

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

#### Feb 4, 2024 – 12:09 PM EST

PDB ID	:	1R3N
Title	:	Crystal structure of beta-alanine synthase from Saccharomyces kluyveri
Authors	:	Lundgren, S.; Gojkovic, Z.; Piskur, J.; Dobritzsch, D.
Deposited on	:	2003-10-02
Resolution	:	2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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)	:	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)
Validation Pipeline (wwPDB-VP)	:	2.36

## 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 2.70 Å.

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



Motrie	Whole archive	Similar resolution
WIEUTIC	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
R <sub>free</sub>	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain		
1	А	462	73%	19%	• 5%
1	В	462	71%	21%	• 6%
1	С	462	76%	16%	• 5%
1	D	462	75%	17%	• 5%
1	Е	462	64% 2	26%	5% 6%
1	F	462	76%	16%	• 5%
1	G	462	65% 2	24%	• 7%



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Mol	Chain	Length	Quality of chain		
1	Н	462	73%	19%	• 5%



## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 27487 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		Atoms					AltConf	Trace
1	Δ	138	Total	С	Ν	0	S	0	0	0
1	A	430	3379	2130	580	653	16	0	0	0
1	В	433	Total	С	Ν	0	S	0	0	0
1	D	400	3344	2108	574	646	16	0	0	0
1	С	138	Total	С	Ν	0	S	0	0	0
1		438	3379	2130	580	653	16	0	0	0
1	Л	437	Total	С	Ν	0	S	0	0	0
1	D	437	3375	2128	579	652	16	0	0	U
1	F	433	Total	С	Ν	0	S	0	0	0
1	Ľ	400	3344	2108	574	646	16	0	0	U
1	Б	138	Total	С	Ν	0	S	0	0	0
1	Г	430	3379	2130	580	653	16	0	0	0
1	C	420	Total	С	Ν	0	S	0	0	0
1	G	430	3327	2097	571	643	16	0	0	0
1	ц	138	Total	С	Ν	0	S	0	0	0
	п	400	3379	2130	580	653	16	0	0	0

• Molecule 1 is a protein called beta-alanine synthase.

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	456	HIS	-	expression tag	UNP Q96W94
А	457	HIS	-	expression tag	UNP Q96W94
А	458	HIS	-	expression tag	UNP Q96W94
А	459	HIS	-	expression tag	UNP Q96W94
А	460	HIS	-	expression tag	UNP Q96W94
А	461	HIS	-	expression tag	UNP Q96W94
А	462	HIS	-	expression tag	UNP Q96W94
А	463	HIS	-	expression tag	UNP Q96W94
В	456	HIS	-	expression tag	UNP Q96W94
В	457	HIS	-	expression tag	UNP Q96W94
В	458	HIS	-	expression tag	UNP Q96W94
В	459	HIS	-	expression tag	UNP Q96W94
В	460	HIS	-	expression tag	UNP Q96W94



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Chain	Residue	Modelled	Actual	Comment	Reference
В	461	HIS	-	expression tag	UNP Q96W94
В	462	HIS	-	expression tag	UNP Q96W94
В	463	HIS	-	expression tag	UNP Q96W94
С	456	HIS	-	expression tag	UNP Q96W94
С	457	HIS	-	expression tag	UNP Q96W94
С	458	HIS	-	expression tag	UNP Q96W94
С	459	HIS	-	expression tag	UNP Q96W94
С	460	HIS	-	expression tag	UNP Q96W94
С	461	HIS	-	expression tag	UNP Q96W94
С	462	HIS	-	expression tag	UNP Q96W94
С	463	HIS	-	expression tag	UNP Q96W94
D	456	HIS	-	expression tag	UNP Q96W94
D	457	HIS	-	expression tag	UNP Q96W94
D	458	HIS	-	expression tag	UNP Q96W94
D	459	HIS	-	expression tag	UNP Q96W94
D	460	HIS	-	expression tag	UNP Q96W94
D	461	HIS	-	expression tag	UNP Q96W94
D	462	HIS	-	expression tag	UNP Q96W94
D	463	HIS	-	expression tag	UNP Q96W94
Е	456	HIS	-	expression tag	UNP Q96W94
Е	457	HIS	-	expression tag	UNP Q96W94
Е	458	HIS	-	expression tag	UNP Q96W94
Е	459	HIS	-	expression tag	UNP Q96W94
Е	460	HIS	-	expression tag	UNP Q96W94
Е	461	HIS	-	expression tag	UNP Q96W94
Е	462	HIS	-	expression tag	UNP Q96W94
Е	463	HIS	-	expression tag	UNP Q96W94
F	456	HIS	-	expression tag	UNP Q96W94
F	457	HIS	-	expression tag	UNP Q96W94
F	458	HIS	-	expression tag	UNP Q96W94
F	459	HIS	-	expression tag	UNP Q96W94
F	460	HIS	-	expression tag	UNP Q96W94
F	461	HIS	-	expression tag	UNP Q96W94
F	462	HIS	-	expression tag	UNP Q96W94
F	463	HIS	-	expression tag	UNP Q96W94
G	456	HIS	-	expression tag	UNP Q96W94
G	457	HIS	-	expression tag	UNP Q96W94
G	458	HIS	-	expression tag	UNP Q96W94
G	459	HIS	-	expression tag	UNP Q96W94
G	460	HIS	-	expression tag	UNP Q96W94
G	461	HIS	-	expression tag	UNP Q96W94
G	462	HIS	-	expression tag	UNP Q96W94

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Chain	Residue	Modelled	Actual	Comment	Reference			
G	463	HIS	-	expression tag	UNP Q96W94			
Н	456	HIS	-	expression tag	UNP Q96W94			
Н	457	HIS	-	expression tag	UNP Q96W94			
Н	458	HIS	-	expression tag	UNP Q96W94			
Н	459	HIS	-	expression tag	UNP Q96W94			
Н	460	HIS	-	expression tag	UNP Q96W94			
Н	461	HIS	-	expression tag	UNP Q96W94			
Н	462	HIS	-	expression tag	UNP Q96W94			
Н	463	HIS	-	expression tag	UNP Q96W94			

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• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	2	Total Zn 2 2	0	0
2	В	2	Total Zn 2 2	0	0
2	С	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	Е	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0
2	G	2	Total Zn 2 2	0	0
2	Н	2	Total Zn 2 2	0	0

• Molecule 3 is BETA-AMINO ISOBUTYRATE (three-letter code: BIB) (formula: C<sub>4</sub>H<sub>8</sub>NO<sub>2</sub>).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccccc} \text{Total} & \text{C} & \text{N} & \text{O} \\ \hline 7 & 4 & 1 & 2 \end{array}$	0	0
3	В	1	$\begin{array}{ccccc} \text{Total} & \text{C} & \text{N} & \text{O} \\ \hline 7 & 4 & 1 & 2 \end{array}$	0	0
3	С	1	$\begin{array}{ccccc} \text{Total} & \text{C} & \text{N} & \text{O} \\ \hline 7 & 4 & 1 & 2 \end{array}$	0	0
3	D	1	$\begin{array}{ccccc} \text{Total} & \text{C} & \text{N} & \text{O} \\ 7 & 4 & 1 & 2 \end{array}$	0	0
3	Е	1	$\begin{array}{ccccc} \text{Total} & \text{C} & \text{N} & \text{O} \\ 7 & 4 & 1 & 2 \end{array}$	0	0
3	Е	1	$\begin{array}{ccccc} \text{Total} & \text{C} & \text{N} & \text{O} \\ 7 & 4 & 1 & 2 \end{array}$	0	0
3	G	1	$\begin{array}{ccccc} \text{Total} & \text{C} & \text{N} & \text{O} \\ 7 & 4 & 1 & 2 \end{array}$	0	0
3	G	1	$\begin{array}{ccccc} \text{Total} & \text{C} & \text{N} & \text{O} \\ 7 & 4 & 1 & 2 \end{array}$	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	109	Total O 109 109	0	0
4	В	60	Total         O           60         60	0	0
4	С	91	Total O 91 91	0	0
4	D	54	$\begin{array}{cc} \text{Total} & \text{O} \\ 54 & 54 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Е	20	TotalO2020	0	0
4	F	101	Total         O           101         101	0	0
4	G	24	$\begin{array}{cc} \text{Total} & \text{O} \\ 24 & 24 \end{array}$	0	0
4	Н	50	Total         O           50         50	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.



 $\bullet$  Molecule 1: beta-alanine synthase

• Molecule 1: beta-alanine synthase





## 1318 P119 1319 1115 1319 1125 1314 1125 13256 1134 1344 1134 1344 1134 1344 1134 1344 1134 1344 1134 1344 1134 1344 1134 1344 1134 1344 1134 1344 1134 1344 1134 1345 1134 1346 1153 1347 1134 1346 1154 1347 1154 1346 1156 1347 1143 1400 1176 1419 1199 1419 1199 1419 1199 1419 1190 1419 1190 1419 1190 1419 1190 1419 1190 1419 1190 1419 1190 1411 1200 1413 1200 1413 1200 1413 1200 1415 1200 1415 1200 <









# F317 F119 F317 F119 T316 1136 T316 1136 T316 1136 D326 1136 D345 1136 T316 1136 T346 1136 T346 1136 N347 1136 N345 1136 N346 1136 N347 1136 N346 1136 N347 1136 N346 1136 N347 1136 N347 1136 N347 1136 N347 1136 N347 1136 N347 1136 N346 1136 N347 1136 N347 1136 N347 1136 N346 1204 N386 1206 N386 1206 N386 1206 N386 1206 N401</t

## SIH

 $\bullet$  Molecule 1: beta-alanine synthase

Chain G:	65%	24% •	7%							
SER LYS ASP ASP ASP ASP ASP THR THR THR THR THR SER ALA ASP ASP ASP ASP ASP ASP ASP ASP ASP AS	LAN PRD ALA ALA ALA ALA ALA P27 P27 P28 P37 P37 P37 P37 P37 P37 P37 P37 P37 P37	R62 R74 E82 E82 S83 K87 K87 K88 K89	K92 193 K103 G106 K107							
T111 512 512 512 612 0118 0118 0118 0125 6128 0128 0139 V130 V130 V130 V144 V144 V144 V144	V146 146 150 150 153 155 155 151 156 1515 171 176 1176 1176	V189 6191 6191 8192 8193 8193 8195 7198 0199	5200 N203 Y206 T207 T210							
K215 E216 E216 E216 F223 F223 F223 F223 F223 F223 F223 F22	42.02 42.02 42.02 42.68 42.66 42.66 42.73 42.66 42.91 42.91 42.95 42.95 42.95 42.95 42.96	S316 F317 F317 T318 T319 D320 F321 R322 R322 R322 R322 R322 S325	V328 M332 K334 K334 E339							
R342 K345 K345 K345 L356 L356 C356 E369 E369 E369 E369 E369 E369 E369 E36	D386 D386 R389 Q390 Q390 Q393 N392 N392 N392 N392 N403 A403 A403 A403 A403 A403 A403 A403 A	D417 C418 C419 S420 Y423 S427 S427 S427 S427 S427 S427 S427	6435 V438 L440 L440 Q441 A442 I444							
N445 7446 H465 H455 H155 H155 H155 H155 H155 H155 H15										
• Molecule 1: beta-alanine synthase										

Ch	ain	H	:												-	73'	%														19	}%			•	59	%				
SER LYS	ASP VAL	SER	THR ILE	THR	THR VAL	SER	ALA	PRO	ASP	G18 T10		S29	130	A31	700	Q37	T38	E41	T42	пле	140	R51	452 653	Q54	H57		R63		D70	M73	R74	F77	T78	KR7		193	96M	0011	K103	G106	K107
T111	D116	E120	K123	Y124	0125 G126	1127	I 1 24	E135	-	R138	K141	D142		V153	V155		C168	S172		S175	V189		D192 K193	P194	Y206		T210	P211	K015	E216		~~~~	1227	1030	2021	E236	1240		09ZN	W268	R269
M281	S286	<mark>q</mark> 290	D302		F317 T318	L319	пала	P324	<b>S325</b>	D326	K334		D341	TOA A	1345 K345	I346	N347	0707	E355	<b>S356</b>	V361		F367	C371	S378	V 06/1	K385	D386	R389		<b>8399</b>	T402	A403	P404 H405	V406	P407	1400 S409	M410	I413		D417
¥423	E433	F436	K437 V438		<mark>1441</mark>	D447	WAE1	T CT- A	H455	HIS	STH	SIH	HIS	HIS	SIH																										



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	117.23Å 77.12Å 225.52Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $95.05^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution (Å)	25.00 - 2.70	Depositor
	24.90 - 2.70	EDS
% Data completeness	95.8 (25.00-2.70)	Depositor
(in resolution range)	95.9(24.90-2.70)	EDS
$R_{merge}$	0.08	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.00 (at 2.72 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R R.	0.208 , $0.266$	Depositor
$\Pi, \Pi_{free}$	0.292 , $0.324$	DCC
$R_{free}$ test set	5296 reflections $(4.99\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	44.8	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.33, 19.4	EDS
L-test for $twinning^2$	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	27487	wwPDB-VP
Average B, all atoms $(Å^2)$	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 56.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5506e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<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: ZN, BIB

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	B	ond angles
	Unain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.56	1/3457~(0.0%)	0.80	15/4689~(0.3%)
1	В	0.43	0/3422	0.75	14/4640~(0.3%)
1	С	0.52	0/3457	0.75	6/4689~(0.1%)
1	D	0.44	0/3453	0.73	8/4684~(0.2%)
1	Е	0.39	0/3422	0.71	10/4640~(0.2%)
1	F	0.49	0/3457	0.73	7/4689~(0.1%)
1	G	0.38	0/3404	0.72	13/4615~(0.3%)
1	Н	0.44	0/3457	0.74	12/4689~(0.3%)
All	All	0.46	1/27529~(0.0%)	0.74	85/37335~(0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	105	GLY	C-O	-9.59	1.08	1.23

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	Н	125	ASP	CB-CG-OD2	9.55	126.90	118.30
1	В	125	ASP	CB-CG-OD2	8.89	126.30	118.30
1	А	105	GLY	CA-C-N	8.52	133.25	116.20
1	D	125	ASP	CB-CG-OD2	7.93	125.44	118.30
1	А	309	ASN	CB-CA-C	-7.89	94.61	110.40

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	3379	0	3264	49	0
1	В	3344	0	3227	39	1
1	С	3379	0	3264	44	0
1	D	3375	0	3261	39	0
1	Е	3344	0	3227	73	0
1	F	3379	0	3264	41	0
1	G	3327	0	3209	51	1
1	Н	3379	0	3264	44	0
2	А	2	0	0	0	0
2	В	2	0	0	0	0
2	С	2	0	0	0	0
2	D	2	0	0	0	0
2	Е	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	Н	2	0	0	0	0
3	А	7	0	8	1	0
3	В	7	0	8	0	0
3	С	7	0	8	0	0
3	D	7	0	8	0	0
3	Е	14	0	16	0	0
3	G	14	0	16	0	0
4	А	109	0	0	4	0
4	В	60	0	0	3	0
4	С	91	0	0	2	0
4	D	54	0	0	3	0
4	Е	20	0	0	0	0
4	F	101	0	0	3	0
4	G	24	0	0	3	0
4	Н	50	0	0	2	0
All	All	27487	0	26044	370	1

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 7.

The worst 5 of 370 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:VAL:HG23	1:D:190:GLY:H	1.24	1.03
1:E:118:GLN:HG3	1:E:119:PRO:HD2	1.47	0.96
1:E:71:GLY:HA3	1:E:204:ILE:CG2	1.97	0.94
1:H:346:ILE:HD11	4:H:511:HOH:O	1.68	0.93
1:B:55:GLU:HB2	1:B:58:GLU:HG3	1.49	0.90

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ASN:ND2	1:G:144:ASN:O[1_565]	1.98	0.22

#### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	А	436/462~(94%)	420 (96%)	16 (4%)	0	100	100
1	В	431/462~(93%)	418 (97%)	11 (3%)	2~(0%)	29	54
1	С	436/462~(94%)	420 (96%)	14 (3%)	2~(0%)	29	54
1	D	435/462~(94%)	419 (96%)	12 (3%)	4 (1%)	17	40
1	Е	431/462 (93%)	417 (97%)	12 (3%)	2(0%)	29	54
1	F	436/462~(94%)	422 (97%)	12 (3%)	2~(0%)	29	54
1	G	428/462 (93%)	411 (96%)	13 (3%)	4 (1%)	17	40
1	Н	436/462~(94%)	422 (97%)	13 (3%)	1 (0%)	47	73
All	All	3469/3696~(94%)	3349 (96%)	103 (3%)	17 (0%)	29	54

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type			
1	D	20	LEU			
Continued on next page						



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	v	-	1 0
Mol	Chain	$\mathbf{Res}$	Type
1	В	106	GLY
1	В	454	GLY
1	С	21	ASN
1	С	106	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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percer	ntiles
1	А	360/383~(94%)	323~(90%)	37~(10%)	7	16
1	В	356/383~(93%)	314 (88%)	42 (12%)	5	12
1	С	360/383~(94%)	332~(92%)	28 (8%)	12	29
1	D	360/383~(94%)	317 (88%)	43 (12%)	5	12
1	Ε	356/383~(93%)	284 (80%)	72 (20%)	1	3
1	F	360/383~(94%)	321 (89%)	39 (11%)	6	15
1	G	355/383~(93%)	289 (81%)	66~(19%)	1	4
1	Н	360/383~(94%)	325 (90%)	35 (10%)	8	19
All	All	2867/3064~(94%)	2505 (87%)	362 (13%)	4	10

5 of 362 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	F	103	LYS
1	G	200	SER
1	F	192	ASP
1	F	455	HIS
1	G	293	ASN

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such side chains are listed below:

Mol	Chain	Res	Type			
1	D	252	GLN			



Continued from previous page...

Mol	Chain	Res	Type
1	G	434	ASN
1	Е	397	HIS
1	G	405	HIS
1	G	118	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)

Of 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 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	Type	Chain	Dog	Tink	B	ond leng	$\operatorname{gths}$	E	Bond ang	gles
	Type	Ullalli	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BIB	G	8502	-	$5,\!6,\!6$	1.00	0	4,7,7	1.04	0
3	BIB	G	7502	-	$5,\!6,\!6$	0.90	0	4,7,7	0.93	0
3	BIB	В	1502	-	5,6,6	1.02	0	4,7,7	1.20	0
3	BIB	А	2502	-	5,6,6	0.99	0	4,7,7	0.79	0
3	BIB	D	4502	-	5,6,6	0.98	0	4,7,7	0.92	0
3	BIB	Е	6502	-	5,6,6	0.87	0	4,7,7	1.19	0
3	BIB	С	3502	-	5,6,6	1.01	0	4,7,7	1.05	0
3	BIB	E	5502	-	5,6,6	1.01	0	4,7,7	0.76	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	BIB	G	8502	-	-	0/5/6/6	-
3	BIB	G	7502	-	-	0/5/6/6	-
3	BIB	В	1502	-	-	1/5/6/6	-
3	BIB	А	2502	-	-	0/5/6/6	-
3	BIB	D	4502	-	-	0/5/6/6	-
3	BIB	Е	6502	-	-	2/5/6/6	-
3	BIB	С	3502	-	-	0/5/6/6	-
3	BIB	Е	5502	-	-	0/5/6/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Е	6502	BIB	C4-C3-C5-O7
3	Е	6502	BIB	C4-C3-C5-O6
3	В	1502	BIB	C2-C3-C4-N1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	2502	BIB	1	0

#### 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)

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.

