

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

#### Dec 20, 2023 – 06:59 AM EST

PDB ID	:	1VDV
Title	:	Bovine Milk Xanthine Dehydrogenase Y-700 Bound Form
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Deposited on	:	2004-03-25
Resolution	:	1.98  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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 Å.

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



Motria	Whole archive	Similar resolution				
wietric	$(\# {\rm Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$				
Clashscore	141614	1014 (1.98-1.98)				
Ramachandran outliers	138981	1006 (1.98-1.98)				
Sidechain outliers	138945	1006 (1.98-1.98)				

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	1332	81%	15%	••
1	В	1332	83%	13%	••

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
5	MOS	В	4004	-	-	Х	-
9	ACY	А	5201	-	-	Х	-
9	ACY	В	5202	-	-	Х	-



#### 1VDV

## 2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 22610 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

• Molecule 1 is a protein called Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues		A	toms		ZeroOcc	AltConf	Trace	
1	Δ	1299	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
1	I A		10077	6404	1728	1884	61	0	0	
1	р	1206	Total	С	Ν	Ο	S	0	0	0
1		1290	10054	6391	1724	1878	61	0	0	U

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	1	MET	-	initiating methionine	UNP P80457
В	1	MET	_	initiating methionine	UNP P80457

• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	2	Total Ca 2 2	0	0
2	В	2	Total Ca 2 2	0	0

• Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $Fe_2S_2$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	TotalFeS422	0	0
3	А	1	TotalFeS422	0	0
3	В	1	TotalFeS422	0	0
3	В	1	Total Fe S 4 2 2	0	0

• Molecule 4 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (three-letter code: MTE) (formula:  $C_{10}H_{14}N_5O_6PS_2$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	
4	Λ Λ	1	Total	С	Ν	Ο	Р	$\mathbf{S}$	0	0	
4 A	L	24	10	5	6	1	2	0	0		
4	D	1	Total	С	Ν	0	Р	S	0	0	
4 D		24	10	5	6	1	2		U		

• Molecule 5 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula:  $HMoO_2S$ ).



Mol	Chain	Residues	I	Atom	S		ZeroOcc	AltConf	
5	Δ	1	Total	Mo	0	$\mathbf{S}$	0	0	
	Π	T	4	1	2	1	0	0	
5	D	1	Total	Mo	Ο	$\mathbf{S}$	0	0	
5	D	L	4	1	2	1	0	0	

• Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $\rm C_{27}H_{33}N_9O_{15}P_2).$ 





Mol	Chain	Residues		Ate	oms		ZeroOcc	AltConf	
6	Δ	1	Total	С	Ν	Ο	Р	0	0
0 A	L	53	27	9	15	2	0	0	
6	D	1	Total	С	Ν	Ο	Р	0	0
0	D	L	53	27	9	15	2	0	0

• Molecule 7 is 1-[3-CYANO-4-(NEOPENTYLOXY)PHENYL]-1H-PYRAZOLE-4-CARBOX YLIC ACID (three-letter code: YSH) (formula:  $C_{16}H_{17}N_3O_3$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf		
7	А	1	Total 22	C 16	N 3	O 3	0	0



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf		
7	В	1	Total	С	Ν	0	0	0
1	D	T	22	16	3	3	0	0

• Molecule 8 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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



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

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

• Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	А	1086	Total O 1086 1086	0	0
10	В	1033	Total O 1033 1033	0	0



## 3 Residue-property plots (i)

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

Note EDS was not executed.

• Molecule 1: Xanthine dehydrogenase/oxidase





#### G528 LYS ASP ASP LYS LYS LYS LYS CYS GLY K537 R508 R509 <mark>S412</mark> K476 Q473 L52: L44 F723 Y743 P753 . L719 E699 L712 K713 F655 A656 K657 D658 D658 E676 A726 A816 173 K81 K84 H74 D951 L952 T909 A910 F911 R912 <mark>G913</mark> F914 V964 P965 F1132 Y1133 92 <mark>96</mark> 66 Q1284 H1285 T1286 N1287 N1288 N1288 K1172 N1173 N1108 P1109 111<u>9</u> G1 L1316 C1317 V1318 T1319 G1320 G1320 G1321 N1322 K1322 K1325 K1326 K1325



## 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	166.82Å 123.94Å 148.89Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $91.16^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	20.00 - 1.98	Depositor
% Data completeness	(Not available) $(20.00-1.98)$	Depositor
(in resolution range)	(100 available) (20.00 1.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
$R, R_{free}$	0.178 , $0.215$	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22610	wwPDB-VP
Average B, all atoms $(Å^2)$	21.0	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: FAD, GOL, ACY, MTE, MOS, YSH, FES, CA

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

Mal	Chain	Bond	lengths	Bond	angles
		RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.32	0/10298	0.60	0/13939
1	В	0.31	0/10275	0.60	0/13909
All	All	0.32	0/20573	0.60	0/27848

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	10077	0	10076	172	0
1	В	10054	0	10053	155	0
2	А	2	0	0	0	0
2	В	2	0	0	0	0
3	А	8	0	0	1	0
3	В	8	0	0	0	0
4	А	24	0	10	1	0
4	В	24	0	10	1	0
5	А	4	0	0	1	0
5	В	4	0	0	2	0
6	А	53	0	31	4	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	В	53	0	31	3	0
7	А	22	0	16	3	0
7	В	22	0	16	3	0
8	А	66	0	88	8	0
8	В	60	0	80	8	0
9	А	4	0	3	4	0
9	В	4	0	3	4	0
10	А	1086	0	0	9	0
10	В	1033	0	0	7	0
All	All	22610	0	20417	331	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 8.

All (331) 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)
7:B:5102:YSH:N2	7:B:5102:YSH:C1	1.70	1.52
7:A:5101:YSH:N2	7:A:5101:YSH:C1	1.68	1.51
1:A:3:ALA:HB1	1:A:228:ARG:H	1.20	1.06
1:A:537:LYS:HG2	1:A:538:LEU:H	1.28	0.98
1:A:955:PHE:HA	1:A:1145:ASN:HD21	1.30	0.97
1:B:1286:THR:HG22	1:B:1287:ASN:H	1.32	0.94
1:A:439:ARG:HH11	1:A:439:ARG:HB3	1.32	0.93
1:A:131:GLN:HE21	1:A:133:GLU:H	1.14	0.90
1:B:955:PHE:HA	1:B:1145:ASN:HD21	1.36	0.89
1:B:1321:ALA:HB1	1:B:1322:PRO:HD2	1.56	0.87
1:A:1211:LEU:HA	1:A:1221:THR:HG21	1.57	0.86
1:B:404:LEU:HD21	1:B:407:ILE:HD11	1.57	0.86
1:A:36:LEU:HD22	1:A:89:GLU:HG3	1.57	0.84
1:A:3:ALA:HB1	1:A:228:ARG:N	1.93	0.83
1:B:131:GLN:HE21	1:B:133:GLU:H	1.26	0.83
1:B:1088:GLN:HG2	1:B:1133:TYR:CD1	2.15	0.82
1:B:328:ARG:HG2	1:B:328:ARG:HH11	1.45	0.80
1:B:551:LYS:NZ	1:B:551:LYS:HA	1.96	0.80
1:A:719:LEU:HD21	1:A:860:GLU:HG2	1.65	0.79
1:A:358:ILE:HD12	1:A:431:ILE:HG23	1.64	0.78
1:A:718:ASP:HB3	1:A:721:LYS:HE2	1.69	0.75
1:A:537:LYS:HG2	1:A:538:LEU:N	2.03	0.73
1:B:551:LYS:HZ2	1:B:552:HIS:H	1.32	0.73
1:B:36:LEU:HD22	1:B:89:GLU:HG3	1.71	0.73



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:1088:GLN:HG2	1:A:1133:TYR:CD1	2.25	0.72
1:B:551:LYS:HA	1:B:551:LYS:HZ2	1.54	0.70
1:A:1118:MET:O	1:A:1122:GLN:HG2	1.92	0.70
1:B:1286:THR:HG22	1:B:1287:ASN:N	2.05	0.69
1:B:154:ARG:HD3	1:B:1196:GLU:OE2	1.92	0.69
1:B:552:HIS:CE1	1:B:1172:LYS:HZ3	2.09	0.69
1:A:406:SER:C	1:A:407:ILE:HD12	2.13	0.68
1:A:264:ILE:HD11	6:A:3005:FAD:H3B	1.75	0.68
1:B:1078:ALA:HB1	5:B:4004:MOS:O1	1.94	0.68
1:A:217:LEU:O	1:A:220:LYS:HG2	1.93	0.68
1:A:911:PHE:H	9:A:5201:ACY:H3	1.59	0.67
1:A:441:LEU:HB3	1:A:451:GLU:HB2	1.76	0.66
1:B:376:SER:HB3	1:B:379:THR:OG1	1.95	0.66
1:B:719:LEU:HD11	1:B:895:ARG:HB2	1.78	0.66
1:A:948:LYS:HG2	1:A:951:ASP:OD2	1.95	0.65
1:A:154:ARG:HD3	1:A:1196:GLU:OE2	1.96	0.65
1:B:948:LYS:HG2	1:B:951:ASP:OD2	1.97	0.65
1:A:538:LEU:HD12	8:A:5002:GOL:H31	1.77	0.65
1:A:193:PRO:HG2	1:A:560:PHE:CE1	2.32	0.65
1:A:428:GLU:OE2	1:A:1233:GLY:HA3	1.96	0.65
1:B:1312:LYS:O	1:B:1316:LEU:HD13	1.97	0.65
1:A:880:ARG:HD2	1:A:914:PHE:HB3	1.79	0.65
1:B:406:SER:O	1:B:407:ILE:HD12	1.97	0.65
1:A:131:GLN:HE21	1:A:133:GLU:N	1.92	0.64
1:A:439:ARG:HB3	1:A:439:ARG:NH1	2.09	0.64
1:B:551:LYS:HZ2	1:B:552:HIS:N	1.96	0.64
1:B:911:PHE:H	9:B:5202:ACY:H3	1.63	0.64
1:B:719:LEU:HD11	1:B:895:ARG:CB	2.28	0.63
1:A:580:LEU:HD13	1:A:1044:THR:HG23	1.80	0.63
1:A:358:ILE:CD1	1:A:431:ILE:HG23	2.28	0.63
1:A:328:ARG:HG2	1:A:328:ARG:HH11	1.63	0.63
1:A:217:LEU:HD12	1:A:220:LYS:HD3	1.82	0.62
1:A:164:ALA:O	1:A:165:LYS:HB2	2.00	0.61
1:B:1286:THR:CG2	1:B:1287:ASN:H	2.11	0.61
1:A:197:ASN:O	1:A:200:GLU:HG2	2.01	0.61
1:A:788:LEU:HB2	8:A:5011:GOL:H12	1.83	0.60
1:B:757:GLU:HB3	1:B:786:ARG:HE	1.66	0.60
5:B:4004:MOS:MO	5:B:4004:MOS:O2	1.73	0.60
1:B:310:LYS:O	1:B:314:GLU:HG3	2.02	0.59
1:B:911:PHE:N	9:B:5202:ACY:H3	2.16	0.59
1:A:3:ALA:HA	1:A:227:LEU:HD22	1.83	0.59



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:4:ASP:HB3	10:A:5928:HOH:O	2.02	0.59
7:A:5101:YSH:C1	7:A:5101:YSH:C6	2.78	0.59
1:A:439:ARG:HH11	1:A:439:ARG:CB	2.13	0.59
1:A:911:PHE:N	9:A:5201:ACY:H3	2.18	0.59
1:A:328:ARG:HG2	10:A:5679:HOH:O	2.03	0.59
1:B:880:ARG:HD2	1:B:914:PHE:HB3	1.84	0.59
1:B:1318:VAL:HG22	1:B:1321:ALA:HB2	1.85	0.59
1:A:966:ARG:O	1:A:970:GLU:HG3	2.02	0.58
1:B:570:GLU:OE2	1:B:1057:PRO:HG3	2.03	0.58
1:A:3:ALA:HA	1:A:227:LEU:CD2	2.32	0.58
1:A:1010:THR:HG23	7:A:5101:YSH:O22	2.04	0.58
1:A:1203:LEU:HD13	1:A:1270:VAL:HG21	1.85	0.58
1:A:1172:LYS:HG3	8:A:5001:GOL:H31	1.87	0.57
1:B:1289:ASN:O	1:B:1290:THR:HB	2.05	0.57
1:B:372:LEU:HD23	1:B:407:ILE:HG13	1.86	0.57
1:A:241:THR:OG1	1:A:244:GLU:HG3	2.05	0.57
1:A:914:PHE:HA	9:A:5201:ACY:H2	1.87	0.56
1:B:473:GLN:O	1:B:476:LYS:HB2	2.05	0.56
1:B:713:LYS:HD3	1:B:897:THR:HG22	1.88	0.56
1:A:552:HIS:CG	1:A:553:PRO:HD2	2.40	0.56
1:B:346:ALA:HB1	6:B:4005:FAD:H4'	1.86	0.56
1:B:1326:LYS:HG3	10:B:5861:HOH:O	2.04	0.56
1:B:197:ASN:O	1:B:200:GLU:HG2	2.04	0.56
1:B:1287:ASN:O	1:B:1288:ASN:HB2	2.06	0.56
1:A:154:ARG:HD2	10:A:5453:HOH:O	2.06	0.56
1:A:1312:LYS:O	1:A:1316:LEU:HD23	2.06	0.56
1:A:651:ASP:CG	1:A:871:ARG:HH11	2.09	0.55
1:A:433:LYS:HE3	1:A:504:MET:SD	2.46	0.55
1:A:569:LYS:NZ	1:A:569:LYS:HB3	2.21	0.55
1:B:509:ARG:HH11	1:B:509:ARG:HG2	1.72	0.55
1:A:1318:VAL:HB	1:A:1322:PRO:HB3	1.88	0.55
1:B:404:LEU:HD21	1:B:407:ILE:CD1	2.33	0.55
1:B:1323:GLY:O	1:B:1325:CYS:N	2.41	0.54
1:A:1212:HIS:H	1:A:1221:THR:HG22	1.72	0.54
1:B:441:LEU:HB3	1:B:451:GLU:HB2	1.90	0.54
1:A:909:THR:O	9:A:5201:ACY:H1	2.08	0.54
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.08	0.54
1:A:753:PRO:HD3	1:A:816:ALA:HB1	1.90	0.53
1:A:269:LYS:HE3	10:A:6386:HOH:O	2.09	0.53
1:A:97:ARG:NH1	1:A:97:ARG:HB2	2.23	0.53
1:B:1010:THR:HG23	7:B:5102:YSH:O22	2.08	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:87:THR:HG1	1:A:89:GLU:HG2	1.74	0.53
1:B:1312:LYS:HG2	10:B:6326:HOH:O	2.10	0.52
1:B:909:THR:O	9:B:5202:ACY:H1	2.08	0.52
1:A:1322:PRO:C	1:A:1324:ASN:H	2.12	0.52
1:A:473:GLN:O	1:A:476:LYS:HB2	2.09	0.52
1:A:599:TYR:HA	1:B:599:TYR:HA	1.91	0.52
1:A:131:GLN:NE2	1:A:133:GLU:H	1.96	0.52
1:B:521:LEU:HD22	1:B:538:LEU:HD11	1.91	0.52
1:B:264:ILE:HD11	6:B:4005:FAD:H3B	1.90	0.52
1:B:551:LYS:HA	1:B:551:LYS:HZ3	1.73	0.52
1:A:389:PHE:O	1:A:391:PRO:HD3	2.10	0.52
7:B:5102:YSH:C1	7:B:5102:YSH:C6	2.81	0.52
1:A:1082:SER:HB2	4:A:3003:MTE:O3P	2.10	0.52
1:B:32:ARG:HH12	1:B:676:GLU:CD	2.13	0.52
1:B:154:ARG:HD2	10:B:5493:HOH:O	2.08	0.52
1:B:164:ALA:O	1:B:165:LYS:HB2	2.09	0.52
1:A:885:MET:HE2	1:A:894:ILE:HD11	1.93	0.51
1:B:406:SER:C	1:B:407:ILE:HD12	2.30	0.51
1:A:338:ALA:HA	1:A:429:ASP:OD1	2.11	0.51
1:A:537:LYS:CG	1:A:538:LEU:H	2.12	0.51
1:A:1078:ALA:HB1	5:A:3004:MOS:O1	2.09	0.51
1:A:505:ILE:N	1:A:505:ILE:HD12	2.25	0.51
1:B:376:SER:HB2	1:B:402:GLU:HG2	1.92	0.51
1:A:1318:VAL:HG12	1:A:1319:THR:H	1.76	0.51
1:B:548:LEU:HA	8:B:5022:GOL:H12	1.93	0.50
1:A:404:LEU:HD21	1:A:407:ILE:HD11	1.92	0.50
1:A:1319:THR:HG23	1:A:1320:GLY:N	2.26	0.50
1:B:723:PHE:CD2	1:B:847:LYS:HE2	2.47	0.50
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.11	0.50
1:B:1281:ALA:O	1:B:1284:GLN:HB3	2.12	0.50
1:A:480:GLU:O	1:A:484:GLN:HG3	2.11	0.50
1:A:747:HIS:CD2	1:A:836:THR:HG21	2.47	0.50
1:B:914:PHE:HA	9:B:5202:ACY:H2	1.92	0.50
1:A:1318:VAL:HG12	1:A:1319:THR:N	2.26	0.50
1:A:1289:ASN:HD22	1:A:1292:GLU:HB2	1.77	0.50
1:B:1289:ASN:HB3	1:B:1292:GLU:HB2	1.94	0.50
1:A:161:ARG:HD3	10:A:5307:HOH:O	2.11	0.49
1:A:598:ARG:HG3	1:B:600:GLU:HG2	1.94	0.49
1:A:604:PHE:CD2	1:A:675:PRO:HG3	2.46	0.49
1:B:747:HIS:CD2	1:B:836:THR:HG21	2.48	0.49
1:B:1172:LYS:HG3	8:B:5008:GOL:H31	1.95	0.49



A + a 1		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:58:TYR:CD2	1:B:220:LYS:HB2	2.47	0.49
1:B:551:LYS:HZ2	1:B:551:LYS:CA	2.23	0.49
1:A:1007:ILE:O	1:A:1008:SER:CB	2.61	0.49
1:B:165:LYS:HB2	1:B:165:LYS:NZ	2.27	0.49
1:B:699:GLU:H	1:B:699:GLU:CD	2.14	0.49
1:B:1173:ASN:O	1:B:1236:PRO:HA	2.13	0.49
1:A:237:ILE:N	1:A:237:ILE:HD12	2.28	0.49
1:A:1088:GLN:HG2	1:A:1133:TYR:CE1	2.48	0.49
1:A:644:ASN:O	1:A:653:THR:HA	2.13	0.49
1:A:856:ILE:HD12	1:A:856:ILE:N	2.27	0.49
1:B:650:ASN:HD21	1:B:778:LYS:HE3	1.78	0.49
1:A:739:GLN:HG2	1:A:911:PHE:CE1	2.48	0.49
1:B:964:VAL:HB	1:B:965:PRO:HD3	1.95	0.49
1:A:1017:ALA:HB1	1:A:1086:TYR:CD2	2.47	0.48
1:A:1106:LYS:NZ	1:A:1106:LYS:HB3	2.27	0.48
1:A:508:ARG:O	1:A:512:THR:HG23	2.13	0.48
1:A:527:LEU:C	1:A:529:LYS:H	2.17	0.48
1:B:655:PHE:CE1	1:B:814:LEU:HD23	2.47	0.48
1:B:826:MET:HB3	8:B:5014:GOL:H31	1.94	0.48
1:B:1007:ILE:O	1:B:1008:SER:CB	2.61	0.48
1:B:1082:SER:HB2	4:B:4003:MTE:O3P	2.13	0.48
1:B:719:LEU:HD13	1:B:860:GLU:OE2	2.14	0.48
1:B:1323:GLY:O	1:B:1324:ASN:C	2.51	0.48
8:A:5011:GOL:O3	1:B:1030:LEU:HD22	2.14	0.48
1:A:211:ILE:HG12	1:A:212:PHE:N	2.29	0.48
1:A:346:ALA:HB1	6:A:3005:FAD:H4'	1.96	0.48
1:A:1318:VAL:HG21	1:A:1322:PRO:CB	2.44	0.48
1:B:726:ALA:HB2	1:B:857:VAL:CG2	2.44	0.48
1:B:1321:ALA:HB1	1:B:1322:PRO:CD	2.38	0.48
1:B:655:PHE:HE1	1:B:814:LEU:HD23	1.78	0.48
1:B:952:LEU:HD23	1:B:958:ARG:HA	1.94	0.48
1:A:310:LYS:O	1:A:314:GLU:HG3	2.14	0.47
1:B:558:GLN:HB3	1:B:1192:ILE:HD13	1.96	0.47
1:A:604:PHE:HE2	8:A:5006:GOL:H31	1.79	0.47
1:B:433:LYS:HG3	10:B:5852:HOH:O	2.14	0.47
1:A:1215:PRO:HD2	1:A:1216:GLU:OE2	2.15	0.47
1:A:555:ALA:HB3	1:A:1238:GLU:HG3	1.95	0.47
1:B:544:SER:HB2	1:B:994:LYS:HD2	1.97	0.47
1:A:374:ILE:HD13	1:A:398:LEU:CD2	2.45	0.47
1:A:529:LYS:O	1:A:530:ASP:HB2	2.14	0.47
1:A:505:ILE:HD12	1:A:505:ILE:H	1.80	0.47



	<b>A t</b> area <b>D</b>	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:1318:VAL:CB	1:A:1322:PRO:HB3	2.44	0.47
1:B:911:PHE:O	1:B:912:ARG:C	2.53	0.47
1:B:325:GLU:HB2	1:B:412:SER:HB3	1.96	0.47
1:A:885:MET:CE	1:A:894:ILE:HD11	2.45	0.47
1:A:987:PHE:CD2	1:A:996:ARG:HG3	2.50	0.47
1:B:1318:VAL:O	1:B:1320:GLY:N	2.47	0.47
1:A:558:GLN:HB3	1:A:1192:ILE:HD13	1.96	0.46
1:A:926:TRP:O	1:A:930:VAL:HG23	2.14	0.46
1:A:655:PHE:HE1	1:A:814:LEU:HD23	1.80	0.46
1:B:328:ARG:HH11	1:B:328:ARG:CG	2.20	0.46
1:B:736:ILE:HG23	1:B:736:ILE:O	2.16	0.46
1:A:1052:LYS:HD3	1:A:1254:TYR:CZ	2.51	0.46
1:B:994:LYS:HE3	8:B:5008:GOL:O2	2.15	0.46
1:B:217:LEU:O	1:B:220:LYS:HG2	2.15	0.46
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.86	0.46
1:A:1322:PRO:C	1:A:1324:ASN:N	2.68	0.46
1:B:117:THR:HB	1:B:118:PRO:HD3	1.97	0.46
1:B:1203:LEU:HD11	10:B:5736:HOH:O	2.14	0.46
1:B:1053:ALA:O	1:B:1098:LEU:HD11	2.16	0.46
1:A:37:ARG:HD3	1:A:595:ASP:O	2.16	0.46
1:A:648:LEU:HD11	1:A:803:THR:HG21	1.97	0.46
1:B:726:ALA:HB2	1:B:857:VAL:HG21	1.98	0.46
1:A:911:PHE:O	1:A:912:ARG:C	2.53	0.46
1:B:635:LEU:HD21	1:B:818:LYS:HG2	1.97	0.45
1:A:757:GLU:HB3	1:A:786:ARG:HE	1.80	0.45
1:B:37:ARG:HD3	8:B:5013:GOL:O3	2.15	0.45
1:B:1261:GLU:N	1:B:1262:PRO:CD	2.79	0.45
1:A:407:ILE:HD12	1:A:407:ILE:N	2.31	0.45
1:A:602:GLU:HA	1:A:822:PRO:HG2	1.99	0.45
1:B:57:LYS:HE2	1:B:83:VAL:HG22	1.98	0.45
1:B:1221:THR:HG22	1:B:1226:THR:HB	1.98	0.45
1:A:193:PRO:HG2	1:A:560:PHE:CZ	2.52	0.45
1:B:389:PHE:O	1:B:391:PRO:HD3	2.16	0.45
1:A:964:VAL:HB	1:A:965:PRO:HD3	1.98	0.45
1:A:1126:SER:HB2	1:B:1132:PHE:CD1	2.52	0.45
1:A:164:ALA:O	1:A:165:LYS:CB	2.64	0.45
1:B:736:ILE:HG13	1:B:1298:SER:HB3	1.99	0.45
1:B:987:PHE:CD2	1:B:996:ARG:HG3	2.52	0.45
1:A:605:LEU:HD23	1:A:605:LEU:C	2.37	0.45
1:B:508:ARG:O	1:B:512:THR:HG23	2.17	0.45
1:A:1261:GLU:N	1:A:1262:PRO:CD	2.80	0.45



	A h o	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:1153:PHE:HB2	1:A:1155:TYR:CZ	2.52	0.45	
1:A:952:LEU:HD23	1:A:958:ARG:HA	2.00	0.44	
1:A:699:GLU:CD	1:A:699:GLU:H	2.21	0.44	
1:A:604:PHE:CE2	8:A:5006:GOL:H31	2.52	0.44	
1:B:1324:ASN:O	1:B:1325:CYS:C	2.56	0.44	
1:A:683:HIS:HA	8:A:5019:GOL:H12	1.99	0.44	
1:A:573:VAL:HG21	1:A:1052:LYS:HD2	2.00	0.44	
1:B:644:ASN:O	1:B:653:THR:HA	2.18	0.44	
1:A:161:ARG:HH12	1:A:556:ASN:ND2	2.16	0.43	
1:B:95:LYS:HG3	1:B:589:GLU:OE1	2.18	0.43	
1:B:328:ARG:HG2	1:B:328:ARG:NH1	2.19	0.43	
1:B:403:ILE:C	1:B:403:ILE:HD12	2.38	0.43	
1:B:1088:GLN:HG2	1:B:1133:TYR:CE1	2.52	0.43	
1:B:1088:GLN:HG3	10:B:5797:HOH:O	2.18	0.43	
1:B:1017:ALA:HB1	1:B:1086:TYR:CD2	2.53	0.43	
6:B:4005:FAD:HM73	10:B:5428:HOH:O	2.18	0.43	
1:A:911:PHE:HD2	1:A:912:ARG:N	2.17	0.43	
1:B:723:PHE:CE2	1:B:847:LYS:HE2	2.52	0.43	
1:B:871:ARG:HG3	1:B:871:ARG:HH11	1.83	0.43	
1:A:374:ILE:HG21	1:A:398:LEU:HD22	2.00	0.43	
6:A:3005:FAD:HM73	10:A:5425:HOH:O	2.18	0.43	
1:B:154:ARG:CD	1:B:1196:GLU:OE2	2.65	0.43	
1:B:61:LEU:C	1:B:61:LEU:HD23	2.38	0.43	
1:B:141:ASP:O	1:B:144:GLN:HG3	2.18	0.43	
1:A:328:ARG:HG3	10:A:5888:HOH:O	2.17	0.43	
1:A:487:CYS:HB3	1:A:513:LEU:HD13	2.00	0.43	
1:A:651:ASP:OD1	1:A:871:ARG:NH1	2.52	0.43	
1:A:1053:ALA:O	1:A:1098:LEU:HD11	2.19	0.43	
1:A:1315:THR:O	1:A:1318:VAL:HG22	2.19	0.43	
1:B:926:TRP:O	1:B:930:VAL:HG23	2.19	0.43	
1:B:955:PHE:CA	1:B:1145:ASN:HD21	2.20	0.43	
1:A:404:LEU:CD2	1:A:407:ILE:HD11	2.49	0.43	
1:B:826:MET:H	8:B:5014:GOL:C3	2.30	0.43	
1:A:1290:THR:O	1:A:1290:THR:HG22	2.19	0.43	
1:B:82:HIS:NE2	1:B:219:LEU:HD13	2.33	0.43	
1:B:1199:PHE:CE1	1:B:1267:GLY:HA2	2.53	0.43	
1:A:570:GLU:CD	1:A:1057:PRO:HG3	2.40	0.43	
1:B:948:LYS:HG2	1:B:951:ASP:CG	2.39	0.43	
1:B:992:CYS:SG	1:B:1285:HIS:NE2	2.92	0.43	
1:A:131:GLN:O	1:A:134:PRO:HD3	2.19	0.42	
1:A:100:PRO:O	1:A:104:ARG:HG3	2.19	0.42	



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:216:LEU:HD23	1:A:219:LEU:HD12	2.00	0.42
1:B:909:THR:OG1	1:B:910:ALA:N	2.51	0.42
1:A:87:THR:OG1	1:A:89:GLU:HG2	2.19	0.42
1:A:491:ALA:O	1:A:509:ARG:NH2	2.52	0.42
1:B:753:PRO:HD3	1:B:816:ALA:HB1	2.01	0.42
1:B:1108:ASN:N	1:B:1109:PRO:HD3	2.34	0.42
1:A:275:PHE:HA	1:A:276:PRO:HD2	1.91	0.42
1:B:257:LEU:HA	1:B:279:ILE:O	2.18	0.42
1:A:519:PHE:O	1:A:523:VAL:HG23	2.20	0.42
1:A:1183:GLY:HA2	1:A:1247:CYS:O	2.19	0.42
1:B:249:LYS:HG3	1:B:403:ILE:CG2	2.50	0.42
1:B:572:THR:HA	1:B:575:ARG:HD2	2.01	0.42
1:B:719:LEU:HD11	1:B:895:ARG:HB3	2.00	0.42
1:A:103:GLU:HG3	1:A:107:LYS:HE2	2.02	0.42
1:A:651:ASP:OD2	1:A:871:ARG:HG3	2.19	0.42
1:B:572:THR:OG1	1:B:1048:GLN:HG2	2.19	0.42
1:A:703:LYS:NZ	1:A:703:LYS:HB3	2.35	0.42
1:A:46:GLY:HA2	3:A:3002:FES:S1	2.60	0.42
1:A:376:SER:HB3	1:A:402:GLU:HG2	2.02	0.42
1:B:316:VAL:HA	1:B:324:THR:HG21	2.01	0.42
1:B:325:GLU:HB2	1:B:412:SER:CB	2.50	0.42
1:B:473:GLN:HA	1:B:473:GLN:NE2	2.35	0.42
1:B:271:LYS:NZ	8:B:5020:GOL:H32	2.35	0.41
1:A:312:LEU:HD12	1:A:312:LEU:HA	1.89	0.41
1:B:217:LEU:HD12	1:B:217:LEU:HA	1.93	0.41
1:B:551:LYS:NZ	1:B:552:HIS:H	2.09	0.41
1:A:1319:THR:HG23	1:A:1320:GLY:H	1.85	0.41
1:B:505:ILE:HD12	1:B:505:ILE:N	2.36	0.41
1:B:518:LYS:HZ3	8:B:5022:GOL:C3	2.32	0.41
1:A:670:VAL:HG11	1:A:681:ALA:HB3	2.01	0.41
1:A:1318:VAL:HG11	1:A:1322:PRO:HA	2.02	0.41
1:B:244:GLU:O	1:B:248:LEU:HG	2.19	0.41
1:B:1325:CYS:O	1:B:1326:LYS:CB	2.67	0.41
1:B:13:LYS:HD3	1:B:13:LYS:C	2.41	0.41
1:B:552:HIS:HB2	1:B:1237:THR:HG21	2.03	0.41
1:B:1287:ASN:O	1:B:1288:ASN:CB	2.67	0.41
1:A:1216:GLU:CD	1:A:1216:GLU:H	2.23	0.41
1:B:657:LYS:O	1:B:658:ASP:HB2	2.21	0.41
1:B:899:ARG:HD2	1:B:899:ARG:HA	1.87	0.41
1:A:923:ALA:HA	1:A:926:TRP:NE1	2.36	0.41
1:A:1088:GLN:HG3	10:A:5686:HOH:O	2.19	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:992:CYS:HA	1:B:1284:GLN:HE21	1.86	0.41
1:B:1289:ASN:O	1:B:1290:THR:CB	2.69	0.41
1:A:32:ARG:HH12	1:A:676:GLU:CD	2.24	0.40
1:A:433:LYS:HD3	1:A:433:LYS:HA	1.81	0.40
1:B:58:TYR:CZ	1:B:220:LYS:HD2	2.56	0.40
1:B:328:ARG:CG	1:B:328:ARG:NH1	2.79	0.40
1:B:1325:CYS:O	1:B:1326:LYS:HB3	2.20	0.40
1:A:284:ILE:HA	1:A:285:PRO:HD2	1.91	0.40
1:B:712:LEU:HD21	1:B:875:HIS:CE1	2.56	0.40
1:A:1212:HIS:H	1:A:1221:THR:CG2	2.34	0.40
1:A:3:ALA:HA	1:A:227:LEU:HD23	2.04	0.40
1:A:490:LEU:HB2	1:A:513:LEU:CD2	2.52	0.40
1:A:539:ASP:H	8:A:5002:GOL:C3	2.35	0.40
1:A:551:LYS:HE3	10:A:6123:HOH:O	2.21	0.40
1:A:556:ASN:O	1:A:557:ILE:HD13	2.21	0.40
1:A:655:PHE:CE1	1:A:814:LEU:HD23	2.57	0.40
1:A:131:GLN:HA	1:A:132:PRO:HD2	1.95	0.40
1:A:263:GLU:HB2	6:A:3005:FAD:H52A	2.02	0.40
1:A:506:GLU:CD	1:A:506:GLU:H	2.24	0.40
1:B:277:MET:HE3	1:B:278:ILE:N	2.35	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	Percen	tiles
1	А	1293/1332~(97%)	1244 (96%)	41 (3%)	8 (1%)	25	14
1	В	1290/1332~(97%)	1234 (96%)	44 (3%)	12 (1%)	17	8
All	All	2583/2664~(97%)	2478 (96%)	85 (3%)	20 (1%)	19	9

All (20) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	А	4	ASP
1	А	1008	SER
1	В	1008	SER
1	В	1287	ASN
1	В	1324	ASN
1	В	1326	LYS
1	А	1319	THR
1	В	244	GLU
1	В	1325	CYS
1	А	912	ARG
1	А	1322	PRO
1	В	912	ARG
1	В	1139	GLY
1	В	1319	THR
1	А	797	GLY
1	А	1318	VAL
1	В	797	GLY
1	В	1322	PRO
1	В	1323	GLY
1	А	1139	GLY

#### 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	1101/1128~(98%)	1086 (99%)	15 (1%)	67 62
1	В	1098/1128~(97%)	1088 (99%)	10 (1%)	78 77
All	All	2199/2256~(98%)	2174~(99%)	25~(1%)	73 70

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	154	ARG
1	А	281	PRO
1	А	312	LEU
1	А	328	ARG



Mol	Chain	Res	Type
1	А	476	LYS
1	А	550	GLN
1	А	565	ASN
1	А	618	LYS
1	А	651	ASP
1	А	743	TYR
1	А	911	PHE
1	А	1002	PRO
1	А	1145	ASN
1	А	1208	LEU
1	А	1239	PHE
1	В	154	ARG
1	В	328	ARG
1	В	551	LYS
1	В	565	ASN
1	В	600	GLU
1	В	743	TYR
1	В	911	PHE
1	В	1002	PRO
1	В	1145	ASN
1	В	1239	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	A 131		GLN
1	А	252	HIS
1	А	272	ASN
1	А	351	ASN
1	А	471	GLN
1	А	473	GLN
1	А	550	GLN
1	А	556	ASN
1	А	565	ASN
1	А	626	GLN
1	А	650	ASN
1	А	1145	ASN
1	А	1212	HIS
1	А	1284	GLN
1	А	1289	ASN
1	А	1324	ASN
1	В	131	GLN



Mol	Chain	Res	Type
1	В	146	ASN
1	В	351	ASN
1	В	471	GLN
1	В	473	GLN
1	В	484	GLN
1	В	565	ASN
1	В	626	GLN
1	В	650	ASN
1	В	875	HIS
1	В	976	GLN
1	В	1145	ASN
1	В	1284	GLN
1	В	1287	ASN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 39 ligands modelled in this entry, 4 are monoatomic - leaving 35 for Mogul analysis.

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

Mal	Turne	Chain	Dec	Tink	B	ond leng	gths	E	Bond ang	gles
Mol Type C	Unam	nes	Res Link	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
8	GOL	В	5022	-	$5,\!5,\!5$	0.23	0	$5,\!5,\!5$	0.36	0



Mal	Trune	Chain	Dec	Timle	B	ond leng	gths	E	ond ang	gles
INIOI	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
9	ACY	В	5202	-	3,3,3	1.13	0	3,3,3	1.73	1 (33%)
8	GOL	А	5019	-	$5,\!5,\!5$	0.32	0	$5,\!5,\!5$	0.29	0
3	FES	В	4001	1	0,4,4	-	-	-		
8	GOL	В	5021	-	$5,\!5,\!5$	0.27	0	$5,\!5,\!5$	0.39	0
7	YSH	В	5102	-	19,23,23	<mark>6.75</mark>	10 (52%)	26,33,33	<mark>3.53</mark>	7 (26%)
6	FAD	В	4005	-	53,58,58	2.44	22 (41%)	68,89,89	2.02	25 (36%)
5	MOS	А	3004	4	0,3,3	-	-	-		
8	GOL	А	5004	-	$5,\!5,\!5$	0.28	0	$5,\!5,\!5$	0.32	0
3	FES	В	4002	1	0,4,4	-	-	-		
8	GOL	А	5011	-	$5,\!5,\!5$	0.21	0	$5,\!5,\!5$	0.36	0
3	FES	А	3001	1	0,4,4	-	-	-		•
8	GOL	А	5006	-	$5,\!5,\!5$	0.24	0	$5,\!5,\!5$	0.41	0
3	FES	А	3002	1	0,4,4	-	-	-		
8	GOL	В	5012	-	$5,\!5,\!5$	0.22	0	$5,\!5,\!5$	0.42	0
8	GOL	А	5018	-	$5,\!5,\!5$	0.34	0	$5,\!5,\!5$	0.27	0
4	MTE	В	4003	5	21,26,26	6.02	13 (61%)	21,40,40	4.41	9 (42%)
6	FAD	А	3005	-	53,58,58	2.33	19 (35%)	68,89,89	2.03	24 (35%)
8	GOL	А	5002	-	$5,\!5,\!5$	0.22	0	$5,\!5,\!5$	0.36	0
8	GOL	А	5016	-	$5,\!5,\!5$	0.27	0	$5,\!5,\!5$	0.48	0
8	GOL	В	5007	-	$5,\!5,\!5$	0.28	0	$5,\!5,\!5$	0.32	0
8	GOL	В	5013	-	$5,\!5,\!5$	0.23	0	$5,\!5,\!5$	0.29	0
4	MTE	А	3003	5	21,26,26	6.25	13 (61%)	21,40,40	4.02	8 (38%)
8	GOL	А	5003	-	$5,\!5,\!5$	0.31	0	$5,\!5,\!5$	0.32	0
8	GOL	В	5015	-	$5,\!5,\!5$	0.26	0	$5,\!5,\!5$	0.30	0
8	GOL	В	5008	-	$5,\!5,\!5$	0.26	0	$5,\!5,\!5$	0.39	0
8	GOL	А	5017	-	$5,\!5,\!5$	0.28	0	$5,\!5,\!5$	0.31	0
8	GOL	В	5020	-	$5,\!5,\!5$	0.25	0	$5,\!5,\!5$	0.34	0
8	GOL	В	5014	-	$5,\!5,\!5$	0.21	0	$5,\!5,\!5$	0.38	0
8	GOL	А	5001	-	$5,\!5,\!5$	0.31	0	$5,\!5,\!5$	0.39	0
9	ACY	А	5201	-	3,3,3	1.03	0	3,3,3	1.80	1 (33%)
7	YSH	А	5101	-	19,23,23	6.67	10 (52%)	26,33,33	3.50	7 (26%)
8	GOL	В	5009	-	$5,\!5,\!5$	0.31	0	$5,\!5,\!5$	0.29	0
8	GOL	А	5005	-	$5,\!5,\!5$	0.31	0	$5,\!5,\!5$	0.34	0
5	MOS	В	4004	4	0,3,3	-	-	-		·

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.



	1	V	D	V
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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	В	5022	-	-	0/4/4/4	-
8	GOL	А	5019	-	-	0/4/4/4	-
3	FES	В	4001	1	-	-	0/1/1/1
8	GOL	В	5021	-	-	0/4/4/4	-
7	YSH	В	5102	-	-	1/10/16/16	0/2/2/2
6	FAD	В	4005	-	-	2/30/50/50	0/6/6/6
8	GOL	А	5004	_	-	0/4/4/4	-
3	FES	В	4002	1	-	_	0/1/1/1
8	GOL	А	5011	_	-	0/4/4/4	-
3	FES	А	3001	1	-	-	0/1/1/1
8	GOL	А	5006	-	-	0/4/4/4	-
3	FES	А	3002	1	-	-	0/1/1/1
8	GOL	В	5012	-	-	0/4/4/4	-
8	GOL	А	5018	-	-	0/4/4/4	-
4	MTE	В	4003	5	-	6/6/34/34	0/3/3/3
6	FAD	А	3005	-	-	4/30/50/50	0/6/6/6
8	GOL	А	5002	-	-	0/4/4/4	-
8	GOL	А	5016	-	-	0/4/4/4	-
8	GOL	В	5007	-	-	0/4/4/4	-
8	GOL	В	5013	-	-	0/4/4/4	-
4	MTE	А	3003	5	-	4/6/34/34	0/3/3/3
8	GOL	А	5003	-	-	0/4/4/4	-
8	GOL	В	5015	-	-	0/4/4/4	-
8	GOL	В	5008	-	-	0/4/4/4	-
8	GOL	А	5017	-	-	0/4/4/4	-
8	GOL	В	5020	-	-	0/4/4/4	-
8	GOL	В	5014	-	-	0/4/4/4	-
8	GOL	А	5001	-	-	0/4/4/4	-
7	YSH	А	5101	-	-	1/10/16/16	0/2/2/2
8	GOL	В	5009	-	-	0/4/4/4	-
8	GOL	А	5005	-	-	0/4/4/4	-

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	А	3003	MTE	C7-C6	19.00	1.68	1.53
4	В	4003	MTE	C7-C6	18.55	1.68	1.53
7	В	5102	YSH	C1-C5	18.40	1.71	1.39
7	А	5101	YSH	C1-C5	18.13	1.71	1.39
7	В	5102	YSH	C11-C6	17.98	1.62	1.41
7	А	5101	YSH	C11-C6	17.86	1.62	1.41
4	А	3003	MTE	C9-N5	11.68	1.62	1.38



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	В	4003	MTE	C9-N5	11.49	1.61	1.38
4	А	3003	MTE	C9-C10	10.82	1.61	1.41
4	В	4003	MTE	C9-C10	10.80	1.61	1.41
7	В	5102	YSH	C10-C9	8.75	1.57	1.39
7	А	5101	YSH	C10-C9	8.52	1.57	1.39
4	В	4003	MTE	P-O4'	-6.93	1.37	1.60
4	А	3003	MTE	P-O4'	-6.77	1.38	1.60
4	А	3003	MTE	C6-N5	-6.52	1.36	1.45
7	А	5101	YSH	C8-C12	5.91	1.53	1.44
6	А	3005	FAD	C10-N1	5.87	1.45	1.33
7	А	5101	YSH	O22-C20	5.79	1.39	1.22
7	В	5102	YSH	C8-C12	5.73	1.53	1.44
7	В	5102	YSH	O22-C20	5.69	1.39	1.22
6	В	4005	FAD	C10-N1	5.60	1.44	1.33
4	В	4003	MTE	P-O3P	-5.05	1.35	1.54
4	А	3003	MTE	P-O3P	-4.99	1.35	1.54
6	В	4005	FAD	C4X-N5	4.91	1.40	1.30
6	А	3005	FAD	C4X-N5	4.73	1.39	1.30
6	В	4005	FAD	C9A-C5X	4.71	1.49	1.41
6	В	4005	FAD	C10-N10	4.68	1.47	1.37
4	В	4003	MTE	C4'-C3'	-4.51	1.45	1.52
7	В	5102	YSH	O14-C9	4.50	1.46	1.37
4	В	4003	MTE	C9-C4	4.45	1.47	1.41
6	В	4005	FAD	C9-C9A	4.41	1.46	1.39
4	А	3003	MTE	C9-C4	4.40	1.47	1.41
4	А	3003	MTE	C4'-C3'	-4.34	1.46	1.52
6	А	3005	FAD	C10-N10	4.30	1.46	1.37
6	В	4005	FAD	C1'-C2'	4.30	1.58	1.52
6	А	3005	FAD	C9-C9A	4.28	1.46	1.39
6	А	3005	FAD	C9A-C5X	4.18	1.48	1.41
7	А	5101	YSH	O14-C9	4.07	1.45	1.37
6	В	4005	FAD	C6-C7	4.07	1.45	1.39
6	А	3005	FAD	C9A-N10	4.05	1.48	1.41
6	В	4005	FAD	C9A-N10	4.03	1.48	1.41
6	В	4005	FAD	C4A-N3A	4.01	1.41	1.35
6	A	3005	FAD	C1'-C2'	3.89	1.58	1.52
6	А	3005	FAD	C6-C7	3.80	1.45	1.39
4	В	4003	MTE	C4-N3	3.78	1.39	1.33
6	A	3005	FAD	C4A-N3A	3.76	1.40	1.35
7	В	5102	YSH	C7-C6	3.60	1.42	1.40
6	В	4005	FAD	O4B-C1B	3.58	1.46	1.41
4	А	3003	MTE	C4-N3	3.57	1.39	1.33



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
6	А	3005	FAD	O4B-C1B	3.53	1.46	1.41
6	В	4005	FAD	C6-C5X	3.52	1.45	1.40
6	А	3005	FAD	C6-C5X	3.51	1.45	1.40
6	В	4005	FAD	C2A-N3A	3.36	1.37	1.32
7	А	5101	YSH	C7-C6	3.31	1.42	1.40
4	А	3003	MTE	O4'-C4'	-3.30	1.32	1.44
6	А	3005	FAD	C2A-N3A	3.26	1.37	1.32
6	В	4005	FAD	C4-N3	3.20	1.44	1.38
6	А	3005	FAD	C4-N3	3.09	1.44	1.38
4	В	4003	MTE	C6-N5	-3.06	1.40	1.45
6	В	4005	FAD	C8-C7	3.01	1.48	1.40
6	А	3005	FAD	C8-C7	2.98	1.48	1.40
4	А	3003	MTE	C2-N1	2.86	1.40	1.35
6	А	3005	FAD	C2A-N1A	2.82	1.39	1.33
7	В	5102	YSH	O14-C15	2.73	1.53	1.42
4	А	3003	MTE	O4-C4	2.72	1.31	1.24
6	В	4005	FAD	C5'-C4'	2.68	1.55	1.51
7	А	5101	YSH	O14-C15	2.66	1.53	1.42
6	В	4005	FAD	C2A-N1A	2.65	1.38	1.33
6	В	4005	FAD	C4'-C3'	2.62	1.58	1.53
7	В	5102	YSH	O21-C20	-2.60	1.22	1.30
7	А	5101	YSH	O21-C20	-2.59	1.22	1.30
4	В	4003	MTE	O3'-C3'	2.55	1.47	1.43
4	В	4003	MTE	C2-N1	2.43	1.39	1.35
6	В	4005	FAD	C2'-C3'	2.42	1.58	1.53
4	В	4003	MTE	O4-C4	2.42	1.30	1.24
6	В	4005	FAD	P-O1P	2.30	1.59	1.50
6	А	3005	FAD	PA-O1A	2.28	1.59	1.50
6	А	3005	FAD	C4'-C3'	2.28	1.57	1.53
6	А	3005	FAD	P-O1P	2.23	1.58	1.50
6	В	4005	FAD	C9-C8	2.22	1.42	1.39
6	В	4005	FAD	PA-O1A	2.21	1.58	1.50
7	В	5102	YSH	C4-N3	2.18	1.40	1.33
4	А	3003	MTE	P-O2P	-2.13	1.46	1.54
6	A	3005	FAD	C5'-C4'	2.13	1.54	1.51
4	В	4003	MTE	P-O2P	-2.12	1.46	1.54
7	А	5101	YSH	C4-N3	2.11	1.39	1.33
6	В	4005	FAD	C8M-C8	2.04	1.55	1.51

All (82) bond angle outliers are listed below:



1	V	D	V

Continued from previous page							
Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
Mol	Chain	Dog	Tuno	Atoms	7	$Observed(^{o})$	Ideal(0)
7	DIIAIII	5102	VCU	C4 N2 N2	<b>1</b> 4 75	114 44	10270
7		5102	VSH	C4 N3 N2	14.70 14.97	114.44	103.70 102.70
1	A	2002	I SII MTE	C4 - N5 - N2	14.27	114.09	103.70
4	A P	4003	MTE	C4-C9-N5	10.22	130.22	119.12
4	D	4003	MTE	$P \Omega 4^{\prime} C 4^{\prime}$	12.09	129.94	119.12
4		4003	VCU	1-04-04	7.06	146.62	110.00 191.70
6	A	2005		$\frac{010-011-00}{N2A}$	-7.00	117.90	121.79
6	A D	3005	FAD FAD	N3A-C2A-NIA	-7.04	117.07	120.00
7	D	4005	FAD Veit	$\frac{\text{N}_{\text{D}}\text{A}-\text{O}_{\text{Z}}\text{A}-\text{N}_{\text{T}}\text{A}}{\text{C}_{10}}$	-0.95	117.01	128.08 121.70
1	В	<u>5102</u>	Y SH MTE	$\frac{10-011-00}{10-04}$	-0.90	110.03	121.79
4	A	3003	MTE	P-04-04	0.09	130.73	118.30
4	В	4003		$\begin{array}{c} \text{C2-N1-C10} \\ \text{C2-N1-C10} \end{array}$	0.82	127.58	114.04
4	A	3003	MIE	C2-N1-C10	5.05	127.21	114.54
(	A	5101	YSH	C1-C5-C20	-4.57	121.00	127.78
4	A	3003	MTE	C2-N3-C4	4.52	123.12	115.93
4	B	4003	MTE	N2-C2-N3	4.40	124.19	117.25
4	В	4003	MTE	C2-N3-C4	4.41	122.94	115.93
4	A	3003	MTE	N2-C2-N3	4.31	123.96	117.25
1	B	5102	YSH	C1-C5-C20	-4.09	121.70	127.78
6	В	4005	FAD	04'-C4'-C3'	4.08	119.01	109.10
6	A	3005	FAD	C5X-N5-C4X	3.99	124.71	118.07
6	A	3005	FAD	O4'-C4'-C3'	3.99	118.79	109.10
6	B	4005	FAD	C5X-N5-C4X	3.94	124.62	118.07
4	В	4003	MTE	N1-C2-N3	-3.79	119.48	125.42
6	В	4005	FAD	C1'-N10-C9A	3.78	126.81	120.51
4	A	3003	MTE	N1-C2-N3	-3.78	119.50	125.42
6	A	3005	FAD	C1'-N10-C9A	3.73	126.73	120.51
6	A	3005	FAD	C3B-C2B-C1B	3.65	106.47	100.98
6	В	4005	FAD	C3B-C2B-C1B	3.50	106.25	100.98
4	В	4003	MTE	O3'-C7-C6	-3.48	106.64	108.96
6	A	3005	FAD	C9A-C5X-N5	-3.43	118.70	122.43
4	A	3003	MTE	O3'-C7-C6	-3.36	106.73	108.96
6	В	4005	FAD	C9A-C5X-N5	-3.34	118.80	122.43
6	А	3005	FAD	C5'-C4'-C3'	-3.31	105.80	112.20
4	А	3003	MTE	O3'-C7-N8	-3.29	105.19	108.57
6	В	4005	FAD	C5'-C4'-C3'	-3.13	$106.1\overline{5}$	112.20
6	В	4005	FAD	C4-C4X-N5	$2.9\overline{2}$	122.38	118.23
6	A	3005	FAD	C4X-C4-N3	2.85	120.44	113.19
6	В	4005	FAD	C4X-C4-N3	2.82	120.35	113.19
6	А	3005	FAD	O3'-C3'-C4'	2.82	115.62	108.81
6	A	3005	FAD	C4-C4X-N5	2.82	122.24	118.23
7	А	5101	YSH	O22-C20-C5	-2.79	114.01	121.45



1	V	D	V

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
7	В	5102	YSH	O22-C20-C5	-2.66	114.36	121.45
7	А	5101	YSH	C7-C6-C11	2.63	123.78	119.87
6	В	4005	FAD	C10-C4X-N5	-2.61	119.32	124.86
6	А	3005	FAD	C8M-C8-C9	-2.59	114.71	119.49
6	А	3005	FAD	C10-C4X-N5	-2.55	119.45	124.86
6	В	4005	FAD	C8M-C8-C9	-2.53	114.81	119.49
6	А	3005	FAD	O3B-C3B-C4B	-2.51	103.80	111.05
6	В	4005	FAD	O3B-C3B-C4B	-2.50	103.81	111.05
6	В	4005	FAD	O3'-C3'-C4'	2.49	114.83	108.81
9	А	5201	ACY	O-C-CH3	-2.48	112.69	122.33
6	В	4005	FAD	C10-N1-C2	2.47	121.85	116.90
6	А	3005	FAD	C8M-C8-C7	2.46	125.77	120.74
6	В	4005	FAD	O2B-C2B-C3B	2.45	119.74	111.82
6	В	4005	FAD	C4-N3-C2	-2.44	121.14	125.64
7	В	5102	YSH	C7-C6-C11	2.43	123.48	119.87
6	В	4005	FAD	C2A-N1A-C6A	2.42	122.90	118.75
6	А	3005	FAD	O2'-C2'-C1'	2.42	115.66	109.80
6	А	3005	FAD	C2A-N1A-C6A	2.42	122.90	118.75
6	А	3005	FAD	O5B-PA-O1A	2.41	118.47	109.07
4	В	4003	MTE	O3'-C7-N8	-2.40	106.10	108.57
6	В	4005	FAD	O2'-C2'-C1'	2.40	115.61	109.80
6	А	3005	FAD	C4-N3-C2	-2.38	121.24	125.64
9	В	5202	ACY	O-C-CH3	-2.37	113.10	122.33
7	А	5101	YSH	C1-C5-C4	2.34	112.35	105.21
6	В	4005	FAD	C8M-C8-C7	2.34	125.52	120.74
7	А	5101	YSH	O21-C20-C5	2.33	120.89	114.85
7	В	5102	YSH	O21-C20-C5	2.33	120.89	114.85
6	А	3005	FAD	O2B-C2B-C3B	2.30	119.27	111.82
6	А	3005	FAD	C10-N1-C2	2.28	121.45	116.90
6	А	3005	FAD	C7M-C7-C6	-2.25	115.34	119.49
6	В	4005	FAD	O5B-PA-O1A	2.24	117.83	109.07
4	В	4003	MTE	O2P-P-O4'	2.23	112.66	106.73
7	В	5102	YSH	C1-C5-C4	2.20	111.94	105.21
6	В	4005	FAD	C4X-C10-N1	-2.19	119.64	124.73
6	А	3005	FAD	O5'-P-O1P	2.15	117.45	109.07
6	А	3005	FAD	C4X-C10-N1	-2.14	119.78	124.73
6	В	4005	FAD	C7M-C7-C6	-2.12	115.58	119.49
6	А	3005	FAD	O2'-C2'-C3'	2.10	114.21	109.10
6	В	4005	FAD	O5'-P-O1P	2.06	117.13	109.07
6	В	4005	FAD	C1B-N9A-C4A	-2.02	123.10	126.64
6	В	4005	FAD	O2'-C2'-C3'	2.02	114.00	109.10

There are no chirality outliers.



1VDV
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Mol	Chain	Res	Type	Atoms
4	А	3003	MTE	C4'-O4'-P-O2P
4	А	3003	MTE	C4'-O4'-P-O3P
4	В	4003	MTE	C2'-C3'-C4'-O4'
4	В	4003	MTE	O3'-C3'-C4'-O4'
4	В	4003	MTE	C3'-C4'-O4'-P
4	В	4003	MTE	C4'-O4'-P-O2P
4	В	4003	MTE	C4'-O4'-P-O3P
6	А	3005	FAD	N10-C1'-C2'-O2'
6	А	3005	FAD	N10-C1'-C2'-C3'
6	В	4005	FAD	N10-C1'-C2'-O2'
6	В	4005	FAD	N10-C1'-C2'-C3'
7	А	5101	YSH	N13-C12-C8-C9
7	В	5102	YSH	N13-C12-C8-C9
4	А	3003	MTE	C4'-O4'-P-O1P
4	В	4003	MTE	C4'-O4'-P-O1P
6	А	3005	FAD	C2'-C3'-C4'-O4'
4	А	3003	MTE	C3'-C4'-O4'-P
6	А	3005	FAD	O3'-C3'-C4'-O4'

All (18) torsion outliers are listed below:

There are no ring outliers.

21 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	В	5022	GOL	2	0
9	В	5202	ACY	4	0
8	А	5019	GOL	1	0
7	В	5102	YSH	3	0
6	В	4005	FAD	3	0
5	А	3004	MOS	1	0
8	А	5011	GOL	2	0
8	А	5006	GOL	2	0
3	А	3002	FES	1	0
4	В	4003	MTE	1	0
6	А	3005	FAD	4	0
8	А	5002	GOL	2	0
8	В	5013	GOL	1	0
4	А	3003	MTE	1	0
8	В	5008	GOL	2	0
8	В	5020	GOL	1	0
8	В	5014	GOL	2	0
8	А	5001	GOL	1	0



Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	А	5201	ACY	4	0
7	А	5101	YSH	3	0
5	В	4004	MOS	2	0

Continued from previous page...

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















## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



## 6 Fit of model and data (i)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

## 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

#### 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

