

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

#### Feb 5, 2024 – 10:12 AM EST

PDB ID	:	1ULB
Title	:	APPLICATION OF CRYSTALLOGRAPHIC AND MODELING METHODS
		IN THE DESIGN OF PURINE NUCLEOSIDE PHOSPHORYLASE IN-
		HIBITORS
Authors	:	Ealick, S.E.; Rule, S.A.; Carter, D.C.; Greenhough, T.J.; Babu, Y.S.; Cook,
		W.J.; Habash, J.; Helliwell, J.R.; Stoeckler, J.D.; Parksjunior, R.E.; Chen,
		SF.; Bugg, C.E.
Deposited on	:	1991-11-05
Resolution	:	2.75 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)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

# 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 2.75 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)

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%

Mol	Chain	Length		Quality of chain							
1	А	289	29%	46%	19%	6%					



#### 1ULB

# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2279 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 PURINE NUCLEOSIDE PHOSPHORYLASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	289	Total 2258	C 1434	N 395	0 413	S 16	0	0	0

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

• Molecule 3 is GUANINE (three-letter code: GUN) (formula:  $C_5H_5N_5O$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	А	1	Total 11	С 5	N 5	0 1	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: PURINE NUCLEOSIDE PHOSPHORYLASE



## 4 Data and refinement statistics (i)

Property	Value	Source	
Space group	H 3 2	Depositor	
Cell constants	142.90Å 142.90Å 165.20Å	Denesitor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor	
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	(Not available) - 2.75	Depositor	
Resolution (A)	29.15 - 2.79	EDS	
% Data completeness	(Not available) ((Not available)-2.75)	Depositor	
(in resolution range)	47.2(29.15-2.79)	EDS	
$R_{merge}$	(Not available)	Depositor	
$R_{sym}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	1.83 (at 2.80Å)	Xtriage	
Refinement program	PROLSQ	Depositor	
P. P.	0.204 , (Not available)	Depositor	
$n, n_{free}$	0.266 , (Not available)	DCC	
$R_{free}$ test set	No test flags present.	wwPDB-VP	
Wilson B-factor $(Å^2)$	68.8	Xtriage	
Anisotropy	0.097	Xtriage	
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34, 53.9	EDS	
L-test for $twinning^2$	$< L >=0.48, < L^2>=0.32$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
$F_o, F_c$ correlation	0.89	EDS	
Total number of atoms	2279	wwPDB-VP	
Average B, all atoms $(Å^2)$	29.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 9.33% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: GUN, SO4

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

Mal	Chain	Bo	nd lengths	Bo	ond angles
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.97	1/2310~(0.0%)	1.48	39/3125~(1.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	239	SER	C-N	-10.16	1.10	1.34

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	239	SER	O-C-N	-13.87	100.51	122.70
1	А	239	SER	CA-C-N	9.43	137.95	117.20
1	А	5	TYR	CB-CG-CD1	-8.97	115.62	121.00
1	А	185	ARG	NE-CZ-NH2	8.02	124.31	120.30
1	А	84	ARG	NE-CZ-NH2	7.76	124.18	120.30
1	А	101	ARG	NE-CZ-NH2	7.74	124.17	120.30
1	А	76	ARG	NE-CZ-NH2	7.66	124.13	120.30
1	А	154	ARG	NE-CZ-NH2	7.60	124.10	120.30
1	А	133	ARG	NE-CZ-NH2	7.53	124.07	120.30
1	А	234	ARG	NE-CZ-NH2	7.43	124.01	120.30
1	А	158	ARG	NE-CZ-NH2	7.34	123.97	120.30
1	А	148	ARG	NE-CZ-NH2	7.30	123.95	120.30
1	А	24	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	А	171	ARG	NE-CZ-NH2	7.20	123.90	120.30
1	А	67	ARG	NE-CZ-NH2	7.01	123.81	120.30
1	А	173	ARG	NE-CZ-NH2	6.44	123.52	120.30
1	A	229	ARG	NE-CZ-NH2	6.30	123.45	120.30
1	А	58	ARG	NE-CZ-NH2	6.28	123.44	120.30
1	А	60	THR	O-C-N	6.20	132.62	122.70
1	A	80	MET	CG-SD-CE	6.14	110.03	100.20



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	А	61	VAL	CB-CA-C	-6.13	99.74	111.40
1	А	130	MET	CG-SD-CE	6.07	109.91	100.20
1	А	81	MET	CG-SD-CE	6.05	109.89	100.20
1	А	87	MET	CG-SD-CE	6.03	109.85	100.20
1	А	181	MET	CG-SD-CE	5.99	109.79	100.20
1	А	260	VAL	O-C-N	5.92	132.17	122.70
1	А	170	MET	CG-SD-CE	5.86	109.58	100.20
1	А	194	MET	CG-SD-CE	5.82	109.52	100.20
1	А	207	ARG	NE-CZ-NH2	5.82	123.21	120.30
1	А	162	MET	CG-SD-CE	5.82	109.50	100.20
1	А	219	MET	CG-SD-CE	5.71	109.34	100.20
1	А	247	MET	CG-SD-CE	5.63	109.20	100.20
1	А	285	PRO	O-C-N	5.54	131.56	122.70
1	А	249	TYR	CB-CA-C	5.53	121.45	110.40
1	А	279	MET	CG-SD-CE	5.51	109.02	100.20
1	A	5	TYR	CB-CG-CD2	5.51	124.31	121.00
1	А	168	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	А	242	THR	O-C-N	-5.14	114.47	122.70
1	А	61	VAL	N-CA-C	5.00	124.51	111.00

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	2258	0	2234	230	0
2	А	10	0	0	1	0
3	А	11	0	5	0	0
All	All	2279	0	2239	230	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 51.

All (230) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



ARONITARONIT2distance (Å)overlap (Å)1:A:33:GLY:O1:A:35:LEU:HD121.361.261:A:60:THR:O1:A:62:PRO:HD1.051.211:A:60:THR:O1:A:62:PRO:HD1.981.111:A:284:LEU:HD211:A:62:PRO:HD1.981.111:A:284:LEU:HD211:A:62:PRO:HD1.981.111:A:284:LEU:HD211:A:289:SER:OG1.481.091:A:148:ARG:O1:A:148:ARG:HG31.561.041:A:22:LYS:HE21:A:23:HIS:CE11.941.021:A:48:ARG:HD121:A:23:HIS:CE11.941.011:A:24:PHE:CD21:A:23:ARG:HG31.460.961:A:47:ILE:HG231:A:231.460.961:A:47:ILE:HG211:A:27:VAL:HG211.420.971:A:47:ILE:HG231:A:67:ARG:HG31.460.951:A:67:HR:C1:A:62:PRO:O1.870.911:A:60:THR:C1:A:62:PRO:O1.870.911:A:60:THR:C1:A:62:PRO:D2.380.861:A:3ASN:O1:A:51'YR:N2.090.851:A:48:ARG:NH21:A:13:VAL:HG231.860.891:A:3ASN:O1:A:51'YR:N2.090.851:A:28:AELEU:CD21:A:28:SER:OG2.240.851:A:3:ASN:O1:A:261:LEU:H1.760.841:A:259:GLU:C1:A:260:GLU:HG21.810.811:A:249:TYR:O1:A:260:GLU:HG21.810.811:A:249:TYR:O1:A:260:GLU:HG21.830.791:A:44:GLN:HG22.090.8	Atom-1	Atom-2	Interatomic	Clash
1:A:34:GLY:O $1:A:35:LEU:HD12$ $1.36$ $1.26$ $1:A:60:THR:O$ $1:A:62:PRO:HD2$ $1.05$ $1.21$ $1:A:60:THR:O$ $1:A:62:PRO:CD$ $1.98$ $1.11$ $1:A:28:LEU:HD21$ $1:A:62:PRO:CD$ $1.98$ $1.11$ $1:A:28:LEU:HD21$ $1:A:62:PRO:CD$ $1.98$ $1.11$ $1:A:28:LEU:HD21$ $1:A:29:SER:OG$ $1.48$ $1.09$ $1:A:124:PHE:HD2$ $1:A:24:I:LE:HG12$ $1.14$ $1.08$ $1:A:29:LYS:HE2$ $1:A:23:HIS:CE1$ $1.94$ $1.02$ $1:A:84:ARG:HE22$ $1:A:13:XAL:HG23$ $1.23$ $1.02$ $1:A:49:THR:RC12$ $1:A:13:XAL:HG23$ $1.23$ $1.02$ $1:A:49:THE:RC12$ $1:A:19:PRO:1D2$ $1.42$ $0.97$ $1:A:49:THE:N$ $1:A:29:PRO:HD2$ $1.81$ $0.95$ $1:A:25:VAL:O$ $1:A:26:PRO:HD2$ $1.81$ $0.95$ $1:A:60:THR:C$ $1:A:62:PRO:O$ $1.87$ $0.91$ $1:A:60:THR:C$ $1:A:62:PRO:HD2$ $1.91$ $0.90$ $1:A:93:LEU:HD23$ $1:A:14:GLN:HG3$ $1.53$ $0.90$ $1:A:98:PHE:N$ $1:A:99:PRO:CD$ $2.38$ $0.86$ $1:A:24:LEU:HD23$ $1:A:61:VAL:O$ $1:A:25:GLU:CD$ $2.38$ $0.86$ $1:A:24:LEU:HD23$ $1:A:24:SER:OG$ $2.24$ $0.85$ $1:A:24:LEU:CD2$ $1:A:254:LYS:HG3$ $1.76$ $0.84$ $1:A:259:GLU:C$ $1:A:261:LEU:H$ $1.73$ $0.84$ $1:A:24:THE1$ $1:A:44:GLN:HG2$ $1.65$ $0.79$ $1:A:34:GLY:C$ $1:A:261:LEU:H$ $1.76$	Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:60:THR:O1:A:62:PRO:HD21.051.211:A:60:THR:O1:A:62:PRO:CD1.981.111:A:284:LEU:HD211:A:62:PRO:CD1.981.111:A:284:LEU:HD211:A:289:SER:OG1.481.091:A:124:PHE:HD21:A:24:LEU:HD221.141.081:A:148:ARG:O1:A:148:ARG:HG31.561.041:A:22.LYS:HE21:A:23:HIS:CE11.941.021:A:148:ARG:HH221:A:11:VAL:HG231.231.021:A:14:PHE:CD21:A:21:LE:HG211.941.011:A:29:PHE:HC231:A:67:ARG:HG31.460.961:A:29:FHE:N1:A:29:PRO:HD21.810.951:A:46:VAL:O1:A:62:PRO:O1.870.911:A:60:THR:C1:A:62:PRO:HD21.910.901:A:61:VAL:O1:A:62:PRO:HD21.910.901:A:60:THR:C1:A:62:PRO:HD21.910.901:A:93:LEU:HD231:A:11:VAL:HG231.860.891:A:93:PHE:N1:A:99:PRO:CD2.380.861:A:34:SN:O1:A:5:TYR:N2.090.851:A:284:LEU:CD21:A:289:SER:GG2.240.851:A:286:GU:CO1:A:26:CULU:H1.730.841:A:223:GLU:O1:A:254:LEU:HD21.590.841:A:249:TYR:O1:A:250:GLU:HE11.810.811:A:249:TYR:O1:A:250:GLU:HE11.810.811:A:249:TYR:O1:A:250:GLU:HE11.830.791:A:240:TYR:O1:A:260:YAL:HG21.660.751:A:240:TYR:O <t< td=""><td>1:A:34:GLY:O</td><td>1:A:35:LEU:HD12</td><td>1.36</td><td>1.26</td></t<>	1:A:34:GLY:O	1:A:35:LEU:HD12	1.36	1.26
1:A:60:THR:O       1:A:62:PRO:CD       1.98       1.11         1:A:284:LEU:HD21       1:A:289:SER:OG       1.48       1.09         1:A:124:PHE:HD2       1:A:249:IEE:HG12       1.14       1.08         1:A:148:ARG:O       1:A:148:ARG:HG3       1.56       1.04         1:A:22:LYS:HE2       1:A:23:HIS:CE1       1.94       1.02         1:A:48:ARG:HD2       1:A:113:VAL:HG23       1.23       1.02         1:A:47:HE:HC21       1:A:241:ILE:HG12       1.94       1.01         1:A:97:THR:HG21       1:A:241:ILE:HG13       1.46       0.96         1:A:98:PHE:N       1:A:262:PRO:HD2       1.81       0.95         1:A:61:VAL:O       1:A:62:PRO:O       1.87       0.91         1:A:61:VAL:O       1:A:62:PRO:HD2       1.91       0.90         1:A:98:PHE:N       1:A:62:PRO:HD2       1.91       0.90         1:A:98:PHE:N       1:A:99:PRO:CD       2.38       0.86         1:A:98:PHE:N       1:A:99:PRO:CD       2.38       0.86         1:A:28:ARG:MH2       1:A:113:VAL:HG23       1.86       0.89         1:A:28:EU:CD2       1:A:261:EU:HD2       1.59       0.84         1:A:29:FRE:N       1:A:261:EU:HD2       1.81       0.81 <t< td=""><td>1:A:60:THR:O</td><td>1:A:62:PRO:HD2</td><td>1.05</td><td>1.21</td></t<>	1:A:60:THR:O	1:A:62:PRO:HD2	1.05	1.21
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1:A:148:ARG:O1:A:148:ARG:HG31.561.041:A:22:LYS:HE21:A:13:VAL:HG231.231.021:A:42:PHE:CD21:A:13:VAL:HG231.231.021:A:41:L2:HG211:A:27:VAL:HG211.420.971:A:47:ILE:HG231:A:67:ARG:HG31.460.961:A:98:PHE:N1:A:99:PRO:HD21.810.951:A:425:VAL:O1:A:62:PRO:O1.870.911:A:61:VAL:O1:A:62:PRO:HD21.870.901:A:93:LEU:HD231:A:61:VAL:O1:A:62:PRO:HD21.860:A33:LEU:HD231:A:113:VAL:HG31.530.901:A:98:PHE:N1:A:99:PRO:CD2.380.861:A:98:PHE:N1:A:99:PRO:CD2.380.861:A:3:ASN:O1:A:5TYR:N2.090.851:A:284:LEU:CD21:A:289:SER:OG2.240.851:A:259:GLU:C1:A:261:LEU:H1.730.841:A:259:GLU:C1:A:250:GLU:HG21.810.811:A:4:249:TYR:O1:A:250:GLU:HG21.810.811:A:4:1:HYS:HD21:A:272:GLU:OE11.810.811:A:4:240:TR:O1:A:267:AL:HB12.090.811:A:4:GLY:C1:A:35:LEU:HD122.030.791:A:24:HEU:CD11:A:267:AL:HB12.160.751:A:124:PHE:HE21:A:23:A:RG:HD21.670.741:A:24:LEU:HD221:A:23:A:RG:HD21.670.731:A:24:LEU:HD221:A:23:A:RG:HD21.670.731:A:24:HE:HE21:A:23:A:RG:HD21.670.731:A	1:A:124:PHE:HD2	1:A:241:ILE:HG12	1.14	1.08
1:A:22:LYS:HE2 $1:A:23:HIS:CE1$ $1.94$ $1.02$ $1:A:84:ARG:HH22$ $1:A:113:VAL:HG23$ $1.23$ $1.02$ $1:A:124:PHE:CD2$ $1:A:241:LE:HG12$ $1.94$ $1.01$ $1:A:97:THR:HG21$ $1:A:227:VAL:HG21$ $1.42$ $0.97$ $1:A:47:LE:HG23$ $1:A:67:ARG:HG3$ $1.46$ $0.96$ $1:A:98:PHE:N$ $1:A:99:PRO:HD2$ $1.81$ $0.95$ $1:A:235:VAL:O$ $1:A:63:PRO:HD2$ $1.81$ $0.95$ $1:A:60:THR:C$ $1:A:62:PRO:O$ $1.87$ $0.91$ $1:A:35:LEU:HD23$ $1:A:14:GLN:HG3$ $1.53$ $0.90$ $1:A:35:LEU:HD23$ $1:A:14:GLN:HG3$ $1.53$ $0.90$ $1:A:35:LEU:HD23$ $1:A:14:GLN:HG3$ $1.53$ $0.90$ $1:A:35:RS:O$ $1:A:5:TYR:N$ $2.09$ $0.85$ $1:A:28:EU:HD21$ $1:A:29:PRO:CD$ $2.38$ $0.86$ $1:A:25:GLU:C$ $1:A:26:EV:H$ $1.73$ $0.84$ $1:A:25:GLU:C$ $1:A:26:LEU:H$ $1.73$ $0.84$ $1:A:25:GLU:C$ $1:A:25:GLU:GLI:HEU:H$ $1.76$ $0.84$ $1:A:24:PTR:O$ $1:A:25:GLU:GLI:HE2$ $1.81$ $0.81$ $1:A:87:MET:CE$ $1:A:4:GLN:HG2$ $2.09$ $0.81$ $1:A:4:LEU:HD2$ $1:A:27:GLU:GLI:GLI:EU:H$ $1.76$ $0.84$ $1:A:24:PHE:H2$ $1:A:27:GLU:GLI:GLI:GLI:EU:H$ $0.79$ $1:A:4:1:LYS:HD2$ $1:A:27:GLU:GLI:GLI:GLI:GLI:GLI:GLI:GLI:GLI:GLI:GLI$	1:A:148:ARG:O	1:A:148:ARG:HG3	1.56	1.04
1:A:84:ARG:HH221:A:113:VAL:HG231.231.021:A:124:PHE:CD21:A:241:LE:HG121.941.011:A:97:THR:HG211:A:227:VAL:HG211.420.971:A:47:LE:HG231:A:67:ARG:HG31.460.961:A:98:PHE:N1:A:99:PR0:HD21.810.951:A:235:VAL:O1:A:236:PHE:HB31.640.951:A:235:VAL:O1:A:62:PRO:O1.870.911:A:60:THR:C1:A:62:PRO:HD21.910.901:A:34:ARG:NH21:A:113:VAL:HG231.860.891:A:93:LEU:HD231:A:144:GLN:HG31.530.901:A:98:PHE:N1:A:99:PRO:CD2.380.861:A:3:ASN:O1:A:5.TYR:N2.090.851:A:28:HEU:CD21:A:261:LEU:H1.730.841:A:250:GLU:C1:A:261:LEU:H1.730.841:A:250:GLU:C1:A:254:LYS:HG31.760.841:A:249:TYR:O1:A:250:GLU:HG21.810.811:A:41:LYS:HD21:A:272:GLU:OE11.810.811:A:41:LYS:HD21:A:67:AL:HB21.830.791:A:42:LEU:HD221:A:66:VAL:HG21.650.791:A:42:LEU:HD221:A:67:AL:HB12.160.751:A:14:LHC:HB12.160.751:A:240:LEU:HD111:A:240:LEU:HD121:A:230.741:A:241:LE:HD111.490.731:A:241:LE:HD112.30.741:A:241:LE:HD112.30.741:A:241:LE:HD112.30.741:A:241:LE:HD112.30	1:A:22:LYS:HE2	1:A:23:HIS:CE1	1.94	1.02
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1:A:249:TYR:O1:A:250:GLU:HG21.810.811:A:87:MET:CE1:A:144:GLN:HG22.090.811:A:41:LYS:HD21:A:272:GLU:OE11.810.811:A:42:LEU:HD221:A:69:VAL:HG221.650.791:A:6:THR:O1:A:9:ASP:HB21.830.791:A:6:THR:O1:A:35:LEU:HD122.030.791:A:124:PHE:HE21:A:241:ILE:HD111.490.781:A:240:LEU:CD11:A:267:ALA:HB12.160.751:A:110:THR:HG231:A:234:ARG:HD21.670.751:A:235:VAL:HG121:A:236:PHE:H1.530.741:A:274:PHE:CZ1:A:278:LEU:HD112.230.741:A:274:PHE:CZ1:A:278:LEU:HD112.230.731:A:202:THR:HG221:A:204:ALA:H1.540.731:A:273:GLN:O1:A:277:ILE:HG121.890.731:A:25:PRO:HB31:A:79:VAL:HG221.700.721:A:25:PRO:C1:A:64:HIS:H1.900.72	1:A:253:GLU:O	1:A:254:LYS:HG3	1.76	0.84
1:A:87:MET:CE1:A:144:GLN:HG22.090.811:A:41:LYS:HD21:A:272:GLU:OE11.810.811:A:42:LEU:HD221:A:69:VAL:HG221.650.791:A:42:LEU:HD221:A:69:VAL:HG221.650.791:A:6:THR:O1:A:9:ASP:HB21.830.791:A:34:GLY:C1:A:35:LEU:HD122.030.791:A:124:PHE:HE21:A:241:ILE:HD111.490.781:A:240:LEU:CD11:A:267:ALA:HB12.160.751:A:10:THR:HG231:A:234:ARG:HD21.670.751:A:25:VAL:HG121:A:236:PHE:H1.530.741:A:2111:LEU:HB21:A:233:LEU:HD231.700.741:A:274:PHE:CZ1:A:278:LEU:HD112.230.741:A:202:THR:HG221:A:204:ALA:H1.540.731:A:202:THR:HG221:A:204:ALA:H1.540.731:A:254:LYS:O1:A:255:ALA:HB31.890.731:A:25:PRO:HB31:A:79:VAL:HG221.700.721:A:62:PRO:C1:A:64:HIS:H1.900.72	1:A:249:TYR:O	1:A:250:GLU:HG2	1.81	0.81
1:A:41:LYS:HD21:A:272:GLU:OE11.810.811:A:42:LEU:HD221:A:69:VAL:HG221.650.791:A:6:THR:O1:A:9:ASP:HB21.830.791:A:6:THR:O1:A:9:ASP:HB21.830.791:A:34:GLY:C1:A:35:LEU:HD122.030.791:A:124:PHE:HE21:A:241:ILE:HD111.490.781:A:240:LEU:CD11:A:267:ALA:HB12.160.751:A:10:THR:HG231:A:234:ARG:HD21.670.751:A:25:VAL:HG121:A:236:PHE:H1.530.741:A:111:LEU:HB21:A:233:LEU:HD231.700.741:A:274:PHE:CZ1:A:278:LEU:HD112.230.741:A:202:THR:HG221:A:204:ALA:H1.540.731:A:273:GLN:O1:A:277:ILE:HG121.890.731:A:25:PRO:HB31:A:79:VAL:HG221.700.721:A:25:PRO:C1:A:64:HIS:H1.900.72	1:A:87:MET:CE	1:A:144:GLN:HG2	2.09	0.81
1:A:42:LEU:HD221:A:69:VAL:HG221.650.791:A:6:THR:O1:A:9:ASP:HB21.830.791:A:6:THR:O1:A:9:ASP:HB21.830.791:A:34:GLY:C1:A:35:LEU:HD122.030.791:A:124:PHE:HE21:A:241:ILE:HD111.490.781:A:240:LEU:CD11:A:267:ALA:HB12.160.751:A:110:THR:HG231:A:234:ARG:HD21.670.751:A:235:VAL:HG121:A:236:PHE:H1.530.741:A:2111:LEU:HB21:A:233:LEU:HD231.700.741:A:274:PHE:CZ1:A:278:LEU:HD112.230.741:A:202:THR:HG221:A:204:ALA:H1.540.731:A:202:THR:HG221:A:204:ALA:H1.540.731:A:254:LYS:O1:A:255:ALA:HB31.890.731:A:25:PRO:HB31:A:79:VAL:HG221.700.721:A:62:PRO:C1:A:64:HIS:H1.900.72	1:A:41:LYS:HD2	1:A:272:GLU:OE1	1.81	0.81
1:A:6:THR:O1:A:9:ASP:HB21.830.791:A:34:GLY:C1:A:35:LEU:HD122.030.791:A:124:PHE:HE21:A:241:ILE:HD111.490.781:A:240:LEU:CD11:A:267:ALA:HB12.160.751:A:110:THR:HG231:A:234:ARG:HD21.670.751:A:235:VAL:HG121:A:236:PHE:H1.530.741:A:2111:LEU:HB21:A:233:LEU:HD231.700.741:A:274:PHE:CZ1:A:278:LEU:HD112.230.741:A:202:THR:HG221:A:204:ALA:H1.540.731:A:273:GLN:O1:A:277:ILE:HG121.890.731:A:25:PRO:HB31:A:79:VAL:HG221.700.721:A:26:PRO:C1:A:64:HIS:H1.900.72	1:A:42:LEU:HD22	1:A:69:VAL:HG22	1.65	0.79
1:A:34:GLY:C1:A:35:LEU:HD122.030.791:A:124:PHE:HE21:A:241:ILE:HD111.490.781:A:240:LEU:CD11:A:267:ALA:HB12.160.751:A:110:THR:HG231:A:234:ARG:HD21.670.751:A:235:VAL:HG121:A:236:PHE:H1.530.741:A:111:LEU:HB21:A:233:LEU:HD231.700.741:A:274:PHE:CZ1:A:278:LEU:HD112.230.741:A:14:ALA:O1:A:18:LEU:HB21.870.731:A:202:THR:HG221:A:204:ALA:H1.540.731:A:254:LYS:O1:A:255:ALA:HB31.890.731:A:25:PRO:HB31:A:79:VAL:HG221.700.721:A:62:PRO:C1:A:64:HIS:H1.900.72	1:A:6:THR:O	1:A:9:ASP:HB2	1.83	0.79
1:A:124:PHE:HE21:A:241:ILE:HD111.490.781:A:240:LEU:CD11:A:267:ALA:HB12.160.751:A:110:THR:HG231:A:234:ARG:HD21.670.751:A:235:VAL:HG121:A:236:PHE:H1.530.741:A:111:LEU:HB21:A:233:LEU:HD231.700.741:A:274:PHE:CZ1:A:278:LEU:HD112.230.741:A:202:THR:HG221:A:18:LEU:HB21.870.731:A:273:GLN:O1:A:277:ILE:HG121.890.731:A:254:LYS:O1:A:255:ALA:HB31.890.731:A:25:PRO:HB31:A:79:VAL:HG221.700.721:A:62:PRO:C1:A:64:HIS:H1.900.72	1:A:34:GLY:C	1:A:35:LEU:HD12	2.03	0.79
1:A:240:LEU:CD11:A:267:ALA:HB12.160.751:A:110:THR:HG231:A:234:ARG:HD21.670.751:A:235:VAL:HG121:A:236:PHE:H1.530.741:A:111:LEU:HB21:A:233:LEU:HD231.700.741:A:274:PHE:CZ1:A:278:LEU:HD112.230.741:A:14:ALA:O1:A:18:LEU:HB21.870.731:A:202:THR:HG221:A:204:ALA:H1.540.731:A:273:GLN:O1:A:277:ILE:HG121.890.731:A:254:LYS:O1:A:255:ALA:HB31.890.731:A:25:PRO:HB31:A:79:VAL:HG221.700.721:A:62:PRO:C1:A:64:HIS:H1.900.72	1:A:124:PHE:HE2	1:A:241:ILE:HD11	1.49	0.78
1:A:110:THR:HG231:A:234:ARG:HD21.670.751:A:235:VAL:HG121:A:236:PHE:H1.530.741:A:111:LEU:HB21:A:233:LEU:HD231.700.741:A:274:PHE:CZ1:A:278:LEU:HD112.230.741:A:14:ALA:O1:A:18:LEU:HB21.870.731:A:202:THR:HG221:A:204:ALA:H1.540.731:A:273:GLN:O1:A:277:ILE:HG121.890.731:A:254:LYS:O1:A:25:ALA:HB31.890.731:A:25:PRO:HB31:A:79:VAL:HG221.700.721:A:62:PRO:C1:A:64:HIS:H1.900.72	1:A:240:LEU:CD1	1:A:267:ALA:HB1	2.16	0.75
1:A:235:VAL:HG121:A:236:PHE:H1.530.741:A:111:LEU:HB21:A:233:LEU:HD231.700.741:A:274:PHE:CZ1:A:278:LEU:HD112.230.741:A:14:ALA:O1:A:18:LEU:HB21.870.731:A:202:THR:HG221:A:204:ALA:H1.540.731:A:273:GLN:O1:A:277:ILE:HG121.890.731:A:254:LYS:O1:A:255:ALA:HB31.890.731:A:25:PRO:HB31:A:79:VAL:HG221.700.721:A:62:PRO:C1:A:64:HIS:H1.900.72	1:A:110:THR:HG23	1:A:234:ARG:HD2	1.67	0.75
1:A:111:LEU:HB21:A:233:LEU:HD231.700.741:A:274:PHE:CZ1:A:278:LEU:HD112.230.741:A:14:ALA:O1:A:18:LEU:HB21.870.731:A:202:THR:HG221:A:204:ALA:H1.540.731:A:273:GLN:O1:A:277:ILE:HG121.890.731:A:254:LYS:O1:A:255:ALA:HB31.890.731:A:25:PRO:HB31:A:79:VAL:HG221.700.721:A:62:PRO:C1:A:64:HIS:H1.900.72	1:A:235:VAL:HG12	1:A:236:PHE:H	1.53	0.74
1:A:274:PHE:CZ1:A:278:LEU:HD112.230.741:A:14:ALA:O1:A:18:LEU:HB21.870.731:A:202:THR:HG221:A:204:ALA:H1.540.731:A:273:GLN:O1:A:277:ILE:HG121.890.731:A:254:LYS:O1:A:255:ALA:HB31.890.731:A:25:PRO:HB31:A:79:VAL:HG221.700.721:A:62:PRO:C1:A:64:HIS:H1.900.72	1:A:111:LEU:HB2	1:A:233:LEU:HD23	1.70	0.74
1:A:14:ALA:O1:A:18:LEU:HB21.870.731:A:202:THR:HG221:A:204:ALA:H1.540.731:A:273:GLN:O1:A:277:ILE:HG121.890.731:A:254:LYS:O1:A:255:ALA:HB31.890.731:A:25:PRO:HB31:A:79:VAL:HG221.700.721:A:62:PRO:C1:A:64:HIS:H1.900.72	1:A:274:PHE:CZ	1:A:278:LEU:HD11	2.23	0.74
1:A:202:THR:HG221:A:204:ALA:H1.540.731:A:273:GLN:O1:A:277:ILE:HG121.890.731:A:254:LYS:O1:A:255:ALA:HB31.890.731:A:25:PRO:HB31:A:79:VAL:HG221.700.721:A:62:PRO:C1:A:64:HIS:H1.900.72	1:A:14:ALA:O	1:A:18:LEU:HB2	1.87	0.73
1:A:273:GLN:O       1:A:277:ILE:HG12       1.89       0.73         1:A:254:LYS:O       1:A:255:ALA:HB3       1.89       0.73         1:A:25:PRO:HB3       1:A:79:VAL:HG22       1.70       0.72         1:A:62:PRO:C       1:A:64:HIS:H       1.90       0.72	1:A:202:THR:HG22	1:A:204:ALA:H	1.54	0.73
1:A:254:LYS:O         1:A:255:ALA:HB3         1.89         0.73           1:A:25:PRO:HB3         1:A:79:VAL:HG22         1.70         0.72           1:A:62:PRO:C         1:A:64:HIS:H         1.90         0.72	1:A:273:GLN:O	1:A:277:ILE:HG12	1.89	0.73
1:A:25:PRO:HB3         1:A:79:VAL:HG22         1.70         0.72           1:A:62:PRO:C         1:A:64:HIS:H         1.90         0.72	1:A:254:LYS:O	1:A:255:ALA:HB3	1.89	0.73
1:A:62:PRO:C         1:A:64:HIS:H         1.90         0.72           1:A 26 CLV O         1:A 20 THD HD         1.00         0.72	1:A:25:PRO:HB3	1:A:79:VAL:HG22	1.70	0.72
	1:A:62:PRO:C	1:A:64:HIS:H	1.90	0.72
1:A:30:GLY:U   1:A:39:THK:HB   1.89   0.72	1:A:36:GLY:O	1:A:39:THR:HB	1.89	0.72



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:178:TRP:CZ2	1:A:183:GLU:HG2	2.25	0.72
1:A:22:LYS:CE	1:A:23:HIS:CE1	2.72	0.70
1:A:187:LEU:HD23	1:A:187:LEU:O	1.92	0.70
1:A:135:HIS:HA	1:A:192:TYR:O	1.92	0.70
1:A:259:GLU:C	1:A:261:LEU:N	2.44	0.70
1:A:6:THR:O	1:A:9:ASP:N	2.24	0.69
1:A:113:VAL:HG21	1:A:221:THR:HG23	1.73	0.69
1:A:254:LYS:O	1:A:255:ALA:CB	2.40	0.69
1:A:97:THR:HG22	1:A:97:THR:O	1.92	0.69
1:A:29:ILE:HD13	1:A:80:MET:HE3	1.75	0.68
1:A:47:ILE:CG2	1:A:67:ARG:HG3	2.21	0.68
1:A:235:VAL:O	1:A:236:PHE:CB	2.41	0.68
1:A:284:LEU:HD21	1:A:289:SER:HG	1.56	0.68
1:A:125:GLU:OE1	1:A:125:GLU:HA	1.95	0.67
1:A:137:ASN:HB2	1:A:222:VAL:HG11	1.76	0.66
1:A:244:LYS:HD3	1:A:245:VAL:H	1.61	0.66
1:A:84:ARG:HH22	1:A:113:VAL:CG2	2.05	0.65
1:A:60:THR:HG23	1:A:91:TYR:OH	1.96	0.65
1:A:28:ALA:HB1	1:A:103:PHE:CE2	2.33	0.64
1:A:248:ASP:C	1:A:250:GLU:N	2.50	0.64
1:A:3:ASN:O	1:A:4:GLY:C	2.37	0.63
1:A:120:LEU:HD23	1:A:206:CYS:SG	2.38	0.63
1:A:240:LEU:HD11	1:A:267:ALA:HB1	1.78	0.63
1:A:249:TYR:O	1:A:250:GLU:CG	2.47	0.63
1:A:64:HIS:O	1:A:66:GLY:N	2.31	0.63
1:A:235:VAL:HG12	1:A:236:PHE:N	2.13	0.63
1:A:248:ASP:C	1:A:250:GLU:H	1.99	0.62
1:A:240:LEU:HD13	1:A:267:ALA:HB1	1.80	0.62
1:A:139:PRO:O	1:A:144:GLN:HB3	1.98	0.61
1:A:25:PRO:HG3	1:A:70:PHE:HE2	1.65	0.61
1:A:22:LYS:H	1:A:22:LYS:HD3	1.66	0.61
1:A:97:THR:C	1:A:99:PRO:HD2	2.20	0.61
1:A:39:THR:HG22	1:A:40:ASP:N	2.15	0.61
1:A:76:ARG:NH1	1:A:76:ARG:HG2	2.15	0.61
1:A:76:ARG:HG2	1:A:76:ARG:HH11	1.66	0.60
1:A:111:LEU:HD12	1:A:235:VAL:HG13	1.83	0.60
1:A:62:PRO:C	1:A:64:HIS:N	2.55	0.60
1:A:124:PHE:CE2	1:A:241:ILE:HD11	2.34	0.60
1:A:222:VAL:O	1:A:226:ILE:HG13	2.01	0.60
1:A:274:PHE:O	$1:\overline{A:278:LEU:HD12}$	2.02	0.59
1:A:61:VAL:HG23	1:A:62:PRO:HD3	1.83	0.58



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:4:GLY:O	1:A:5:TYR:C	2.39	0.58
1:A:89:GLU:OE1	1:A:91:TYR:HE2	1.86	0.58
1:A:244:LYS:HG3	1:A:245:VAL:N	2.17	0.58
1:A:138:LEU:N	1:A:139:PRO:HD2	2.19	0.58
1:A:168:ARG:O	1:A:172:GLN:HG3	2.03	0.58
1:A:112:VAL:HA	1:A:236:PHE:O	2.04	0.57
1:A:125:GLU:O	1:A:126:VAL:C	2.43	0.57
1:A:271:LEU:HD12	1:A:271:LEU:O	2.05	0.57
1:A:128:ASP:O	1:A:129:ILE:HG12	2.05	0.57
1:A:131:LEU:CD1	1:A:171:ARG:HD2	2.34	0.57
1:A:207:ARG:NH1	1:A:246:ILE:O	2.37	0.57
1:A:120:LEU:HD11	1:A:217:VAL:HB	1.87	0.57
1:A:6:THR:H	1:A:9:ASP:HB2	1.70	0.57
1:A:238:PHE:CE1	1:A:274:PHE:HE2	2.23	0.56
1:A:44:GLN:HB2	1:A:72:PHE:HD2	1.70	0.56
1:A:89:GLU:HB3	1:A:91:TYR:CE2	2.39	0.56
1:A:97:THR:O	1:A:97:THR:CG2	2.53	0.56
1:A:234:ARG:HG3	1:A:234:ARG:HH11	1.71	0.56
1:A:138:LEU:N	1:A:139:PRO:CD	2.69	0.56
1:A:242:THR:O	1:A:243:ASN:CB	2.53	0.56
1:A:42:LEU:HD13	1:A:80:MET:SD	2.46	0.56
1:A:174:ALA:HA	1:A:278:LEU:HD21	1.87	0.55
1:A:167:ASP:O	1:A:171:ARG:HG3	2.07	0.55
1:A:92:PRO:HB2	1:A:94:TRP:NE1	2.22	0.55
1:A:73:LEU:HD11	1:A:276:SER:OG	2.07	0.55
1:A:202:THR:HG22	1:A:204:ALA:N	2.22	0.54
1:A:160:PRO:HG3	1:A:230:HIS:HD2	1.72	0.54
1:A:22:LYS:HD3	1:A:22:LYS:N	2.23	0.54
1:A:274:PHE:CE2	1:A:278:LEU:HD11	2.43	0.53
1:A:244:LYS:HG3	1:A:245:VAL:O	2.08	0.53
1:A:60:THR:C	1:A:62:PRO:CD	2.63	0.53
1:A:238:PHE:CZ	1:A:278:LEU:HD13	2.43	0.53
1:A:194:MET:HB3	1:A:222:VAL:HG21	1.91	0.53
1:A:244:LYS:CG	1:A:245:VAL:N	2.72	0.53
1:A:242:THR:O	1:A:243:ASN:HB3	2.09	0.52
1:A:123:LYS:O	1:A:123:LYS:HD3	2.09	0.52
1:A:194:MET:CB	1:A:222:VAL:HG21	2.39	0.52
1:A:271:LEU:O	1:A:275:VAL:HG12	2.09	0.52
1:A:238:PHE:HZ	1:A:278:LEU:HD13	1.72	0.52
1:A:42:LEU:HD23	1:A:71:GLY:HA3	1.90	0.52
1:A:121:ASN:ND2	1:A:215:ASP:OD1	2.42	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:251:SER:O	1:A:252:LEU:CB	2.58	0.52
1:A:31:CYS:HA	1:A:114:THR:OG1	2.11	0.52
1:A:69:VAL:HG13	1:A:80:MET:HB3	1.92	0.52
1:A:251:SER:O	1:A:252:LEU:HB2	2.10	0.51
1:A:42:LEU:CD2	1:A:69:VAL:HG22	2.39	0.51
1:A:73:LEU:HB3	1:A:78:CYS:SG	2.50	0.51
1:A:235:VAL:CG1	1:A:236:PHE:H	2.22	0.51
1:A:263:ALA:O	1:A:268:ALA:HB2	2.11	0.51
1:A:43:THR:CG2	1:A:44:GLN:N	2.74	0.50
1:A:124:PHE:CE2	1:A:241:ILE:CD1	2.94	0.50
1:A:124:PHE:CD2	1:A:241:ILE:CG1	2.81	0.50
1:A:127:GLY:O	1:A:128:ASP:O	2.28	0.50
1:A:22:LYS:HE2	1:A:23:HIS:ND1	2.24	0.50
1:A:34:GLY:C	1:A:35:LEU:CD1	2.77	0.50
1:A:222:VAL:HB	1:A:223:PRO:HD3	1.94	0.50
1:A:207:ARG:O	1:A:211:LYS:HB2	2.11	0.50
1:A:84:ARG:NH2	1:A:113:VAL:CG2	2.68	0.50
1:A:137:ASN:HB2	1:A:222:VAL:CG1	2.41	0.50
1:A:152:ASP:C	1:A:154:ARG:H	2.15	0.50
1:A:103:PHE:O	1:A:106:LEU:HB2	2.12	0.49
1:A:113:VAL:CG2	1:A:221:THR:HG23	2.42	0.49
1:A:111:LEU:CB	1:A:233:LEU:HD23	2.41	0.49
1:A:89:GLU:CB	1:A:91:TYR:CE2	2.96	0.49
1:A:206:CYS:SG	1:A:244:LYS:HD2	2.52	0.49
1:A:96:VAL:CG2	1:A:97:THR:N	2.76	0.49
1:A:287:LYS:O	1:A:288:ALA:HB3	2.13	0.49
1:A:92:PRO:HB2	1:A:94:TRP:CE2	2.48	0.48
1:A:49:ASP:C	1:A:51:SER:H	2.16	0.48
1:A:97:THR:CG2	1:A:227:VAL:HG21	2.28	0.48
1:A:165:ALA:HB3	1:A:166:TYR:CD1	2.48	0.48
1:A:128:ASP:C	1:A:129:ILE:HG12	2.35	0.47
1:A:176:SER:O	1:A:179:LYS:HB2	2.14	0.47
1:A:202:THR:HB	1:A:205:GLU:HG3	1.96	0.47
1:A:193:VAL:HG13	1:A:193:VAL:O	2.15	0.47
1:A:227:VAL:HG12	1:A:227:VAL:O	2.15	0.47
1:A:242:THR:O	1:A:242:THR:OG1	2.31	0.47
1:A:25:PRO:HG3	1:A:70:PHE:CE2	2.47	0.47
1:A:42:LEU:HD22	1:A:69:VAL:CG2	2.39	0.47
1:A:120:LEU:CD2	1:A:206:CYS:SG	3.02	0.47
1:A:184:GLN:HE21	1:A:184:GLN:C	2.17	0.47
1:A:240:LEU:O	1:A:240:LEU:HG	2.13	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:249:TYR:C	1:A:250:GLU:HG2	2.34	0.47
1:A:42:LEU:CD2	1:A:71:GLY:HA3	2.45	0.47
1:A:37:GLY:C	1:A:39:THR:H	2.17	0.46
1:A:50:TYR:OH	1:A:81:MET:HG2	2.15	0.46
1:A:29:ILE:HD13	1:A:80:MET:CE	2.44	0.46
1:A:152:ASP:O	1:A:154:ARG:N	2.49	0.46
1:A:98:PHE:O	1:A:102:VAL:HG13	2.15	0.46
1:A:243:ASN:HB2	1:A:244:LYS:H	1.36	0.46
1:A:43:THR:HG23	1:A:44:GLN:N	2.31	0.45
1:A:252:LEU:HD23	1:A:252:LEU:HA	1.73	0.45
1:A:2:GLU:HG3	1:A:4:GLY:H	1.81	0.45
1:A:251:SER:O	1:A:252:LEU:HG	2.16	0.45
1:A:38:LEU:CD2	1:A:275:VAL:HG11	2.46	0.45
1:A:98:PHE:H	1:A:99:PRO:HD2	1.75	0.45
1:A:137:ASN:CB	1:A:222:VAL:HG11	2.46	0.45
1:A:126:VAL:HG22	1:A:242:THR:HA	1.98	0.45
1:A:195:VAL:O	1:A:219:MET:HA	2.16	0.45
1:A:87:MET:HE3	1:A:144:GLN:HG2	1.97	0.45
1:A:25:PRO:CB	1:A:79:VAL:HG22	2.43	0.44
1:A:131:LEU:CD2	1:A:238:PHE:CD1	3.00	0.44
1:A:139:PRO:CG	1:A:194:MET:HG2	2.47	0.44
1:A:131:LEU:HB2	1:A:188:GLN:O	2.17	0.44
1:A:34:GLY:O	1:A:35:LEU:CD1	2.31	0.44
1:A:66:GLY:HA2	1:A:82:GLN:O	2.18	0.44
1:A:22:LYS:H	1:A:22:LYS:CD	2.30	0.44
1:A:23:HIS:O	1:A:25:PRO:HD3	2.17	0.44
1:A:34:GLY:N	2:A:292:SO4:O3	2.50	0.44
1:A:21:THR:HG23	1:A:23:HIS:H	1.82	0.44
1:A:131:LEU:HD23	1:A:238:PHE:CD1	2.53	0.43
1:A:38:LEU:HD12	1:A:38:LEU:O	2.19	0.43
1:A:178:TRP:CE2	1:A:183:GLU:HG2	2.54	0.43
1:A:119:GLY:O	1:A:244:LYS:CB	2.66	0.43
1:A:38:LEU:HD22	1:A:275:VAL:HG11	2.01	0.43
1:A:74:ASN:CG	1:A:74:ASN:O	2.56	0.43
1:A:81:MET:SD	1:A:99:PRO:HB3	2.58	0.43
1:A:25:PRO:HG2	1:A:106:LEU:HD23	2.01	0.43
1:A:117:ALA:O	1:A:241:ILE:HA	2.19	0.43
1:A:131:LEU:CD2	1:A:238:PHE:CE1	3.02	0.43
1:A:160:PRO:HG3	1:A:230:HIS:CD2	2.54	0.42
1:A:257:HIS:O	1:A:257:HIS:CG	2.71	0.42
1:A:49:ASP:HA	1:A:67:ARG:HB2	2.02	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:93:LEU:HD13	1:A:93:LEU:HA	1.73	0.42
1:A:6:THR:HG23	1:A:8:GLU:HB2	2.02	0.42
1:A:7:TYR:HD2	1:A:155:PHE:CE2	2.37	0.42
1:A:208:VAL:CG2	1:A:209:LEU:N	2.83	0.42
1:A:37:GLY:C	1:A:39:THR:N	2.73	0.42
1:A:38:LEU:HA	1:A:272:GLU:HG2	2.00	0.42
1:A:176:SER:O	1:A:179:LYS:N	2.52	0.42
1:A:175:LEU:HD12	1:A:175:LEU:HA	1.73	0.42
1:A:152:ASP:C	1:A:154:ARG:N	2.73	0.41
1:A:202:THR:HB	1:A:205:GLU:CG	2.50	0.41
1:A:38:LEU:HG	1:A:80:MET:CE	2.50	0.41
1:A:285:PRO:CG	1:A:286:ASP:H	2.27	0.41
1:A:114:THR:O	1:A:115:ASN:HB3	2.20	0.41
1:A:240:LEU:HD21	1:A:263:ALA:HA	2.02	0.41
1:A:235:VAL:CG1	1:A:236:PHE:N	2.79	0.41
1:A:248:ASP:O	1:A:250:GLU:N	2.54	0.41
1:A:28:ALA:CB	1:A:103:PHE:CD2	3.04	0.41
1:A:132:ILE:HD13	1:A:132:ILE:HG21	1.87	0.41
1:A:93:LEU:HD23	1:A:144:GLN:CG	2.38	0.41
1:A:203:VAL:O	1:A:207:ARG:HG2	2.21	0.41
1:A:222:VAL:H	1:A:222:VAL:HG23	1.62	0.41
1:A:41:LYS:O	1:A:42:LEU:C	2.57	0.40
1:A:224:GLU:H	1:A:224:GLU:HG2	1.47	0.40
1:A:220:SER:O	1:A:221:THR:HB	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	287/289~(99%)	218 (76%)	46 (16%)	23~(8%)	1 0



Mol	Chain	Res	Type
1	А	2	GLU
1	А	4	GLY
1	А	61	VAL
1	А	62	PRO
1	А	65	ALA
1	А	128	ASP
1	А	236	PHE
1	А	243	ASN
1	А	250	GLU
1	А	252	LEU
1	А	285	PRO
1	А	33	SER
1	А	118	GLY
1	А	246	ILE
1	А	255	ALA
1	А	153	GLU
1	А	180	GLN
1	А	221	THR
1	A	288	ALA
1	А	254	LYS
1	А	108	VAL
1	A	126	VAL
1	А	182	GLY

All (23) Ramachandran outliers are listed below:

#### 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	240/240~(100%)	176 (73%)	64 (27%)	0 0

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	1	MET
1	А	2	GLU



Mol	Chain	Res	Type
1	А	6	THR
1	А	21	THR
1	А	22	LYS
1	А	31	CYS
1	А	39	THR
1	А	40	ASP
1	А	42	LEU
1	А	43	THR
1	А	44	GLN
1	А	56	PHE
1	А	58	ARG
1	А	59	SER
1	А	61	VAL
1	А	67	ARG
1	А	69	VAL
1	А	78	CYS
1	А	79	VAL
1	А	80	MET
1	А	86	HIS
1	А	93	LEU
1	А	96	VAL
1	А	102	VAL
1	А	105	LEU
1	А	112	VAL
1	А	123	LYS
1	А	126	VAL
1	А	128	ASP
1	А	129	ILE
1	А	131	LEU
1	А	135	HIS
1	А	147	LEU
1	A	148	ARG
1	А	151	ASN
1	A	$15\overline{2}$	ASP
1	А	153	GLU
1	A	158	ARG
1	A	167	ASP
1	А	168	ARG
1	A	175	LEU
1	А	184	GLN
1	A	185	ARG
1	А	187	LEU



Mol	Chain	Res	Type
1	А	207	ARG
1	А	208	VAL
1	А	219	MET
1	А	224	GLU
1	А	229	ARG
1	А	234	ARG
1	А	236	PHE
1	А	239	SER
1	А	242	THR
1	А	246	ILE
1	А	249	TYR
1	А	256	ASN
1	А	261	LEU
1	А	266	GLN
1	A	269	GLN
1	A	271	LEU
1	А	273	GLN
1	А	276	SER
1	А	281	SER
1	А	284	LEU

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

Mol	Chain	Res	Type
1	А	23	HIS
1	А	151	ASN
1	А	184	GLN
1	А	256	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)

3 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 Tuno	Chain	Dog	Link	В	Bond lengths			Bond angles		
IVIOI	Type Chain Res	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
2	SO4	А	292	-	4,4,4	0.70	0	$6,\!6,\!6$	0.21	0
3	GUN	А	290	-	7,12,12	1.52	1 (14%)	8,17,17	0.78	0
2	SO4	А	291	-	4,4,4	0.68	0	6,6,6	0.46	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
3	GUN	А	290	-	-	-	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
3	А	290	GUN	C5-C6	-3.42	1.40	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	292	SO4	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	А	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	А	239:SER	С	240:LEU	N	1.10



## 6 Fit of model and data (i)

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

