:1102:FME:HE2	2.33	0.49
1:B:3:ILE:O	1:B:4:PRO:C	2.49	0.49
1:C:22:ARG:HH11	1:C:25:ARG:HH11	1.59	0.49
1:D:45:ALA:HB1	1:E:19:ILE:HD12	1.94	0.49
5:D:1106:FME:HCN	6:G:1008:HOH:O	2.11	0.49
5:D:1106:FME:C	1:G:68:GLY:O	2.60	0.49
6:D:1144:HOH:O	2:E:803:DIO:H12	2.13	0.49
1:B:2:LEU:O	1:B:4:PRO:CD	2.56	0.49
1:E:189:LEU:CD2	1:E:202:LEU:HD22	2.43	0.49
1:F:17:TYR:OH	1:G:17:TYR:OH	2.31	0.49
1:F:42:LEU:HD11	1:G:4:PRO:CD	2.43	0.49
1:A:1:PRO:O	1:A:2:LEU:C	2.51	0.48
1:E:17:TYR:HB3	1:E:21:SER:CB	2.40	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:C:6:VAL:HG13	1:C:18:ASP:CA	2.44	0.48
1:C:88:CYS:SG	1:C:112:HIS:CD2	3.07	0.48
1:F:113:SER:HB2	1:F:185:LEU:HD22	1.96	0.48
1:G:5:ILE:CG2	1:G:17:TYR:HE2	1.77	0.48
1:G:55:ASN:HA	1:G:85:ASN:ND2	2.28	0.48
1:C:68:GLY:N	5:D:1102:FME:O	2.39	0.47
1:F:83:ILE:HD11	1:F:87:ILE:HD11	1.96	0.47
1:F:49:PHE:CZ	1:G:6:VAL:HG21	2.48	0.47
1:B:5:ILE:HB	1:B:17:TYR:O	2.15	0.47
1:D:177:MET:HG2	6:D:1194:HOH:O	2.14	0.47
1:G:17:TYR:HD2	1:G:18:ASP:N	2.11	0.47
4:B:1001:GOL:O1	1:C:175:SER:HA	2.14	0.47
1:C:42:LEU:HD11	1:D:2:LEU:CA	2.43	0.47
1:F:78:ASP:HB3	1:G:114:LEU:HD13	1.95	0.47
1:E:17:TYR:HB2	1:F:5:ILE:HG12	1.95	0.47
1:A:75:ALA:HB1	1:B:92:VAL:HG12	1.95	0.47
1:B:2:LEU:HD12	1:B:2:LEU:HA	1.64	0.47
1:B:41:SER:HB2	1:C:32:MET:CE	2.39	0.47
4:F:1005:GOL:O1	1:G:175:SER:HA	2.15	0.47
1:D:2:LEU:HD21	1:D:20:TYR:CE2	2.50	0.47
1:E:5:ILE:HG13	1:E:6:VAL:N	2.29	0.47
1:B:22:ARG:HG2	1:B:22:ARG:NH1	2.29	0.47
1:C:30:CYS:HB3	1:C:32:MET:HE3	1.98	0.47
1:C:156:HIS:HD2	6:C:1012:HOH:O	1.98	0.47
1:C:19:ILE:O	1:C:23:LEU:HD13	2.15	0.46
1:E:18:ASP:HB3	1:E:21:SER:HB2	1.97	0.46
1:D:17:TYR:HB3	1:D:18:ASP:HB3	1.96	0.46
1:B:97:SER:HB3	5:D:1101:FME:O	2.15	0.46
1:B:161:LEU:HG	1:B:165:GLU:OE2	2.15	0.46
1:C:30:CYS:HB3	1:C:32:MET:HE2	1.98	0.46
1:D:3:ILE:O	1:D:4:PRO:O	2.33	0.46
1:B:39:VAL:O	1:B:43:VAL:HG23	2.16	0.46
1:B:97:SER:HB3	5:D:1101:FME:C	2.46	0.46
1:E:54:SER:O	1:E:85:ASN:ND2	2.41	0.46
1:G:55:ASN:N	1:G:55:ASN:HD22	2.13	0.46
1:B:189:LEU:HD12	1:B:189:LEU:N	2.31	0.45
1:D:140:GLU:HA	1:D:143:MET:HG2	1.96	0.45
1:F:78:ASP:HB3	1:G:114:LEU:CD1	2.46	0.45
1:A:1:PRO:O	1:A:3:ILE:HD13	2.15	0.45
1:C:42:LEU:HD21	1:D:2:LEU:HA	1.96	0.45
1:C:157:THR:O	1:C:158:LYS:HB2	2.17	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:C:19:ILE:HG23	1:C:20:TYR:CD1	2.51	0.45
1:D:118:ARG:C	1:D:119:ILE:HD12	2.36	0.45
1:D:88:CYS:SG	1:D:112:HIS:NE2	2.90	0.45
1:F:82:TYR:CZ	1:G:192:PRO:HD3	2.52	0.45
1:A:115:PRO:HG3	1:A:190:VAL:HG22	1.98	0.45
1:B:122:HIS:O	5:D:1101:FME:CE	2.63	0.45
1:D:78:ASP:HB3	1:E:114:LEU:HD13	1.98	0.45
1:D:97:SER:HB3	5:D:1103:FME:O	2.17	0.45
1:C:101:LEU:HD23	1:C:101:LEU:C	2.37	0.45
1:B:139:ALA:O	1:B:143:MET:HG2	2.17	0.45
1:C:41:SER:OG	1:D:32:MET:HG3	2.16	0.44
1:G:17:TYR:HB3	1:G:18:ASP:H	1.28	0.44
1:E:24:LEU:C	1:E:24:LEU:HD13	2.37	0.44
1:F:51:GLN:HG3	1:F:85:ASN:OD1	2.18	0.44
1:B:156:HIS:HD2	6:B:1028:HOH:O	1.99	0.44
1:D:123:GLN:C	5:D:1103:FME:HE2	2.38	0.44
1:D:140:GLU:O	1:D:143:MET:HG2	2.17	0.44
1:F:77:TYR:O	1:F:81:GLN:HG2	2.18	0.44
1:G:55:ASN:ND2	1:G:55:ASN:H	2.16	0.44
1:G:120:MET:HA	1:G:172:ARG:O	2.17	0.44
1:A:1:PRO:O	1:A:3:ILE:N	2.51	0.44
1:B:6:VAL:HB	1:B:7:VAL:H	0.89	0.44
5:D:1104:FME:O	1:E:68:GLY:N	2.40	0.44
1:D:97:SER:OG	5:D:1103:FME:CA	2.49	0.44
5:D:1106:FME:CE	1:G:149:LEU:HD13	2.45	0.44
1:E:177:MET:CE	1:E:205:LYS:HB3	2.48	0.44
1:G:151:ASN:ND2	1:G:161:LEU:HD21	2.31	0.44
1:G:28:ILE:HD13	1:G:62:TYR:OH	2.18	0.44
1:G:175:SER:OG	1:G:178:GLU:HG3	2.18	0.44
1:C:6:VAL:HG13	1:C:18:ASP:HA	1.99	0.43
1:G:122:HIS:HB3	1:G:171:ASP:HA	2.00	0.43
1:G:55:ASN:HD22	1:G:55:ASN:C	2.21	0.43
1:C:190:VAL:HG12	1:C:191:HIS:CD2	2.53	0.43
1:C:191:HIS:HB3	1:C:192:PRO:HD2	2.00	0.43
1:A:119:ILE:HD12	1:A:119:ILE:N	2.34	0.43
1:C:30:CYS:CB	1:C:32:MET:HE3	2.48	0.43
1:C:81:GLN:O	1:D:192:PRO:HD2	2.19	0.43
1:E:4:PRO:O	1:E:5:ILE:CB	2.63	0.43
1:C:88:CYS:SG	1:C:90:TRP:NE1	2.91	0.43
1:B:97:SER:HB3	5:D:1101:FME:CA	2.49	0.43
4:B:1001:GOL:H12	6:C:1027:HOH:O	2.19	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:C:127:GLY:O	1:C:128:ALA:HB2	2.19	0.43
1:E:5:ILE:HA	1:E:6:VAL:HG22	1.99	0.43
1:E:17:TYR:CB	1:E:21:SER:HB2	2.41	0.43
1:F:25:ARG:HH21	1:G:7:VAL:CG2	2.25	0.43
1:A:122:HIS:O	5:D:1100:FME:HE2	2.18	0.43
5:D:1106:FME:HB2	1:G:98:MET:HG2	1.99	0.43
1:B:124:PRO:HA	5:D:1101:FME:HG3	2.01	0.42
1:D:51:GLN:HG3	1:D:85:ASN:OD1	2.18	0.42
1:A:1:PRO:O	1:A:3:ILE:CG1	2.67	0.42
1:A:22:ARG:O	1:A:22:ARG:HD3	2.19	0.42
1:C:179:ALA:HB3	1:C:185:LEU:HD11	2.01	0.42
1:G:95:ALA:O	1:G:100:SER:HB3	2.20	0.42
1:A:5:ILE:CD1	1:G:18:ASP:HB3	2.49	0.42
1:D:6:VAL:CG1	1:D:18:ASP:C	2.88	0.42
5:D:1104:FME:N	1:E:122:HIS:NE2	2.68	0.42
5:D:1104:FME:HB2	1:E:98:MET:HG2	2.00	0.42
5:D:1106:FME:CE	1:G:122:HIS:O	2.67	0.42
1:B:17:TYR:CE1	1:C:5:ILE:HG12	2.55	0.42
1:C:48:LEU:HD11	2:D:802:DIO:H22	2.01	0.42
1:C:129:ARG:CZ	1:C:129:ARG:HB2	2.49	0.42
1:E:101:LEU:HD23	1:E:101:LEU:C	2.40	0.42
1:F:44:ILE:HG13	1:F:76:ILE:CD1	2.47	0.42
1:A:157:THR:O	1:A:158:LYS:HB2	2.19	0.42
1:D:119:ILE:HD12	1:D:119:ILE:N	2.35	0.42
1:A:105:ALA:HA	1:A:156:HIS:CD2	2.55	0.42
1:E:97:SER:HB3	1:E:98:MET:H	1.48	0.42
1:C:2:LEU:H	1:C:2:LEU:HG	1.56	0.42
1:G:51:GLN:HG3	1:G:85:ASN:ND2	2.34	0.42
1:B:101:LEU:C	1:B:101:LEU:HD23	2.41	0.41
5:D:1104:FME:HA	1:E:97:SER:OG	2.19	0.41
1:A:115:PRO:CG	1:A:190:VAL:HG22	2.49	0.41
1:A:161:LEU:O	1:A:165:GLU:HG3	2.20	0.41
1:F:148:GLN:NE2	6:F:1082:HOH:O	2.53	0.41
5:D:1105:FME:HG3	1:F:98:MET:SD	2.60	0.41
1:E:77:TYR:OH	1:E:156:HIS:HE1	2.03	0.41
4:D:1003:GOL:O1	1:E:175:SER:HA	2.19	0.41
1:G:24:LEU:HD12	6:G:924:HOH:O	2.19	0.41
1:G:119:ILE:N	1:G:119:ILE:HD12	2.36	0.41
1:A:27:ARG:HG2	1:A:27:ARG:HH11	1.85	0.41
1:A:77:TYR:OH	1:A:156:HIS:CE1	2.71	0.41
1:A:114:LEU:HD23	1:A:114:LEU:HA	1.91	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	$distance (\text{\AA})$	overlap (Å)
1:G:42:LEU:HD13	1:G:42:LEU:HA	1.86	0.41
1:B:54:SER:OG	1:B:57:LYS:HG3	2.21	0.41
1:C:160:SER:OG	1:C:163:VAL:HG23	2.21	0.41
1:D:2:LEU:N	1:D:3:ILE:HG13	2.36	0.41
1:B:114:LEU:N	1:B:114:LEU:HD22	2.35	0.41
1:D:122:HIS:HB3	1:D:171:ASP:HA	2.02	0.41
1:G:55:ASN:N	1:G:55:ASN:ND2	2.68	0.41
1:A:3:ILE:O	1:A:4:PRO:O	2.39	0.41
5:D:1104:FME:C	1:E:68:GLY:O	2.69	0.41
1:E:2:LEU:HD23	1:E:2:LEU:N	2.35	0.41
1:G:6:VAL:CG1	1:G:7:VAL:CA	2.88	0.41
1:B:146:LYS:HE3	1:B:150:TYR:OH	2.21	0.40
1:D:122:HIS:O	5:D:1103:FME:CE	2.69	0.40
1:G:19:ILE:HG23	1:G:20:TYR:N	2.36	0.40
1:E:3:ILE:H	1:E:3:ILE:HG13	1.61	0.40
1:E:175:SER:OG	1:E:178:GLU:HG3	2.20	0.40
1:B:175:SER:HA	4:B:1000:GOL:O1	2.21	0.40
1:D:141:GLU:OE2	4:D:1003:GOL:C3	2.70	0.40
5:D:1103:FME:HCN	6:D:1208:HOH:O	2.21	0.40
1:F:17:TYR:O	1:F:18:ASP:O	2.39	0.40
1:D:24:LEU:HD11	1:D:49:PHE:CE2	2.57	0.40
1:D:35:ILE:O	1:D:68:GLY:HA3	2.21	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	Percentiles
1	А	180/277~(65%)	172 (96%)	4 (2%)	4 (2%)	6 2
1	В	179/277~(65%)	170 (95%)	5(3%)	4 (2%)	6 2
1	С	179/277~(65%)	172 (96%)	5 (3%)	2(1%)	14 9



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	180/277~(65%)	174 (97%)	2(1%)	4(2%)	6 2
1	Е	192/277~(69%)	186~(97%)	5(3%)	1 (0%)	29 26
1	F	183/277~(66%)	174 (95%)	6 (3%)	3~(2%)	9 5
1	G	190/277~(69%)	181 (95%)	8 (4%)	1 (0%)	29 26
All	All	1283/1939~(66%)	1229 (96%)	35~(3%)	19~(2%)	10 5

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	2	LEU
1	А	4	PRO
1	В	2	LEU
1	В	3	ILE
1	С	18	ASP
1	D	2	LEU
1	D	3	ILE
1	F	18	ASP
1	G	6	VAL
1	А	6	VAL
1	В	52	SER
1	F	2	LEU
1	А	3	ILE
1	Е	18	ASP
1	В	6	VAL
1	D	6	VAL
1	С	6	VAL
1	D	4	PRO
1	F	6	VAL

#### 5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	А	157/226~(70%)	149 (95%)	8 (5%)	24 22	



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	В	156/226~(69%)	148~(95%)	8 (5%)	24 22
1	С	156/226~(69%)	146~(94%)	10 (6%)	17 14
1	D	157/226~(70%)	150~(96%)	7~(4%)	27 27
1	Ε	168/226~(74%)	159~(95%)	9~(5%)	22 20
1	F	159/226~(70%)	151~(95%)	8 (5%)	24 23
1	G	166/226~(74%)	158~(95%)	8 (5%)	25 24
All	All	1119/1582~(71%)	1061 (95%)	58 (5%)	23 21

Continued from previous page...

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	2	LEU
1	А	3	ILE
1	А	5	ILE
1	А	17	TYR
1	А	18	ASP
1	А	22	ARG
1	А	25	ARG
1	А	122	HIS
1	В	2	LEU
1	В	3	ILE
1	В	6	VAL
1	В	17	TYR
1	В	18	ASP
1	В	22	ARG
1	В	122	HIS
1	В	177	MET
1	С	1	PRO
1	С	2	LEU
1	С	18	ASP
1	С	24	LEU
1	С	26	GLU
1	С	97	SER
1	С	122	HIS
1	С	161	LEU
1	C	172	ARG
1	С	185	LEU
1	D	3	ILE
1	D	4	PRO
1	D	5	ILE



Mol	Chain	Res	Type
1	D	18	ASP
1	D	97	SER
1	D	122	HIS
1	D	172	ARG
1	Е	1	PRO
1	Е	2	LEU
1	Е	4	PRO
1	Е	5	ILE
1	Е	6	VAL
1	Е	19	ILE
1	Е	22	ARG
1	Е	122	HIS
1	Е	142	ILE
1	F	2	LEU
1	F	3	ILE
1	F	4	PRO
1	F	5	ILE
1	F	6	VAL
1	F	42	LEU
1	F	97	SER
1	F	122	HIS
1	G	2	LEU
1	G	5	ILE
1	G	18	ASP
1	G	32	MET
1	G	42	LEU
1	G	55	ASN
1	G	85	ASN
1	G	122	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	51	GLN
1	А	81	GLN
1	А	148	GLN
1	А	151	ASN
1	А	156	HIS
1	В	51	GLN
1	В	148	GLN
1	В	151	ASN
1	В	156	HIS



	ů		
Mol	Chain	Res	Type
1	В	180	GLN
1	С	112	HIS
1	С	148	GLN
1	С	156	HIS
1	С	191	HIS
1	D	156	HIS
1	Е	112	HIS
1	Е	148	GLN
1	Е	156	HIS
1	F	46	GLN
1	F	112	HIS
1	F	148	GLN
1	F	156	HIS
1	F	180	GLN
1	F	191	HIS
1	G	51	GLN
1	G	55	ASN
1	G	85	ASN
1	G	112	HIS
1	G	148	GLN
1	G	151	ASN
1	G	156	HIS
1	G	194	GLN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

27 ligands are modelled in this entry.



1TG6

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	B	Bond lengths Bond ang		gles		
WIOI	туре	Ullalli	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
4	GOL	В	1000	-	$5,\!5,\!5$	3.80	3 (60%)	$5,\!5,\!5$	<mark>5.55</mark>	2 (40%)
3	EDO	В	901	-	3,3,3	1.05	0	2,2,2	0.29	0
4	GOL	F	1005	-	$5,\!5,\!5$	3.67	3(60%)	$5,\!5,\!5$	<b>5.56</b>	2(40%)
5	FME	D	1103	-	8,9,10	1.09	1 (12%)	7,9,11	1.63	1 (14%)
2	DIO	F	804	-	6,6,6	1.66	1 (16%)	6,6,6	0.43	0
3	EDO	D	905	-	3,3,3	1.07	0	2,2,2	0.26	0
5	FME	D	1106	-	8,9,10	1.14	1 (12%)	7,9,11	1.60	2 (28%)
4	GOL	Е	1004	-	5,5,5	<mark>3.92</mark>	3 (60%)	$5,\!5,\!5$	<mark>5.60</mark>	2 (40%)
4	GOL	В	1001	-	5,5,5	<mark>3.90</mark>	3 (60%)	$5,\!5,\!5$	<mark>5.55</mark>	2 (40%)
3	EDO	В	902	-	3,3,3	1.07	0	2,2,2	0.29	0
3	EDO	F	906	-	3,3,3	1.09	0	2,2,2	0.25	0
2	DIO	Е	803	-	6,6,6	1.73	1 (16%)	$6,\!6,\!6$	0.43	0
5	FME	D	1104	-	8,9,10	0.97	0	7,9,11	1.75	1 (14%)
2	DIO	D	802	-	6,6,6	1.66	1 (16%)	6,6,6	0.45	0
5	FME	D	1102	-	8,9,10	1.11	1 (12%)	7,9,11	2.01	2 (28%)
5	FME	D	1105	-	8,9,10	0.90	0	7,9,11	1.77	1 (14%)
3	EDO	G	907	-	3,3,3	1.05	0	2,2,2	0.24	0
5	FME	D	1100	-	8,9,10	1.03	0	7, 9, 11	1.79	1 (14%)
4	GOL	D	1003	-	$5,\!5,\!5$	<mark>3.83</mark>	3 (60%)	$5,\!5,\!5$	<mark>5.56</mark>	2 (40%)
3	EDO	С	904	-	3,3,3	1.02	0	2,2,2	0.23	0
3	EDO	А	900	-	3,3,3	1.09	0	$2,\!2,\!2$	0.29	0
5	FME	D	1101	-	8,9,10	0.88	0	7, 9, 11	1.98	1 (14%)
2	DIO	G	805	-	$6,\!6,\!6$	1.66	1 (16%)	$6,\!6,\!6$	0.42	0
3	EDO	С	903	-	3,3,3	1.08	0	2,2,2	0.29	0
2	DIO	В	801	-	6,6,6	1.66	1 (16%)	6,6,6	0.44	0
2	DIO	А	800	-	6,6,6	1.69	1 (16%)	6,6,6	0.45	0
4	GOL	С	1002	-	5,5,5	<mark>3.75</mark>	3 (60%)	5, 5, 5	<mark>5.56</mark>	2 (40%)

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.



1	TCG	
T	1G0	

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	В	1000	-	-	2/4/4/4	-
3	EDO	В	901	-	-	0/1/1/1	-
4	GOL	F	1005	-	-	2/4/4/4	-
5	FME	D	1103	-	-	2/7/9/11	-
2	DIO	F	804	-	-	-	0/1/1/1
3	EDO	D	905	-	-	0/1/1/1	-
5	FME	D	1106	-	-	2/7/9/11	-
4	GOL	Е	1004	-	-	2/4/4/4	-
4	GOL	В	1001	-	-	2/4/4/4	-
3	EDO	В	902	-	-	0/1/1/1	-
3	EDO	F	906	-	-	1/1/1/1	-
2	DIO	Е	803	-	-	-	0/1/1/1
5	FME	D	1104	-	-	1/7/9/11	-
2	DIO	D	802	-	-	-	0/1/1/1
5	FME	D	1102	-	-	2/7/9/11	-
5	FME	D	1105	-	-	2/7/9/11	-
3	EDO	G	907	-	-	0/1/1/1	-
5	FME	D	1100	-	-	1/7/9/11	-
4	GOL	D	1003	-	-	2/4/4/4	-
3	EDO	С	904	-	-	0/1/1/1	-
3	EDO	А	900	-	-	0/1/1/1	-
5	FME	D	1101	-	-	2/7/9/11	-
2	DIO	G	805	-	-	-	0/1/1/1
3	EDO	С	903	-	-	0/1/1/1	-
2	DIO	В	801	-	-	-	0/1/1/1
2	DIO	A	800	-	-	_	0/1/1/1
4	GOL	С	1002	-	-	2/4/4/4	-

'-' means no outliers of that kind were identified.

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Е	1004	GOL	C3-C2	-7.67	1.20	1.51
4	D	1003	GOL	C3-C2	-7.63	1.20	1.51
4	В	1001	GOL	C3-C2	-7.61	1.20	1.51
4	В	1000	GOL	C3-C2	-7.40	1.21	1.51
4	С	1002	GOL	C3-C2	-7.36	1.21	1.51
4	F	1005	GOL	C3-C2	-7.15	1.22	1.51
2	Е	803	DIO	O1-C2	-3.96	1.26	1.42
2	А	800	DIO	O1-C2	-3.82	1.27	1.42



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	802	DIO	O1-C2	-3.77	1.27	1.42
2	F	804	DIO	O1-C2	-3.75	1.27	1.42
2	В	801	DIO	O1-C2	-3.75	1.27	1.42
2	G	805	DIO	O1-C2	-3.74	1.27	1.42
4	В	1000	GOL	O2-C2	-3.21	1.33	1.43
4	Е	1004	GOL	C1-C2	-3.07	1.39	1.51
4	В	1001	GOL	C1-C2	-3.06	1.39	1.51
4	С	1002	GOL	O2-C2	-2.98	1.34	1.43
4	F	1005	GOL	C1-C2	-2.96	1.39	1.51
4	В	1001	GOL	O2-C2	-2.89	1.34	1.43
4	Е	1004	GOL	O2-C2	-2.85	1.34	1.43
4	F	1005	GOL	O2-C2	-2.72	1.35	1.43
4	D	1003	GOL	C1-C2	-2.71	1.40	1.51
4	D	1003	GOL	O2-C2	-2.68	1.35	1.43
4	В	1000	GOL	C1-C2	-2.65	1.40	1.51
4	С	1002	GOL	C1-C2	-2.64	1.40	1.51
5	D	1103	FME	CB-CA	-2.30	1.49	1.53
5	D	1106	FME	CB-CG	2.09	1.59	1.51
5	D	1102	FME	CA-N	-2.02	1.43	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	Е	1004	GOL	O3-C3-C2	10.56	160.82	110.20
4	D	1003	GOL	O3-C3-C2	10.50	160.53	110.20
4	В	1001	GOL	O3-C3-C2	10.49	160.48	110.20
4	С	1002	GOL	O3-C3-C2	10.49	160.47	110.20
4	В	1000	GOL	O3-C3-C2	10.44	160.27	110.20
4	F	1005	GOL	O3-C3-C2	10.39	160.01	110.20
4	F	1005	GOL	O2-C2-C3	6.81	139.14	109.12
4	В	1000	GOL	O2-C2-C3	6.69	138.58	109.12
4	Е	1004	GOL	O2-C2-C3	6.68	138.54	109.12
4	С	1002	GOL	O2-C2-C3	6.64	138.37	109.12
4	D	1003	GOL	O2-C2-C3	6.62	138.28	109.12
4	В	1001	GOL	O2-C2-C3	6.61	138.25	109.12
5	D	1101	FME	CA-N-CN	4.29	129.41	122.82
5	D	1102	FME	CA-N-CN	3.94	128.89	122.82
5	D	1105	FME	CA-N-CN	3.94	128.89	122.82
5	D	1100	FME	CA-N-CN	3.81	128.67	122.82
5	D	1104	FME	CA-N-CN	3.78	128.63	122.82
5	D	1103	FME	CA-N-CN	3.05	127.51	122.82
5	D	1106	FME	CA-N-CN	2.99	127.42	122.82



Control	continued from precious page								
Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$		
5	D	1102	FME	O-C-CA	-2.76	117.55	124.78		
5	D	1106	FME	O-C-CA	-2.14	119.18	124.78		

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	В	1000	GOL	O1-C1-C2-O2
4	В	1000	GOL	C1-C2-C3-O3
4	В	1001	GOL	O1-C1-C2-O2
4	В	1001	GOL	C1-C2-C3-O3
4	С	1002	GOL	C1-C2-C3-O3
4	D	1003	GOL	C1-C2-C3-O3
4	Е	1004	GOL	O1-C1-C2-O2
4	Е	1004	GOL	C1-C2-C3-O3
4	F	1005	GOL	O1-C1-C2-O2
4	F	1005	GOL	C1-C2-C3-O3
5	D	1101	FME	CB-CA-N-CN
5	D	1102	FME	O1-CN-N-CA
5	D	1105	FME	CA-CB-CG-SD
4	С	1002	GOL	O1-C1-C2-O2
4	D	1003	GOL	O1-C1-C2-O2
5	D	1101	FME	O1-CN-N-CA
5	D	1103	FME	O1-CN-N-CA
5	D	1104	FME	O1-CN-N-CA
5	D	1105	FME	O1-CN-N-CA
5	D	1106	FME	O1-CN-N-CA
5	D	1100	FME	CA-CB-CG-SD
5	D	1102	FME	CA-CB-CG-SD
5	D	1103	FME	CB-CA-N-CN
3	F	906	EDO	O1-C1-C2-O2
5	D	1106	FME	CB-CA-N-CN

There are no ring outliers.

20 monomers are involved in 72 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	1000	GOL	1	0
3	В	901	EDO	1	0
4	F	1005	GOL	1	0
5	D	1103	FME	10	0



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Mol	Chain	Res	Type	Clashes	Symm-Clashes					
2	F	804	DIO	1	0					
5	D	1106	FME	9	0					
4	В	1001	GOL	2	0					
3	В	902	EDO	1	0					
2	Е	803	DIO	2	0					
5	D	1104	FME	12	0					
2	D	802	DIO	1	0					
5	D	1102	FME	6	0					
5	D	1105	FME	5	0					
5	D	1100	FME	3	0					
4	D	1003	GOL	2	0					
3	А	900	EDO	1	0					
5	D	1101	FME	10	0					
3	С	903	EDO	1	0					
2	В	801	DIO	2	0					
2	А	800	DIO	1	0					

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	Ε	1
1	G	1
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Ε	6:VAL	С	7:VAL	N	1.15
1	G	6:VAL	С	7:VAL	N	1.03
1	F	6:VAL	С	7:VAL	N	0.62



## 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

#### 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

#### 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

