



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:11 PM GMT

PDB ID : 1J4T  
Title : Structure of Artocarpin: a Lectin with Mannose Specificity (Form 2)  
Authors : Pratap, J.V.; Jeyaprakash, A.A.; Rani, P.G.; Sekar, K.; Surolia, A.; Vijayan, M.  
Deposited on : 2001-10-30  
Resolution : 2.40 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

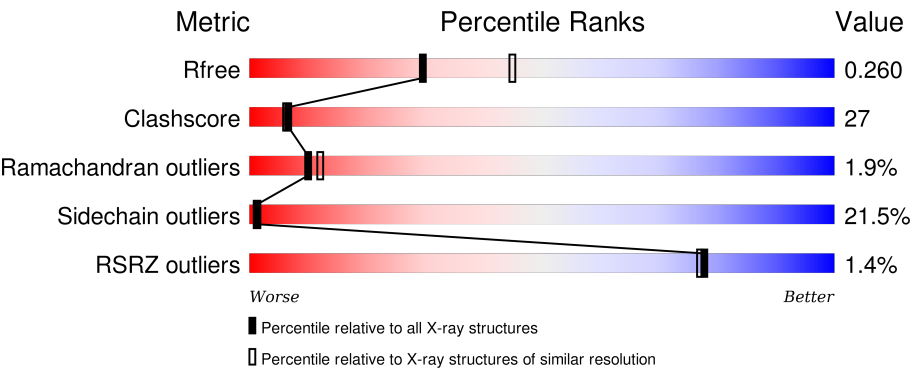
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	149	<div><div>%</div><div><div></div><div>26%</div><div>46%</div><div>22%</div><div>7%</div></div></div>
1	B	149	<div><div></div><div>28%</div><div>46%</div><div>19%</div><div>6%</div></div>
1	C	149	<div><div>%</div><div><div></div><div>28%</div><div>46%</div><div>19%</div><div>7%</div></div></div>
1	D	149	<div><div>3%</div><div><div></div><div>27%</div><div>40%</div><div>27%</div><div>7%</div></div></div>
1	E	149	<div><div>%</div><div><div></div><div>36%</div><div>40%</div><div>20%</div><div>5%</div></div></div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	149	
1	G	149	
1	H	149	

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
1	AYA	A	1	X	-	-	-
1	AYA	B	1	X	X	X	-
1	AYA	C	1	X	-	-	-
1	AYA	E	1	X	-	-	-
1	AYA	G	1	X	-	-	-
1	AYA	H	1	X	-	-	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9922 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 Artocarpin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	0	0
			1132	727	182	222	1			
1	B	149	Total	C	N	O	S	0	0	0
			1132	727	182	222	1			
1	C	149	Total	C	N	O	S	0	0	0
			1132	727	182	222	1			
1	D	149	Total	C	N	O	S	0	0	0
			1132	727	182	222	1			
1	E	149	Total	C	N	O	S	0	0	0
			1128	724	181	222	1			
1	F	149	Total	C	N	O	S	0	0	0
			1128	724	181	222	1			
1	G	149	Total	C	N	O	S	0	0	0
			1132	727	182	222	1			
1	H	149	Total	C	N	O	S	0	0	0
			1132	727	182	222	1			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	AYA	ALA	MODIFIED RESIDUE	UNP Q7M1T4
A	9	SER	PRO	CONFLICT	UNP Q7M1T4
A	20	GLU	ASP	CONFLICT	UNP Q7M1T4
A	49	ASP	GLU	CONFLICT	UNP Q7M1T4
A	70	LYS	ARG	CONFLICT	UNP Q7M1T4
A	84	GLY	ALA	CONFLICT	UNP Q7M1T4
A	145	ILE	VAL	CONFLICT	UNP Q7M1T4
A	148	SER	ALA	CONFLICT	UNP Q7M1T4
B	1	AYA	ALA	MODIFIED RESIDUE	UNP Q7M1T4
B	9	SER	PRO	CONFLICT	UNP Q7M1T4
B	20	GLU	ASP	CONFLICT	UNP Q7M1T4
B	49	ASP	GLU	CONFLICT	UNP Q7M1T4
B	70	LYS	ARG	CONFLICT	UNP Q7M1T4

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	84	GLY	ALA	CONFLICT	UNP Q7M1T4
B	145	ILE	VAL	CONFLICT	UNP Q7M1T4
B	148	SER	ALA	CONFLICT	UNP Q7M1T4
C	1	AYA	ALA	MODIFIED RESIDUE	UNP Q7M1T4
C	9	SER	PRO	CONFLICT	UNP Q7M1T4
C	20	GLU	ASP	CONFLICT	UNP Q7M1T4
C	49	ASP	GLU	CONFLICT	UNP Q7M1T4
C	70	LYS	ARG	CONFLICT	UNP Q7M1T4
C	84	GLY	ALA	CONFLICT	UNP Q7M1T4
C	145	ILE	VAL	CONFLICT	UNP Q7M1T4
C	148	SER	ALA	CONFLICT	UNP Q7M1T4
D	1	AYA	ALA	MODIFIED RESIDUE	UNP Q7M1T4
D	9	SER	PRO	CONFLICT	UNP Q7M1T4
D	20	GLU	ASP	CONFLICT	UNP Q7M1T4
D	49	ASP	GLU	CONFLICT	UNP Q7M1T4
D	70	LYS	ARG	CONFLICT	UNP Q7M1T4
D	84	GLY	ALA	CONFLICT	UNP Q7M1T4
D	145	ILE	VAL	CONFLICT	UNP Q7M1T4
D	148	SER	ALA	CONFLICT	UNP Q7M1T4
E	1	AYA	ALA	MODIFIED RESIDUE	UNP Q7M1T4
E	9	SER	PRO	CONFLICT	UNP Q7M1T4
E	20	GLU	ASP	CONFLICT	UNP Q7M1T4
E	49	ASP	GLU	CONFLICT	UNP Q7M1T4
E	70	LYS	ARG	CONFLICT	UNP Q7M1T4
E	84	GLY	ALA	CONFLICT	UNP Q7M1T4
E	145	ILE	VAL	CONFLICT	UNP Q7M1T4
E	148	SER	ALA	CONFLICT	UNP Q7M1T4
F	1	AYA	ALA	MODIFIED RESIDUE	UNP Q7M1T4
F	9	SER	PRO	CONFLICT	UNP Q7M1T4
F	20	GLU	ASP	CONFLICT	UNP Q7M1T4
F	49	ASP	GLU	CONFLICT	UNP Q7M1T4
F	70	LYS	ARG	CONFLICT	UNP Q7M1T4
F	84	GLY	ALA	CONFLICT	UNP Q7M1T4
F	145	ILE	VAL	CONFLICT	UNP Q7M1T4
F	148	SER	ALA	CONFLICT	UNP Q7M1T4
G	1	AYA	ALA	MODIFIED RESIDUE	UNP Q7M1T4
G	9	SER	PRO	CONFLICT	UNP Q7M1T4
G	20	GLU	ASP	CONFLICT	UNP Q7M1T4
G	49	ASP	GLU	CONFLICT	UNP Q7M1T4
G	70	LYS	ARG	CONFLICT	UNP Q7M1T4
G	84	GLY	ALA	CONFLICT	UNP Q7M1T4
G	145	ILE	VAL	CONFLICT	UNP Q7M1T4

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
G	148	SER	ALA	CONFLICT	UNP Q7M1T4
H	1	AYA	ALA	MODIFIED RESIDUE	UNP Q7M1T4
H	9	SER	PRO	CONFLICT	UNP Q7M1T4
H	20	GLU	ASP	CONFLICT	UNP Q7M1T4
H	49	ASP	GLU	CONFLICT	UNP Q7M1T4
H	70	LYS	ARG	CONFLICT	UNP Q7M1T4
H	84	GLY	ALA	CONFLICT	UNP Q7M1T4
H	145	ILE	VAL	CONFLICT	UNP Q7M1T4
H	148	SER	ALA	CONFLICT	UNP Q7M1T4

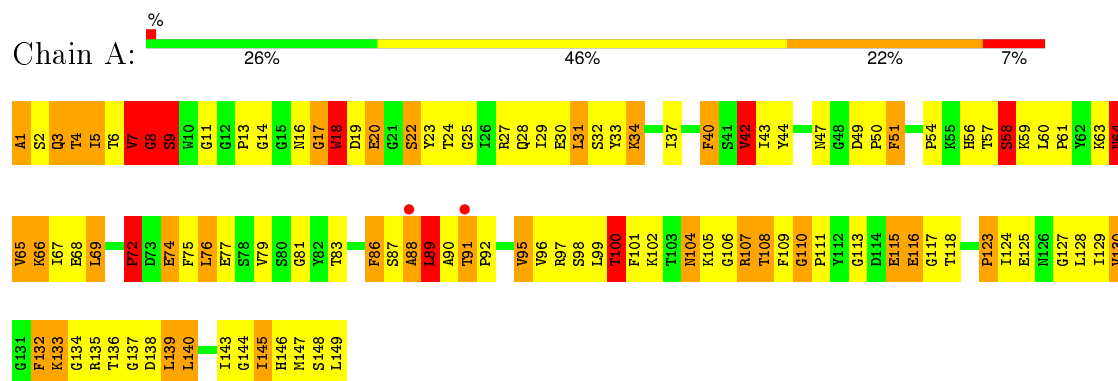
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	118	Total O 118 118	0	0
2	B	123	Total O 123 123	0	0
2	C	121	Total O 121 121	0	0
2	D	121	Total O 121 121	0	0
2	E	93	Total O 93 93	0	0
2	F	115	Total O 115 115	0	0
2	G	102	Total O 102 102	0	0
2	H	81	Total O 81 81	0	0

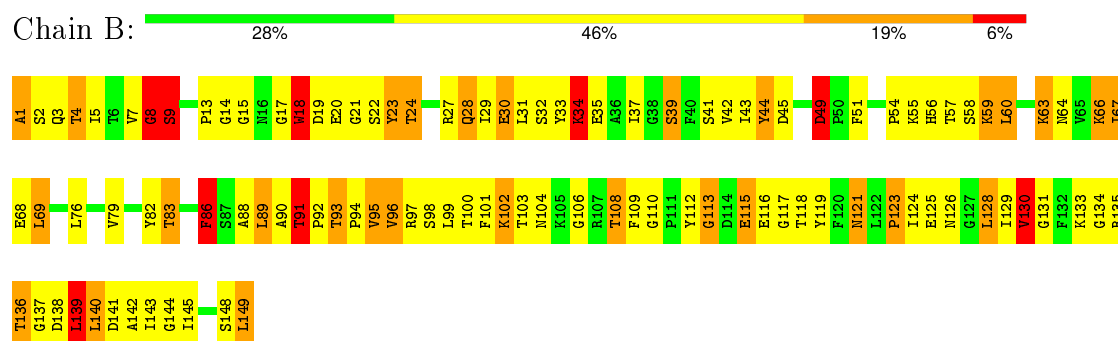
### 3 Residue-property plots [i](#)

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

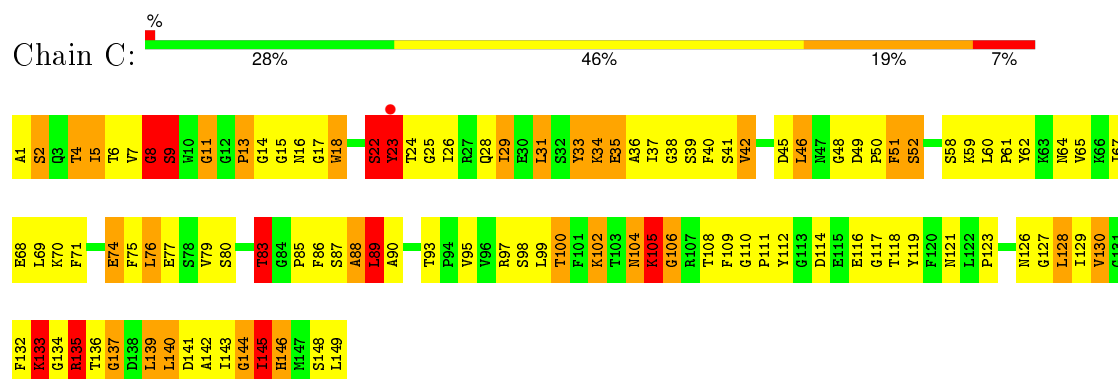
#### • Molecule 1: Artocarpin



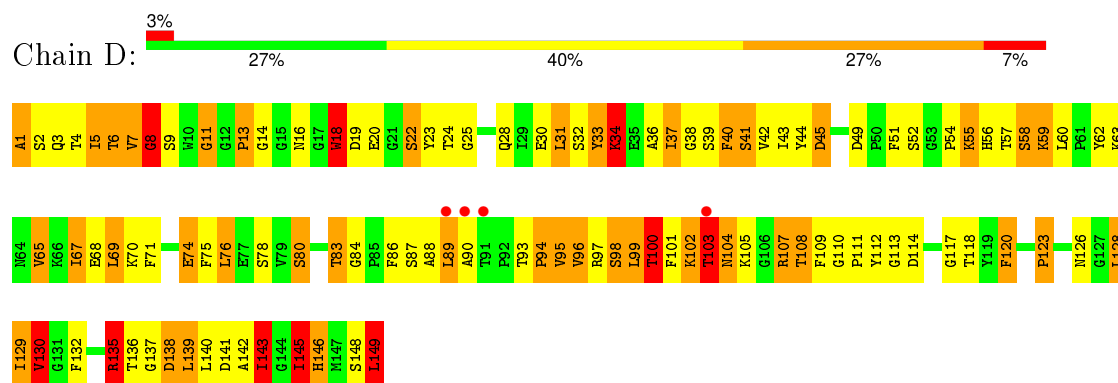
#### • Molecule 1: Artocarpin



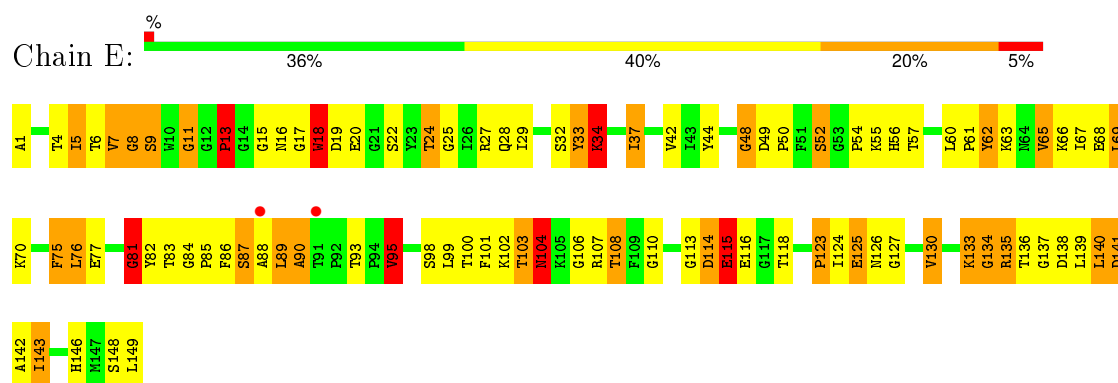
#### • Molecule 1: Artocarpin



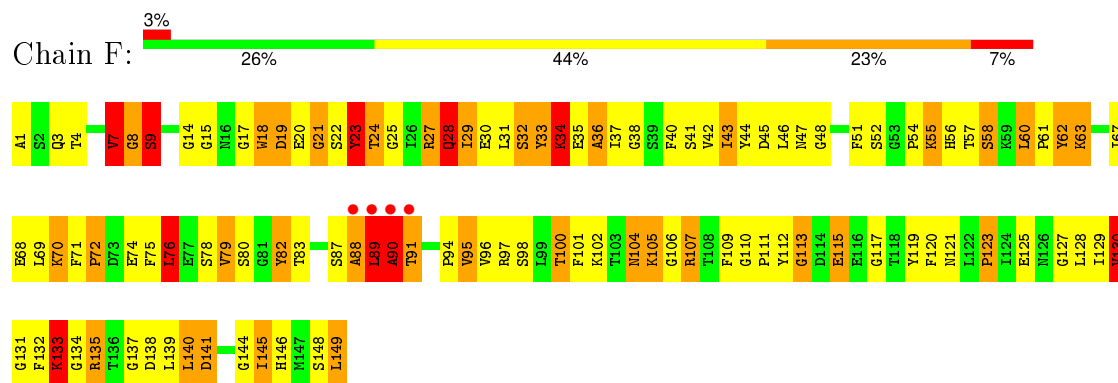
- Molecule 1: Artocarpin



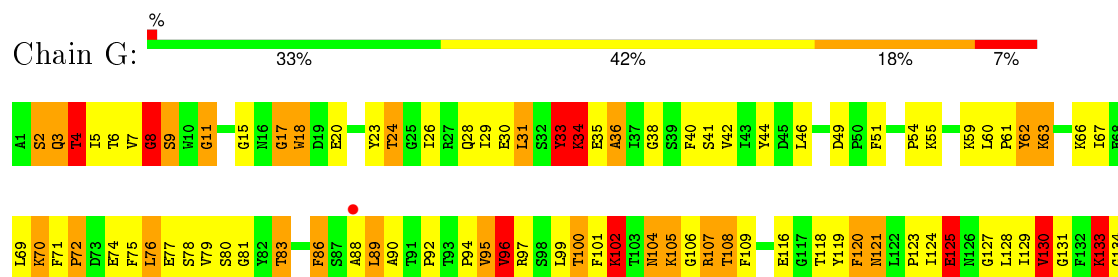
- Molecule 1: Artocarpin



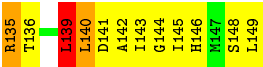
- Molecule 1: Artocarpin



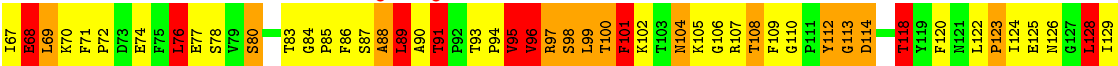
- Molecule 1: Artocarpin







● Molecule 1: Artocarpin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.69Å 72.19Å 92.63Å 90.00° 101.15° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 10.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.40) 83.5 (10.00-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.91 (at 2.41Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.191 , 0.258 0.203 , 0.260	Depositor DCC
$R_{free}$ test set	1536 reflections (4.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.7	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 73.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 36759 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9922	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	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 64.61 % 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 8.0588e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: AYA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.08	4/1155 (0.3%)	2.09	74/1569 (4.7%)
1	B	1.03	6/1155 (0.5%)	2.09	66/1569 (4.2%)
1	C	1.06	5/1155 (0.4%)	2.21	79/1569 (5.0%)
1	D	0.97	5/1155 (0.4%)	2.31	82/1569 (5.2%)
1	E	0.99	3/1151 (0.3%)	2.40	77/1565 (4.9%)
1	F	1.50	6/1151 (0.5%)	2.31	70/1565 (4.5%)
1	G	1.52	3/1155 (0.3%)	2.20	68/1569 (4.3%)
1	H	0.96	1/1155 (0.1%)	2.31	73/1569 (4.7%)
All	All	1.16	33/9232 (0.4%)	2.24	589/12544 (4.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	8
1	B	1	4
1	C	1	8
1	D	0	5
1	E	1	5
1	F	0	7
1	G	1	5
1	H	1	4
All	All	6	46

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	70	LYS	CD-CE	39.71	2.50	1.51
1	F	70	LYS	CD-CE	37.27	2.44	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	33	TYR	C-N	11.14	1.59	1.34
1	A	34	LYS	C-N	10.43	1.58	1.34
1	C	33	TYR	C-N	9.15	1.55	1.34
1	F	34	LYS	C-N	8.37	1.53	1.34
1	F	90	ALA	C-N	-8.32	1.15	1.34
1	A	68	GLU	CD-OE1	6.63	1.32	1.25
1	B	89	LEU	C-N	-6.58	1.19	1.34
1	C	68	GLU	CD-OE1	6.46	1.32	1.25
1	E	68	GLU	CD-OE2	6.42	1.32	1.25
1	C	133	LYS	CE-NZ	6.37	1.65	1.49
1	E	33	TYR	C-N	6.25	1.48	1.34
1	B	59	LYS	C-O	-6.16	1.11	1.23
1	D	8	GLY	C-N	-6.10	1.20	1.34
1	C	22	SER	C-N	-6.08	1.20	1.34
1	B	68	GLU	CD-OE1	6.01	1.32	1.25
1	F	9	SER	C-N	-5.96	1.20	1.34
1	H	68	GLU	CG-CD	5.96	1.60	1.51
1	F	70	LYS	CE-NZ	-5.91	1.34	1.49
1	F	22	SER	C-N	-5.79	1.20	1.34
1	E	133	LYS	CE-NZ	5.72	1.63	1.49
1	C	68	GLU	CD-OE2	5.69	1.31	1.25
1	A	68	GLU	CD-OE2	5.66	1.31	1.25
1	B	34	LYS	CE-NZ	5.61	1.63	1.49
1	D	34	LYS	CE-NZ	5.58	1.62	1.49
1	G	70	LYS	CE-NZ	-5.51	1.35	1.49
1	B	68	GLU	CD-OE2	5.44	1.31	1.25
1	D	33	TYR	C-N	-5.41	1.21	1.34
1	D	68	GLU	CD-OE2	5.35	1.31	1.25
1	A	68	GLU	CB-CG	-5.25	1.42	1.52
1	G	96	VAL	CA-CB	5.04	1.65	1.54
1	D	34	LYS	C-N	-5.04	1.22	1.34

All (589) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	34	LYS	O-C-N	-36.39	64.47	122.70
1	G	70	LYS	CD-CE-NZ	-35.79	29.38	111.70
1	F	70	LYS	CD-CE-NZ	-35.17	30.80	111.70
1	D	34	LYS	O-C-N	-28.27	77.46	122.70
1	H	9	SER	O-C-N	-27.94	77.99	122.70
1	E	34	LYS	CA-C-N	22.48	166.66	117.20
1	H	89	LEU	O-C-N	-19.77	91.07	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	9	SER	CA-C-N	18.79	158.54	117.20
1	C	89	LEU	O-C-N	-18.52	93.07	122.70
1	C	9	SER	O-C-N	-18.40	93.26	122.70
1	F	9	SER	O-C-N	-17.72	94.35	122.70
1	D	8	GLY	C-N-CA	17.15	164.58	121.70
1	D	8	GLY	O-C-N	-16.94	95.60	122.70
1	B	9	SER	O-C-N	-16.78	95.85	122.70
1	E	8	GLY	O-C-N	-16.09	96.96	122.70
1	A	33	TYR	O-C-N	-15.50	97.90	122.70
1	D	34	LYS	CA-C-N	15.37	151.01	117.20
1	A	34	LYS	O-C-N	-14.96	98.76	122.70
1	F	90	ALA	O-C-N	-14.56	99.40	122.70
1	E	8	GLY	C-N-CA	14.16	157.10	121.70
1	B	8	GLY	O-C-N	-14.02	100.28	122.70
1	F	89	LEU	CA-CB-CG	13.90	147.26	115.30
1	D	33	TYR	O-C-N	-13.73	100.74	122.70
1	E	34	LYS	CB-CA-C	-13.32	83.77	110.40
1	B	34	LYS	O-C-N	-12.86	102.12	122.70
1	G	8	GLY	O-C-N	-12.60	102.54	122.70
1	H	90	ALA	O-C-N	12.29	142.36	122.70
1	E	33	TYR	C-N-CA	-11.85	92.07	121.70
1	C	23	TYR	O-C-N	-11.29	104.63	122.70
1	H	90	ALA	CA-C-N	-11.27	92.41	117.20
1	D	9	SER	O-C-N	-11.03	105.05	122.70
1	E	9	SER	O-C-N	-10.89	105.27	122.70
1	H	89	LEU	CB-CG-CD1	10.81	129.38	111.00
1	D	22	SER	O-C-N	-9.93	106.82	122.70
1	C	8	GLY	O-C-N	-9.69	107.19	122.70
1	E	34	LYS	C-N-CA	9.66	145.85	121.70
1	F	70	LYS	CG-CD-CE	9.62	140.76	111.90
1	B	8	GLY	C-N-CA	9.53	145.52	121.70
1	B	33	TYR	C-N-CA	-9.24	98.59	121.70
1	E	8	GLY	CA-C-N	9.20	137.44	117.20
1	B	89	LEU	C-N-CA	9.09	144.42	121.70
1	H	8	GLY	O-C-N	-8.91	108.44	122.70
1	A	33	TYR	CA-C-N	8.84	136.64	117.20
1	F	89	LEU	C-N-CA	8.83	143.78	121.70
1	F	9	SER	CA-C-N	8.81	136.58	117.20
1	A	8	GLY	O-C-N	-8.75	108.70	122.70
1	C	89	LEU	C-N-CA	8.73	143.53	121.70
1	H	135	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	G	8	GLY	C-N-CA	8.30	142.45	121.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	34	LYS	O-C-N	-8.20	109.58	122.70
1	C	22	SER	O-C-N	-8.17	109.62	122.70
1	H	9	SER	C-N-CA	8.13	142.03	121.70
1	G	88	ALA	O-C-N	-8.10	109.75	122.70
1	B	89	LEU	O-C-N	-8.05	109.83	122.70
1	H	135	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	C	128	LEU	CA-CB-CG	8.01	133.73	115.30
1	E	81	GLY	N-CA-C	7.97	133.03	113.10
1	F	33	TYR	O-C-N	-7.90	110.06	122.70
1	F	22	SER	O-C-N	-7.87	110.11	122.70
1	D	9	SER	N-CA-C	-7.81	89.91	111.00
1	D	8	GLY	CA-C-N	7.78	134.31	117.20
1	G	9	SER	N-CA-C	-7.75	90.07	111.00
1	C	9	SER	CA-C-N	7.75	134.24	117.20
1	H	149	LEU	CA-CB-CG	7.71	133.03	115.30
1	C	89	LEU	CA-C-N	7.70	134.14	117.20
1	C	8	GLY	C-N-CA	7.66	140.84	121.70
1	C	89	LEU	CA-CB-CG	7.62	132.83	115.30
1	A	99	LEU	CA-CB-CG	7.61	132.80	115.30
1	H	9	SER	N-CA-C	-7.54	90.63	111.00
1	F	89	LEU	O-C-N	-7.50	110.70	122.70
1	H	8	GLY	C-N-CA	7.45	140.31	121.70
1	E	81	GLY	O-C-N	-7.41	110.84	122.70
1	B	89	LEU	CA-CB-CG	7.34	132.19	115.30
1	D	129	ILE	O-C-N	-7.30	111.01	122.70
1	D	123	PRO	O-C-N	-7.27	111.07	122.70
1	C	149	LEU	CA-CB-CG	7.27	132.01	115.30
1	B	9	SER	CA-C-N	7.25	133.16	117.20
1	B	69	LEU	CA-CB-CG	7.13	131.70	115.30
1	C	49	ASP	CB-CG-OD1	7.09	124.68	118.30
1	E	9	SER	N-CA-C	-7.03	92.02	111.00
1	A	81	GLY	O-C-N	-7.02	111.47	122.70
1	H	146	HIS	O-C-N	-6.97	111.55	122.70
1	F	38	GLY	O-C-N	-6.95	111.58	122.70
1	D	22	SER	C-N-CA	6.94	139.05	121.70
1	B	89	LEU	CB-CA-C	6.93	123.36	110.20
1	G	29	ILE	O-C-N	-6.92	111.62	122.70
1	H	113	GLY	O-C-N	-6.89	111.67	122.70
1	B	41	SER	O-C-N	-6.89	111.68	122.70
1	D	34	LYS	C-N-CA	6.86	138.85	121.70
1	A	17	GLY	O-C-N	-6.85	111.75	122.70
1	A	4	THR	O-C-N	-6.84	111.76	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	95	VAL	O-C-N	-6.83	111.77	122.70
1	C	99	LEU	O-C-N	-6.79	111.84	122.70
1	D	83	THR	O-C-N	-6.78	111.67	123.20
1	H	99	LEU	CA-CB-CG	6.78	130.89	115.30
1	E	101	PHE	O-C-N	-6.75	111.89	122.70
1	D	9	SER	CA-C-N	6.75	132.05	117.20
1	D	33	TYR	CA-C-N	6.75	132.05	117.20
1	A	37	ILE	O-C-N	-6.73	111.75	123.20
1	A	133	LYS	O-C-N	-6.72	111.78	123.20
1	E	123	PRO	O-C-N	-6.67	112.02	122.70
1	G	4	THR	O-C-N	-6.67	112.03	122.70
1	F	89	LEU	CB-CG-CD2	-6.66	99.67	111.00
1	A	113	GLY	O-C-N	-6.66	112.04	122.70
1	C	95	VAL	O-C-N	-6.66	112.05	122.70
1	G	15	GLY	O-C-N	-6.64	112.07	122.70
1	F	29	ILE	O-C-N	-6.61	112.13	122.70
1	G	33	TYR	O-C-N	-6.59	112.16	122.70
1	F	130	VAL	O-C-N	-6.57	112.03	123.20
1	C	139	LEU	O-C-N	-6.57	112.19	122.70
1	B	143	ILE	O-C-N	-6.55	112.06	123.20
1	H	90	ALA	C-N-CA	-6.54	105.35	121.70
1	G	76	LEU	O-C-N	-6.52	112.26	122.70
1	D	128	LEU	CA-CB-CG	6.52	130.30	115.30
1	G	6	THR	O-C-N	-6.50	112.30	122.70
1	D	24	THR	O-C-N	-6.50	112.15	123.20
1	E	55	LYS	O-C-N	-6.49	112.33	122.70
1	C	129	ILE	O-C-N	-6.48	112.33	122.70
1	F	69	LEU	O-C-N	-6.48	112.33	122.70
1	B	139	LEU	CA-CB-CG	6.47	130.19	115.30
1	H	88	ALA	O-C-N	-6.42	112.42	122.70
1	A	9	SER	N-CA-C	-6.42	93.66	111.00
1	H	32	SER	O-C-N	-6.42	112.43	122.70
1	F	91	THR	N-CA-C	-6.41	93.69	111.00
1	G	99	LEU	O-C-N	-6.41	112.44	122.70
1	C	22	SER	C-N-CA	6.39	137.67	121.70
1	C	106	GLY	O-C-N	-6.39	112.48	122.70
1	C	114	ASP	O-C-N	-6.38	112.50	122.70
1	H	46	LEU	O-C-N	-6.37	112.52	122.70
1	B	106	GLY	O-C-N	-6.36	112.52	122.70
1	B	134	GLY	O-C-N	-6.36	112.53	122.70
1	E	100	THR	O-C-N	-6.34	112.55	122.70
1	A	127	GLY	O-C-N	-6.34	112.55	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	149	LEU	CA-CB-CG	6.32	129.84	115.30
1	D	100	THR	O-C-N	-6.32	112.59	122.70
1	H	120	PHE	O-C-N	-6.29	112.64	122.70
1	C	99	LEU	CA-CB-CG	6.28	129.75	115.30
1	F	134	GLY	O-C-N	-6.28	112.65	122.70
1	H	135	ARG	O-C-N	-6.28	112.66	122.70
1	A	68	GLU	O-C-N	-6.27	112.67	122.70
1	E	17	GLY	O-C-N	-6.25	112.70	122.70
1	A	13	PRO	O-C-N	-6.23	112.60	123.20
1	G	51	PHE	O-C-N	-6.23	112.73	122.70
1	B	89	LEU	CB-CG-CD1	-6.23	100.41	111.00
1	H	98	SER	O-C-N	-6.23	112.73	122.70
1	E	62	TYR	O-C-N	-6.23	112.73	122.70
1	F	89	LEU	CB-CA-C	6.23	122.03	110.20
1	D	114	ASP	O-C-N	-6.22	112.75	122.70
1	G	121	ASN	O-C-N	-6.22	112.75	122.70
1	A	146	HIS	O-C-N	-6.21	112.77	122.70
1	B	144	GLY	O-C-N	-6.20	112.78	122.70
1	F	140	LEU	O-C-N	-6.19	112.79	122.70
1	B	86	PHE	O-C-N	-6.18	112.81	122.70
1	C	135	ARG	O-C-N	-6.16	112.84	122.70
1	B	29	ILE	O-C-N	-6.15	112.86	122.70
1	E	141	ASP	O-C-N	-6.15	112.86	122.70
1	F	76	LEU	O-C-N	-6.14	112.87	122.70
1	D	108	THR	O-C-N	-6.14	112.88	122.70
1	F	55	LYS	O-C-N	-6.13	112.88	122.70
1	H	128	LEU	O-C-N	-6.13	112.89	122.70
1	B	133	LYS	O-C-N	-6.13	112.78	123.20
1	H	91	THR	N-CA-C	-6.13	94.46	111.00
1	E	146	HIS	O-C-N	-6.12	112.91	122.70
1	F	95	VAL	O-C-N	-6.12	112.91	122.70
1	D	87	SER	O-C-N	-6.12	112.92	122.70
1	E	104	ASN	O-C-N	-6.11	112.93	122.70
1	F	3	GLN	O-C-N	-6.09	112.96	122.70
1	H	54	PRO	O-C-N	-6.09	112.96	122.70
1	D	101	PHE	O-C-N	-6.08	112.97	122.70
1	F	27	ARG	O-C-N	-6.08	112.97	122.70
1	C	130	VAL	O-C-N	-6.07	112.88	123.20
1	H	45	ASP	CB-CG-OD2	6.07	123.76	118.30
1	C	14	GLY	O-C-N	-6.06	112.90	123.20
1	C	126	ASN	O-C-N	-6.06	112.90	123.20
1	A	74	GLU	O-C-N	-6.05	113.01	122.70

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	70	LYS	O-C-N	-6.05	113.01	122.70
1	G	66	LYS	O-C-N	-6.05	113.01	122.70
1	H	80	SER	O-C-N	-6.05	112.91	123.20
1	G	101	PHE	O-C-N	-6.05	113.02	122.70
1	G	106	GLY	O-C-N	-6.04	113.04	122.70
1	D	65	VAL	O-C-N	-6.04	113.04	122.70
1	H	102	LYS	O-C-N	-6.04	113.04	122.70
1	C	137	GLY	N-CA-C	-6.03	98.02	113.10
1	D	18	TRP	O-C-N	-6.03	113.06	122.70
1	D	80	SER	O-C-N	-6.03	112.95	123.20
1	F	115	GLU	O-C-N	-6.03	113.06	122.70
1	F	144	GLY	O-C-N	-6.03	113.06	122.70
1	H	11	GLY	O-C-N	-6.00	113.00	123.20
1	C	24	THR	O-C-N	-5.98	113.03	123.20
1	C	77	GLU	O-C-N	-5.97	113.15	122.70
1	C	144	GLY	O-C-N	-5.97	113.15	122.70
1	E	77	GLU	O-C-N	-5.96	113.16	122.70
1	A	33	TYR	C-N-CA	5.96	136.59	121.70
1	D	97	ARG	O-C-N	-5.96	113.17	122.70
1	B	119	TYR	O-C-N	-5.95	113.18	122.70
1	A	137	GLY	N-CA-C	-5.94	98.26	113.10
1	C	51	PHE	O-C-N	-5.94	113.20	122.70
1	D	22	SER	CA-C-N	5.93	130.25	117.20
1	B	15	GLY	O-C-N	-5.92	113.22	122.70
1	D	117	GLY	O-C-N	-5.92	113.23	122.70
1	E	87	SER	O-C-N	-5.91	113.24	122.70
1	B	88	ALA	O-C-N	-5.90	113.26	122.70
1	B	121	ASN	O-C-N	-5.89	113.28	122.70
1	G	40	PHE	O-C-N	-5.89	113.28	122.70
1	G	62	TYR	O-C-N	-5.88	113.28	122.70
1	A	99	LEU	O-C-N	-5.88	113.30	122.70
1	D	19	ASP	O-C-N	-5.87	113.30	122.70
1	H	99	LEU	O-C-N	-5.87	113.31	122.70
1	D	25	GLY	O-C-N	-5.87	113.31	122.70
1	D	84	GLY	N-CA-C	-5.87	98.43	113.10
1	E	130	VAL	O-C-N	-5.87	113.22	123.20
1	F	15	GLY	O-C-N	-5.87	113.31	122.70
1	C	40	PHE	O-C-N	-5.86	113.33	122.70
1	C	41	SER	O-C-N	-5.86	113.33	122.70
1	C	83	THR	O-C-N	-5.84	113.27	123.20
1	E	52	SER	O-C-N	-5.84	113.28	123.20
1	F	25	GLY	O-C-N	-5.83	113.38	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	VAL	O-C-N	-5.82	113.30	123.20
1	F	82	TYR	O-C-N	-5.82	113.39	122.70
1	H	6	THR	O-C-N	-5.81	113.40	122.70
1	A	16	ASN	O-C-N	-5.81	113.33	123.20
1	G	130	VAL	O-C-N	-5.81	113.33	123.20
1	E	27	ARG	O-C-N	-5.80	113.41	122.70
1	D	55	LYS	O-C-N	-5.80	113.42	122.70
1	G	81	GLY	O-C-N	-5.80	113.42	122.70
1	E	9	SER	CA-C-N	5.79	129.95	117.20
1	E	69	LEU	O-C-N	-5.79	113.43	122.70
1	H	124	ILE	O-C-N	-5.79	113.44	122.70
1	B	101	PHE	O-C-N	-5.78	113.44	122.70
1	B	137	GLY	O-C-N	-5.78	113.45	122.70
1	G	55	LYS	O-C-N	-5.78	113.45	122.70
1	B	24	THR	O-C-N	-5.78	113.38	123.20
1	B	130	VAL	O-C-N	-5.78	113.38	123.20
1	B	123	PRO	O-C-N	-5.78	113.46	122.70
1	C	18	TRP	O-C-N	-5.78	113.46	122.70
1	C	148	SER	O-C-N	-5.78	113.46	122.70
1	G	144	GLY	O-C-N	-5.77	113.47	122.70
1	E	88	ALA	O-C-N	-5.76	113.48	122.70
1	F	19	ASP	O-C-N	-5.76	113.48	122.70
1	A	132	PHE	O-C-N	-5.76	113.48	122.70
1	G	38	GLY	O-C-N	-5.76	113.49	122.70
1	E	136	THR	O-C-N	-5.76	113.41	123.20
1	B	137	GLY	N-CA-C	-5.75	98.72	113.10
1	A	20	GLU	O-C-N	-5.75	113.42	123.20
1	E	133	LYS	O-C-N	-5.75	113.43	123.20
1	C	15	GLY	O-C-N	-5.74	113.51	122.70
1	D	120	PHE	O-C-N	-5.74	113.52	122.70
1	C	9	SER	N-CA-C	-5.74	95.51	111.00
1	A	125	GLU	O-C-N	-5.73	113.53	122.70
1	H	144	GLY	O-C-N	-5.73	113.53	122.70
1	B	125	GLU	O-C-N	-5.72	113.55	122.70
1	H	69	LEU	CA-CB-CG	5.71	128.44	115.30
1	A	14	GLY	O-C-N	-5.70	113.50	123.20
1	C	37	ILE	O-C-N	-5.70	113.50	123.20
1	H	129	ILE	O-C-N	-5.70	113.58	122.70
1	B	14	GLY	O-C-N	-5.70	113.51	123.20
1	C	52	SER	O-C-N	-5.70	113.51	123.20
1	D	113	GLY	O-C-N	-5.70	113.58	122.70
1	G	94	PRO	O-C-N	-5.70	113.59	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	76	LEU	O-C-N	-5.70	113.59	122.70
1	A	95	VAL	O-C-N	-5.69	113.60	122.70
1	H	101	PHE	O-C-N	-5.68	113.61	122.70
1	B	17	GLY	O-C-N	-5.68	113.61	122.70
1	B	23	TYR	O-C-N	-5.68	113.61	122.70
1	G	149	LEU	CA-CB-CG	5.68	128.37	115.30
1	G	5	ILE	O-C-N	-5.68	113.61	122.70
1	D	3	GLN	O-C-N	-5.68	113.62	122.70
1	F	63	LYS	O-C-N	-5.68	113.61	122.70
1	D	142	ALA	O-C-N	-5.68	113.62	122.70
1	C	127	GLY	O-C-N	-5.67	113.62	122.70
1	E	15	GLY	O-C-N	-5.67	113.62	122.70
1	B	113	GLY	O-C-N	-5.67	113.63	122.70
1	C	42	VAL	O-C-N	-5.67	113.63	122.70
1	F	88	ALA	O-C-N	-5.67	113.63	122.70
1	D	95	VAL	O-C-N	-5.66	113.64	122.70
1	A	31	LEU	O-C-N	-5.66	113.64	122.70
1	C	48	GLY	O-C-N	-5.66	113.65	122.70
1	F	21	GLY	O-C-N	-5.65	113.65	122.70
1	B	117	GLY	O-C-N	-5.65	113.66	122.70
1	D	102	LYS	O-C-N	-5.65	113.66	122.70
1	E	63	LYS	O-C-N	-5.65	113.66	122.70
1	C	74	GLU	O-C-N	-5.65	113.66	122.70
1	C	38	GLY	O-C-N	-5.64	113.67	122.70
1	H	5	ILE	O-C-N	-5.64	113.67	122.70
1	E	107	ARG	O-C-N	-5.64	113.67	122.70
1	A	107	ARG	O-C-N	-5.64	113.67	122.70
1	G	70	LYS	O-C-N	-5.64	113.67	122.70
1	F	45	ASP	O-C-N	-5.64	113.68	122.70
1	E	50	PRO	O-C-N	-5.64	113.68	122.70
1	H	106	GLY	O-C-N	-5.63	113.69	122.70
1	A	115	GLU	O-C-N	-5.63	113.69	122.70
1	B	63	LYS	O-C-N	-5.63	113.70	122.70
1	C	45	ASP	O-C-N	-5.63	113.70	122.70
1	E	114	ASP	O-C-N	-5.63	113.70	122.70
1	G	42	VAL	O-C-N	-5.62	113.71	122.70
1	H	48	GLY	O-C-N	-5.62	113.71	122.70
1	A	27	ARG	O-C-N	-5.61	113.72	122.70
1	C	61	PRO	O-C-N	-5.61	113.72	122.70
1	D	90	ALA	O-C-N	-5.61	113.72	122.70
1	F	72	PRO	O-C-N	-5.61	113.72	122.70
1	C	29	ILE	O-C-N	-5.61	113.73	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	141	ASP	O-C-N	-5.61	113.73	122.70
1	G	67	ILE	O-C-N	-5.61	113.73	122.70
1	G	86	PHE	O-C-N	-5.60	113.73	122.70
1	F	52	SER	O-C-N	-5.60	113.69	123.20
1	A	101	PHE	O-C-N	-5.59	113.76	122.70
1	E	90	ALA	O-C-N	-5.59	113.76	122.70
1	G	128	LEU	CA-CB-CG	5.58	128.14	115.30
1	E	106	GLY	O-C-N	-5.58	113.77	122.70
1	A	88	ALA	O-C-N	-5.58	113.78	122.70
1	C	2	SER	O-C-N	-5.58	113.78	122.70
1	D	145	ILE	O-C-N	-5.58	113.78	122.70
1	F	48	GLY	O-C-N	-5.57	113.78	122.70
1	C	16	ASN	O-C-N	-5.57	113.73	123.20
1	G	141	ASP	O-C-N	-5.56	113.80	122.70
1	A	44	TYR	O-C-N	-5.56	113.80	122.70
1	F	23	TYR	O-C-N	-5.56	113.81	122.70
1	H	105	LYS	O-C-N	-5.56	113.75	123.20
1	D	128	LEU	O-C-N	-5.56	113.81	122.70
1	H	126	ASN	O-C-N	-5.55	113.76	123.20
1	A	123	PRO	O-C-N	-5.55	113.82	122.70
1	B	18	TRP	O-C-N	-5.55	113.82	122.70
1	C	133	LYS	O-C-N	-5.55	113.77	123.20
1	F	133	LYS	O-C-N	-5.55	113.77	123.20
1	H	3	GLN	O-C-N	-5.55	113.83	122.70
1	G	77	GLU	O-C-N	-5.54	113.83	122.70
1	B	44	TYR	O-C-N	-5.54	113.83	122.70
1	B	115	GLU	O-C-N	-5.54	113.84	122.70
1	D	57	THR	O-C-N	-5.54	113.84	122.70
1	D	135	ARG	O-C-N	-5.54	113.83	122.70
1	E	135	ARG	O-C-N	-5.54	113.84	122.70
1	C	28	GLN	O-C-N	-5.54	113.84	122.70
1	D	11	GLY	O-C-N	-5.53	113.80	123.20
1	D	30	GLU	O-C-N	-5.53	113.85	122.70
1	G	24	THR	O-C-N	-5.53	113.79	123.20
1	G	107	ARG	O-C-N	-5.53	113.85	122.70
1	G	133	LYS	O-C-N	-5.52	113.81	123.20
1	H	17	GLY	O-C-N	-5.52	113.87	122.70
1	H	112	TYR	O-C-N	-5.52	113.82	123.20
1	H	95	VAL	O-C-N	-5.52	113.87	122.70
1	H	89	LEU	CA-C-N	5.51	129.33	117.20
1	G	95	VAL	O-C-N	-5.51	113.88	122.70
1	A	51	PHE	O-C-N	-5.51	113.88	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	23	TYR	O-C-N	-5.51	113.89	122.70
1	F	120	PHE	O-C-N	-5.51	113.89	122.70
1	D	51	PHE	O-C-N	-5.50	113.89	122.70
1	F	146	HIS	O-C-N	-5.50	113.90	122.70
1	D	107	ARG	O-C-N	-5.50	113.90	122.70
1	H	133	LYS	O-C-N	-5.49	113.86	123.20
1	F	123	PRO	O-C-N	-5.49	113.91	122.70
1	B	124	ILE	O-C-N	-5.49	113.92	122.70
1	G	127	GLY	O-C-N	-5.49	113.92	122.70
1	D	76	LEU	O-C-N	-5.48	113.93	122.70
1	A	86	PHE	O-C-N	-5.48	113.94	122.70
1	G	46	LEU	O-C-N	-5.48	113.93	122.70
1	D	59	LYS	O-C-N	-5.47	113.94	122.70
1	G	129	ILE	N-CA-C	-5.47	96.23	111.00
1	C	76	LEU	O-C-N	-5.47	113.95	122.70
1	B	99	LEU	O-C-N	-5.46	113.96	122.70
1	B	100	THR	O-C-N	-5.46	113.96	122.70
1	E	18	TRP	O-C-N	-5.46	113.97	122.70
1	F	105	LYS	O-C-N	-5.46	113.92	123.20
1	G	17	GLY	O-C-N	-5.46	113.97	122.70
1	B	138	ASP	O-C-N	-5.45	113.98	122.70
1	G	143	ILE	O-C-N	-5.45	113.94	123.20
1	F	89	LEU	CA-C-N	-5.44	105.23	117.20
1	B	67	ILE	O-C-N	-5.43	114.01	122.70
1	D	4	THR	O-C-N	-5.43	114.01	122.70
1	F	40	PHE	O-C-N	-5.43	114.01	122.70
1	A	72	PRO	O-C-N	-5.43	114.02	122.70
1	A	22	SER	O-C-N	-5.42	114.03	122.70
1	A	40	PHE	O-C-N	-5.42	114.03	122.70
1	C	140	LEU	O-C-N	-5.42	114.03	122.70
1	G	140	LEU	O-C-N	-5.41	114.04	122.70
1	C	79	VAL	O-C-N	-5.41	114.05	122.70
1	F	128	LEU	O-C-N	-5.41	114.05	122.70
1	C	11	GLY	O-C-N	-5.41	114.01	123.20
1	D	143	ILE	CB-CA-C	-5.41	100.79	111.60
1	C	68	GLU	O-C-N	-5.40	114.06	122.70
1	C	80	SER	O-C-N	-5.40	114.02	123.20
1	H	137	GLY	N-CA-C	-5.40	99.60	113.10
1	D	67	ILE	O-C-N	-5.39	114.07	122.70
1	E	137	GLY	O-C-N	-5.39	114.07	122.70
1	G	36	ALA	O-C-N	-5.39	114.07	122.70
1	E	13	PRO	O-C-N	-5.39	114.04	123.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	TRP	O-C-N	-5.39	114.08	122.70
1	H	96	VAL	O-C-N	-5.38	114.09	122.70
1	G	131	GLY	O-C-N	-5.38	114.09	122.70
1	G	11	GLY	O-C-N	-5.38	114.05	123.20
1	A	134	GLY	O-C-N	-5.38	114.09	122.70
1	F	135	ARG	O-C-N	-5.38	114.09	122.70
1	A	2	SER	O-C-N	-5.38	114.10	122.70
1	B	129	ILE	N-CA-C	-5.38	96.48	111.00
1	G	105	LYS	O-C-N	-5.38	114.06	123.20
1	D	13	PRO	O-C-N	-5.37	114.06	123.20
1	H	129	ILE	N-CA-C	-5.37	96.49	111.00
1	E	124	ILE	O-C-N	-5.37	114.11	122.70
1	E	66	LYS	O-C-N	-5.37	114.11	122.70
1	G	61	PRO	O-C-N	-5.37	114.11	122.70
1	F	100	THR	O-C-N	-5.37	114.11	122.70
1	G	41	SER	O-C-N	-5.37	114.11	122.70
1	A	11	GLY	O-C-N	-5.36	114.09	123.20
1	A	76	LEU	O-C-N	-5.36	114.12	122.70
1	A	117	GLY	O-C-N	-5.36	114.13	122.70
1	H	62	TYR	O-C-N	-5.36	114.13	122.70
1	E	108	THR	O-C-N	-5.35	114.13	122.70
1	E	140	LEU	O-C-N	-5.35	114.13	122.70
1	C	145	ILE	O-C-N	-5.35	114.14	122.70
1	E	113	GLY	O-C-N	-5.35	114.14	122.70
1	B	45	ASP	O-C-N	-5.34	114.15	122.70
1	C	119	TYR	O-C-N	-5.34	114.15	122.70
1	C	141	ASP	O-C-N	-5.34	114.15	122.70
1	E	115	GLU	O-C-N	-5.34	114.15	122.70
1	A	63	LYS	O-C-N	-5.34	114.16	122.70
1	C	36	ALA	O-C-N	-5.34	114.16	122.70
1	G	30	GLU	O-C-N	-5.34	114.16	122.70
1	H	123	PRO	O-C-N	-5.34	114.16	122.70
1	D	139	LEU	O-C-N	-5.33	114.17	122.70
1	E	75	PHE	O-C-N	-5.33	114.17	122.70
1	E	16	ASN	O-C-N	-5.33	114.15	123.20
1	C	105	LYS	O-C-N	-5.32	114.16	123.20
1	F	32	SER	O-C-N	-5.32	114.19	122.70
1	E	11	GLY	O-C-N	-5.32	114.16	123.20
1	H	51	PHE	O-C-N	-5.32	114.20	122.70
1	F	107	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	A	6	THR	O-C-N	-5.31	114.20	122.70
1	C	100	THR	O-C-N	-5.31	114.21	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	79	VAL	O-C-N	-5.31	114.21	122.70
1	A	140	LEU	O-C-N	-5.31	114.21	122.70
1	C	85	PRO	O-C-N	-5.31	114.21	122.70
1	A	97	ARG	O-C-N	-5.30	114.21	122.70
1	H	58	SER	O-C-N	-5.30	114.21	122.70
1	C	17	GLY	O-C-N	-5.30	114.22	122.70
1	A	29	ILE	O-C-N	-5.30	114.22	122.70
1	B	103	THR	O-C-N	-5.30	114.22	122.70
1	A	8	GLY	C-N-CA	5.30	134.95	121.70
1	E	126	ASN	O-C-N	-5.30	114.19	123.20
1	A	139	LEU	CA-CB-CG	5.29	127.48	115.30
1	E	67	ILE	O-C-N	-5.29	114.23	122.70
1	E	102	LYS	O-C-N	-5.29	114.24	122.70
1	B	140	LEU	O-C-N	-5.29	114.24	122.70
1	G	139	LEU	O-C-N	-5.29	114.24	122.70
1	F	4	THR	O-C-N	-5.28	114.25	122.70
1	E	22	SER	O-C-N	-5.28	114.26	122.70
1	F	62	TYR	O-C-N	-5.27	114.26	122.70
1	D	32	SER	O-C-N	-5.27	114.26	122.70
1	F	30	GLU	O-C-N	-5.27	114.27	122.70
1	D	89	LEU	CB-CG-CD1	-5.27	102.04	111.00
1	F	119	TYR	O-C-N	-5.27	114.27	122.70
1	A	50	PRO	O-C-N	-5.26	114.28	122.70
1	D	31	LEU	O-C-N	-5.26	114.28	122.70
1	F	14	GLY	O-C-N	-5.26	114.25	123.20
1	D	45	ASP	O-C-N	-5.25	114.29	122.70
1	A	64	ASN	O-C-N	-5.25	114.29	122.70
1	D	74	GLU	O-C-N	-5.25	114.30	122.70
1	E	142	ALA	O-C-N	-5.25	114.29	122.70
1	F	79	VAL	O-C-N	-5.25	114.30	122.70
1	D	94	PRO	O-C-N	-5.25	114.30	122.70
1	G	102	LYS	O-C-N	-5.25	114.30	122.70
1	A	129	ILE	O-C-N	-5.25	114.30	122.70
1	E	37	ILE	O-C-N	-5.25	114.28	123.20
1	A	24	THR	O-C-N	-5.25	114.28	123.20
1	A	69	LEU	O-C-N	-5.24	114.31	122.70
1	E	81	GLY	CA-C-N	5.24	128.74	117.20
1	B	95	VAL	O-C-N	-5.24	114.32	122.70
1	E	143	ILE	O-C-N	-5.24	114.30	123.20
1	E	7	VAL	O-C-N	-5.23	114.31	123.20
1	B	30	GLU	O-C-N	-5.23	114.33	122.70
1	D	40	PHE	O-C-N	-5.23	114.33	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	SER	O-C-N	-5.23	114.33	122.70
1	E	103	THR	O-C-N	-5.23	114.33	122.70
1	D	62	TYR	O-C-N	-5.22	114.34	122.70
1	A	89	LEU	N-CA-C	-5.22	96.90	111.00
1	F	117	GLY	O-C-N	-5.22	114.35	122.70
1	H	23	TYR	O-C-N	-5.22	114.35	122.70
1	H	89	LEU	N-CA-C	-5.22	96.91	111.00
1	B	91	THR	N-CA-C	-5.21	96.92	111.00
1	B	128	LEU	CA-CB-CG	5.21	127.29	115.30
1	A	65	VAL	O-C-N	-5.21	114.36	122.70
1	B	21	GLY	O-C-N	-5.21	114.36	122.70
1	F	36	ALA	O-C-N	-5.20	114.38	122.70
1	F	125	GLU	O-C-N	-5.20	114.38	122.70
1	E	32	SER	O-C-N	-5.20	114.38	122.70
1	C	117	GLY	O-C-N	-5.20	114.39	122.70
1	D	126	ASN	O-C-N	-5.19	114.37	123.20
1	G	120	PHE	O-C-N	-5.19	114.39	122.70
1	B	136	THR	O-C-N	-5.19	114.38	123.20
1	D	128	LEU	CB-CG-CD2	-5.19	102.18	111.00
1	E	76	LEU	O-C-N	-5.19	114.40	122.70
1	C	88	ALA	O-C-N	-5.19	114.40	122.70
1	D	38	GLY	O-C-N	-5.18	114.41	122.70
1	E	48	GLY	O-C-N	-5.18	114.41	122.70
1	B	3	GLN	O-C-N	-5.18	114.41	122.70
1	G	92	PRO	O-C-N	-5.17	114.42	122.70
1	D	5	ILE	O-C-N	-5.17	114.42	122.70
1	H	97	ARG	O-C-N	-5.17	114.42	122.70
1	H	45	ASP	N-CA-C	-5.17	97.04	111.00
1	C	134	GLY	O-C-N	-5.17	114.43	122.70
1	D	137	GLY	N-CA-C	-5.17	100.18	113.10
1	G	31	LEU	O-C-N	-5.17	114.44	122.70
1	C	90	ALA	N-CA-C	5.16	124.94	111.00
1	F	37	ILE	O-C-N	-5.16	114.42	123.20
1	H	85	PRO	O-C-N	-5.16	114.45	122.70
1	G	63	LYS	O-C-N	-5.16	114.45	122.70
1	G	72	PRO	O-C-N	-5.15	114.45	122.70
1	H	31	LEU	O-C-N	-5.15	114.46	122.70
1	F	58	SER	O-C-N	-5.15	114.46	122.70
1	D	146	HIS	O-C-N	-5.15	114.46	122.70
1	A	25	GLY	O-C-N	-5.14	114.47	122.70
1	A	57	THR	O-C-N	-5.14	114.47	122.70
1	A	147	MET	O-C-N	-5.14	114.47	122.70

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	25	GLY	O-C-N	-5.14	114.47	122.70
1	B	49	ASP	CB-CG-OD1	5.14	122.93	118.30
1	G	80	SER	O-C-N	-5.14	114.46	123.20
1	C	31	LEU	O-C-N	-5.14	114.48	122.70
1	G	134	GLY	O-C-N	-5.14	114.48	122.70
1	A	42	VAL	O-C-N	-5.13	114.49	122.70
1	A	124	ILE	O-C-N	-5.13	114.49	122.70
1	F	113	GLY	O-C-N	-5.13	114.49	122.70
1	F	137	GLY	O-C-N	-5.13	114.49	122.70
1	C	106	GLY	N-CA-C	5.13	125.92	113.10
1	C	6	THR	O-C-N	-5.13	114.50	122.70
1	A	100	THR	O-C-N	-5.12	114.50	122.70
1	E	65	VAL	CB-CA-C	-5.12	101.67	111.40
1	D	99	LEU	O-C-N	-5.12	114.50	122.70
1	C	25	GLY	O-C-N	-5.12	114.51	122.70
1	E	134	GLY	O-C-N	-5.12	114.51	122.70
1	E	127	GLY	O-C-N	-5.12	114.51	122.70
1	A	136	THR	O-C-N	-5.11	114.51	123.20
1	B	34	LYS	N-CA-CB	5.11	119.80	110.60
1	G	3	GLN	O-C-N	-5.11	114.52	122.70
1	H	70	LYS	O-C-N	-5.11	114.52	122.70
1	F	127	GLY	O-C-N	-5.11	114.53	122.70
1	C	121	ASN	O-C-N	-5.11	114.53	122.70
1	G	125	GLU	O-C-N	-5.11	114.53	122.70
1	H	55	LYS	O-C-N	-5.10	114.53	122.70
1	B	79	VAL	CB-CA-C	-5.10	101.71	111.40
1	D	63	LYS	O-C-N	-5.10	114.54	122.70
1	D	141	ASP	O-C-N	-5.10	114.54	122.70
1	H	108	THR	O-C-N	-5.09	114.55	122.70
1	B	128	LEU	CB-CG-CD1	-5.09	102.34	111.00
1	C	26	ILE	O-C-N	-5.09	114.56	122.70
1	G	109	PHE	O-C-N	-5.09	114.55	123.20
1	E	33	TYR	CA-C-N	-5.09	106.01	117.20
1	B	90	ALA	O-C-N	-5.08	114.56	122.70
1	F	78	SER	O-C-N	-5.08	114.57	122.70
1	C	34	LYS	O-C-N	-5.08	114.57	122.70
1	F	111	PRO	O-C-N	-5.08	114.57	122.70
1	A	5	ILE	O-C-N	-5.08	114.57	122.70
1	D	103	THR	O-C-N	-5.08	114.57	122.70
1	E	6	THR	O-C-N	-5.07	114.58	122.70
1	A	106	GLY	O-C-N	-5.07	114.59	122.70
1	H	15	GLY	O-C-N	-5.07	114.59	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2	SER	O-C-N	-5.07	114.60	122.70
1	B	37	ILE	O-C-N	-5.06	114.59	123.20
1	C	102	LYS	O-C-N	-5.06	114.60	122.70
1	A	79	VAL	O-C-N	-5.06	114.61	122.70
1	E	29	ILE	O-C-N	-5.06	114.61	122.70
1	H	45	ASP	O-C-N	-5.06	114.61	122.70
1	A	66	LYS	O-C-N	-5.05	114.61	122.70
1	B	19	ASP	O-C-N	-5.05	114.61	122.70
1	H	39	SER	O-C-N	-5.05	114.62	122.70
1	H	130	VAL	O-C-N	-5.05	114.62	123.20
1	C	90	ALA	C-N-CA	-5.05	109.08	121.70
1	D	70	LYS	O-C-N	-5.04	114.64	122.70
1	H	78	SER	O-C-N	-5.04	114.63	122.70
1	E	85	PRO	O-C-N	-5.04	114.64	122.70
1	B	27	ARG	O-C-N	-5.03	114.65	122.70
1	E	28	GLN	O-C-N	-5.03	114.65	122.70
1	F	24	THR	O-C-N	-5.03	114.65	123.20
1	C	146	HIS	O-C-N	-5.03	114.66	122.70
1	F	83	THR	O-C-N	-5.03	114.66	123.20
1	H	41	SER	O-C-N	-5.03	114.66	122.70
1	G	28	GLN	O-C-N	-5.02	114.66	122.70
1	G	135	ARG	O-C-N	-5.02	114.66	122.70
1	D	130	VAL	O-C-N	-5.02	114.66	123.20
1	E	61	PRO	O-C-N	-5.02	114.67	122.70
1	D	58	SER	O-C-N	-5.02	114.67	122.70
1	H	114	ASP	O-C-N	-5.02	114.67	122.70
1	E	4	THR	O-C-N	-5.01	114.68	122.70
1	F	28	GLN	O-C-N	-5.01	114.68	122.70
1	D	37	ILE	O-C-N	-5.01	114.68	123.20
1	G	124	ILE	O-C-N	-5.01	114.68	122.70
1	A	7	VAL	O-C-N	-5.01	114.68	123.20
1	D	6	THR	O-C-N	-5.01	114.68	122.70
1	D	28	GLN	O-C-N	-5.01	114.68	122.70
1	D	41	SER	O-C-N	-5.01	114.68	122.70
1	D	39	SER	O-C-N	-5.01	114.69	122.70
1	A	98	SER	O-C-N	-5.01	114.69	122.70

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1	AYA	CA
1	B	1	AYA	CA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
1	C	1	AYA	CA
1	E	1	AYA	CA
1	G	1	AYA	CA
1	H	1	AYA	CA

All (46) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	AYA	Mainchain
1	A	115	GLU	Mainchain
1	A	34	LYS	Mainchain
1	A	42	VAL	Mainchain
1	A	72	PRO	Mainchain
1	A	8	GLY	Mainchain,Peptide
1	A	9	SER	Mainchain
1	B	1	AYA	Mainchain
1	B	34	LYS	Mainchain
1	B	8	GLY	Mainchain
1	B	9	SER	Mainchain
1	C	109	PHE	Mainchain
1	C	144	GLY	Mainchain
1	C	23	TYR	Mainchain
1	C	34	LYS	Mainchain
1	C	7	VAL	Mainchain
1	C	8	GLY	Mainchain
1	C	89	LEU	Mainchain
1	C	9	SER	Mainchain
1	D	1	AYA	Mainchain
1	D	23	TYR	Mainchain
1	D	34	LYS	Mainchain
1	D	8	GLY	Mainchain,Peptide
1	E	34	LYS	Mainchain,Peptide
1	E	8	GLY	Peptide
1	E	9	SER	Mainchain
1	E	99	LEU	Mainchain
1	F	23	TYR	Mainchain
1	F	7	VAL	Mainchain
1	F	8	GLY	Mainchain
1	F	88	ALA	Mainchain
1	F	89	LEU	Mainchain
1	F	9	SER	Mainchain
1	F	90	ALA	Mainchain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	G	3	GLN	Mainchain
1	G	33	TYR	Mainchain
1	G	7	VAL	Mainchain
1	G	8	GLY	Mainchain
1	G	89	LEU	Mainchain
1	H	1	AYA	Mainchain
1	H	118	THR	Mainchain
1	H	89	LEU	Mainchain
1	H	9	SER	Mainchain

## 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	A	1132	0	1084	69	0
1	B	1132	0	1083	59	0
1	C	1132	0	1084	58	0
1	D	1132	0	1080	86	0
1	E	1128	0	1071	48	0
1	F	1128	0	1067	69	0
1	G	1132	0	1081	55	0
1	H	1132	0	1082	72	0
2	A	118	0	0	7	0
2	B	123	0	0	9	0
2	C	121	0	0	4	0
2	D	121	0	0	7	0
2	E	93	0	0	4	0
2	F	115	0	0	6	0
2	G	102	0	0	6	0
2	H	81	0	0	6	0
All	All	9922	0	8632	481	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 27.

All (481) 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:C:8:GLY:HA2	1:D:123:PRO:HG2	1.22	1.18
1:D:18:TRP:HZ3	1:D:136:THR:HG23	0.98	1.10
1:D:18:TRP:CZ3	1:D:136:THR:HG23	1.89	1.07
1:A:61:PRO:HD2	2:A:181:HOH:O	1.57	1.04
1:E:60:LEU:HD11	1:E:89:LEU:HD11	1.47	0.97
1:F:28:GLN:HG2	1:F:43:ILE:HB	1.47	0.95
1:D:20:GLU:HG2	1:D:54:PRO:HD2	1.50	0.92
1:D:74:GLU:HA	1:D:104:ASN:HD21	1.33	0.92
1:D:99:LEU:HD11	1:D:143:ILE:HD11	1.51	0.91
1:C:8:GLY:CA	1:D:123:PRO:HG2	2.00	0.90
1:A:92:PRO:HD2	2:A:240:HOH:O	1.72	0.88
1:H:86:PHE:CZ	1:H:88:ALA:HB3	2.10	0.86
1:G:123:PRO:HG2	1:H:8:GLY:HA2	1.55	0.86
1:C:60:LEU:HD11	1:C:89:LEU:HD11	1.56	0.86
1:G:8:GLY:HA2	1:H:123:PRO:HB2	1.55	0.86
1:H:74:GLU:HA	1:H:104:ASN:HD21	1.42	0.84
1:D:18:TRP:HZ3	1:D:136:THR:CG2	1.88	0.84
1:D:60:LEU:HD12	1:D:139:LEU:HD13	1.59	0.83
1:D:14:GLY:O	1:D:135:ARG:HG2	1.78	0.82
1:G:34:LYS:HG3	2:G:246:HOH:O	1.78	0.82
1:F:79:VAL:HG13	1:F:101:PHE:CE1	2.14	0.82
1:C:74:GLU:HA	1:C:104:ASN:HD21	1.43	0.82
2:B:212:HOH:O	1:D:1:AYA:HM3	1.82	0.80
1:E:86:PHE:HD2	1:E:89:LEU:HB2	1.46	0.78
1:E:86:PHE:CD2	1:E:89:LEU:HB2	2.19	0.78
1:F:60:LEU:H	1:F:60:LEU:HD22	1.48	0.78
1:D:60:LEU:HD12	1:D:139:LEU:CD1	2.14	0.78
1:E:123:PRO:HG2	1:F:8:GLY:HA2	1.66	0.78
1:F:67:ILE:HG23	1:F:109:PHE:CD2	2.19	0.77
1:G:18:TRP:HZ3	1:G:136:THR:HG1	1.32	0.77
1:F:75:PHE:H	1:F:104:ASN:ND2	1.83	0.76
1:A:133:LYS:HE3	1:A:144:GLY:HA3	1.66	0.76
1:A:89:LEU:O	1:A:91:THR:HG22	1.86	0.76
1:D:41:SER:OG	1:D:55:LYS:HD3	1.86	0.76
1:D:75:PHE:H	1:D:104:ASN:ND2	1.84	0.75
1:H:18:TRP:HZ3	1:H:136:THR:OG1	1.71	0.74
1:E:52:SER:HB2	2:E:153:HOH:O	1.87	0.74
1:A:102:LYS:HG2	1:A:108:THR:HB	1.70	0.73
1:D:60:LEU:CD1	1:D:139:LEU:HD13	2.17	0.73
1:H:91:THR:HG21	1:H:95:VAL:HG21	1.69	0.73
1:G:74:GLU:HA	1:G:104:ASN:HD21	1.54	0.73
1:F:7:VAL:HG12	1:F:145:ILE:HG22	1.69	0.73

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:THR:HG22	1:A:111:PRO:HA	1.70	0.73
1:C:8:GLY:HA2	1:D:123:PRO:CG	2.12	0.73
1:B:20:GLU:HG2	1:B:54:PRO:HD2	1.69	0.72
1:C:35:GLU:HG3	1:C:86:PHE:CZ	2.24	0.72
1:E:48:GLY:HA3	2:E:172:HOH:O	1.89	0.72
1:C:133:LYS:HE2	2:C:218:HOH:O	1.90	0.72
1:F:20:GLU:HG2	1:F:54:PRO:HD2	1.71	0.72
1:H:109:PHE:HB3	1:H:112:TYR:OH	1.90	0.71
1:D:89:LEU:HA	2:D:223:HOH:O	1.90	0.71
1:C:4:THR:HG21	1:C:146:HIS:HB3	1.73	0.71
1:A:88:ALA:C	1:A:90:ALA:H	1.90	0.71
1:B:39:SER:HB3	1:B:57:THR:HA	1.73	0.71
1:H:18:TRP:HZ3	1:H:136:THR:HG1	1.38	0.70
1:E:60:LEU:CD1	1:E:89:LEU:HD11	2.20	0.70
1:B:28:GLN:HG2	1:B:43:ILE:HG13	1.74	0.70
1:G:133:LYS:HE3	1:H:125:GLU:OE2	1.92	0.69
1:C:65:VAL:HG21	1:C:112:TYR:CE1	2.28	0.68
1:H:135:ARG:HD2	2:H:205:HOH:O	1.95	0.67
1:C:74:GLU:HB2	1:C:105:LYS:HG3	1.75	0.67
1:A:60:LEU:H	1:A:60:LEU:HD22	1.59	0.67
1:F:67:ILE:HG23	1:F:109:PHE:CE2	2.30	0.67
1:H:71:PHE:CD1	1:H:72:PRO:HA	2.30	0.66
1:D:78:SER:HB3	1:D:102:LYS:HB2	1.77	0.66
1:F:34:LYS:HD2	1:F:62:TYR:HA	1.76	0.66
1:B:30:GLU:OE2	1:B:66:LYS:HG3	1.95	0.66
1:F:79:VAL:HG13	1:F:101:PHE:HE1	1.57	0.66
1:F:89:LEU:O	1:F:91:THR:HG22	1.94	0.66
1:A:92:PRO:HD3	2:A:256:HOH:O	1.95	0.66
1:H:18:TRP:CZ3	1:H:136:THR:OG1	2.48	0.66
1:D:136:THR:HG22	1:D:140:LEU:HD12	1.78	0.66
1:G:83:THR:HG22	1:G:118:THR:HG23	1.77	0.66
1:G:18:TRP:HZ3	1:G:136:THR:OG1	1.78	0.66
1:F:74:GLU:HA	1:F:104:ASN:HD21	1.60	0.65
1:C:18:TRP:HH2	1:C:140:LEU:CD1	2.09	0.65
1:E:82:TYR:HB2	1:E:98:SER:HB3	1.79	0.65
1:C:5:ILE:HD13	1:D:5:ILE:HD12	1.77	0.65
1:G:104:ASN:HD22	1:G:104:ASN:H	1.45	0.65
1:D:74:GLU:OE2	1:D:103:THR:HG21	1.98	0.64
1:D:60:LEU:HD11	1:D:89:LEU:HD11	1.78	0.64
1:E:123:PRO:HG2	1:F:8:GLY:CA	2.26	0.64
1:H:58:SER:HB2	1:H:138:ASP:O	1.98	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:LEU:CD1	1:D:89:LEU:HD11	2.28	0.63
1:F:20:GLU:HB2	1:F:132:PHE:O	1.98	0.63
1:D:99:LEU:HD11	1:D:143:ILE:CD1	2.28	0.63
1:B:1:AYA:H	1:D:128:LEU:HD21	1.63	0.63
1:A:1:AYA:HM3	1:C:128:LEU:HD11	1.81	0.63
1:D:74:GLU:OE2	1:D:107:ARG:HD3	1.99	0.63
1:B:89:LEU:O	1:B:91:THR:HG22	1.99	0.63
1:A:132:PHE:CE1	1:A:145:ILE:HD11	2.33	0.63
1:F:34:LYS:CD	1:F:62:TYR:HA	2.29	0.63
1:A:20:GLU:HG2	1:A:54:PRO:HD2	1.80	0.63
1:F:1:AYA:HM2	1:H:128:LEU:HG	1.81	0.62
1:D:37:ILE:O	1:D:139:LEU:HG	1.99	0.62
1:C:86:PHE:CZ	1:C:88:ALA:HB3	2.35	0.62
1:G:116:GLU:HB3	2:G:203:HOH:O	1.97	0.62
1:E:82:TYR:CE2	1:E:115:GLU:HG2	2.34	0.61
1:E:81:GLY:O	1:E:98:SER:HB3	2.00	0.61
1:A:40:PHE:O	1:A:56:HIS:HB2	2.00	0.61
1:B:102:LYS:HD3	1:B:108:THR:HB	1.81	0.61
1:C:11:GLY:HA2	1:C:83:THR:HG21	1.83	0.61
1:A:8:GLY:HA2	1:B:123:PRO:HD2	1.82	0.61
1:H:60:LEU:HD21	2:H:227:HOH:O	2.01	0.60
1:B:130:VAL:HG11	1:B:148:SER:OG	2.01	0.60
1:F:34:LYS:HB2	1:F:62:TYR:CD1	2.35	0.60
1:A:60:LEU:HD11	1:A:89:LEU:HD11	1.83	0.60
1:D:98:SER:HA	1:D:112:TYR:O	2.01	0.60
1:D:59:LYS:HG3	2:D:186:HOH:O	2.00	0.59
1:G:18:TRP:HH2	1:G:140:LEU:HD13	1.66	0.59
1:B:135:ARG:HB2	1:B:141:ASP:HB2	1.85	0.59
1:D:67:ILE:HG23	1:D:109:PHE:CD2	2.37	0.59
1:E:20:GLU:HG2	1:E:54:PRO:HD2	1.84	0.59
1:H:28:GLN:NE2	1:H:66:LYS:HE3	2.17	0.59
1:A:123:PRO:HD2	1:B:8:GLY:HA2	1.84	0.59
1:H:74:GLU:OE2	1:H:107:ARG:HD3	2.03	0.59
1:D:136:THR:CG2	1:D:140:LEU:HD12	2.34	0.58
1:D:13:PRO:HB3	2:D:162:HOH:O	2.02	0.58
1:B:128:LEU:HD12	1:D:2:SER:HB3	1.85	0.58
1:D:74:GLU:CA	1:D:104:ASN:HD21	2.11	0.58
1:C:135:ARG:CG	1:C:142:ALA:HB3	2.34	0.58
1:E:133:LYS:NZ	2:E:166:HOH:O	2.37	0.58
1:B:98:SER:HA	1:B:112:TYR:O	2.03	0.58
1:H:28:GLN:HE22	1:H:66:LYS:HE3	1.68	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ASP:HB3	2:A:172:HOH:O	2.03	0.58
1:A:18:TRP:CD1	1:A:19:ASP:N	2.72	0.58
1:B:23:TYR:HE2	1:B:51:PHE:CE2	2.21	0.58
1:B:1:AYA:HM3	2:D:150:HOH:O	2.04	0.57
1:A:18:TRP:HD1	1:A:19:ASP:N	2.02	0.57
1:C:135:ARG:HG3	1:C:142:ALA:HB3	1.84	0.57
1:D:58:SER:HB2	1:D:138:ASP:O	2.04	0.57
1:D:18:TRP:HH2	1:D:140:LEU:HD11	1.69	0.57
1:D:136:THR:HG22	1:D:140:LEU:HA	1.86	0.57
1:G:139:LEU:HD23	2:G:212:HOH:O	2.03	0.57
1:F:96:VAL:HG21	1:F:140:LEU:HD23	1.86	0.57
1:H:86:PHE:CE2	1:H:88:ALA:HB3	2.39	0.57
1:D:75:PHE:N	1:D:104:ASN:ND2	2.52	0.57
1:D:99:LEU:CD1	1:D:143:ILE:HD11	2.32	0.57
1:H:27:ARG:HD3	1:H:71:PHE:CD2	2.40	0.57
1:F:104:ASN:HD22	1:F:104:ASN:H	1.51	0.57
1:F:8:GLY:O	1:F:9:SER:HB2	2.04	0.57
1:G:18:TRP:C	1:G:18:TRP:CD1	2.78	0.57
1:G:78:SER:HB3	1:G:102:LYS:HB3	1.86	0.57
1:G:135:ARG:HB2	1:G:142:ALA:HB3	1.87	0.57
1:G:121:ASN:HB3	2:G:214:HOH:O	2.04	0.57
1:C:60:LEU:CD1	1:C:89:LEU:HD11	2.31	0.56
1:B:83:THR:O	1:B:118:THR:HG22	2.05	0.56
1:B:35:GLU:HB2	1:B:86:PHE:CZ	2.40	0.56
1:D:36:ALA:HB3	1:D:139:LEU:HD21	1.88	0.56
1:A:74:GLU:HA	1:A:104:ASN:HD21	1.70	0.56
1:G:139:LEU:HD23	1:G:139:LEU:N	2.20	0.56
1:H:138:ASP:HB2	1:H:139:LEU:HD12	1.88	0.56
1:C:11:GLY:HA2	1:C:83:THR:CG2	2.36	0.56
1:A:17:GLY:HA2	1:A:135:ARG:HG2	1.87	0.56
1:C:46:LEU:HB2	1:C:51:PHE:HB2	1.88	0.56
1:B:93:THR:CG2	2:B:195:HOH:O	2.53	0.56
1:H:104:ASN:HD22	1:H:104:ASN:H	1.52	0.56
1:H:26:ILE:HG23	1:H:42:VAL:HG23	1.87	0.56
1:D:11:GLY:HA2	1:D:83:THR:OG1	2.06	0.55
1:D:132:PHE:CE1	1:D:145:ILE:HD12	2.41	0.55
1:D:74:GLU:HG3	1:D:105:LYS:HG2	1.88	0.55
1:G:74:GLU:OE2	1:G:107:ARG:HD3	2.06	0.55
1:A:88:ALA:C	1:A:90:ALA:N	2.60	0.55
1:B:22:SER:HB2	2:B:156:HOH:O	2.07	0.55
1:A:28:GLN:NE2	1:A:66:LYS:HE3	2.21	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLN:NE2	1:A:66:LYS:CE	2.69	0.55
1:F:23:TYR:O	1:F:130:VAL:HG22	2.07	0.55
1:C:67:ILE:O	1:C:67:ILE:HG22	2.06	0.55
1:F:19:ASP:HA	1:F:133:LYS:HB2	1.87	0.55
1:E:75:PHE:H	1:E:104:ASN:ND2	2.04	0.55
1:B:102:LYS:CD	1:B:108:THR:HB	2.36	0.55
1:E:104:ASN:N	1:E:104:ASN:HD22	2.03	0.55
1:G:34:LYS:NZ	1:G:34:LYS:HB3	2.22	0.54
1:H:13:PRO:HD2	1:H:93:THR:OG1	2.07	0.54
1:A:7:VAL:HG12	1:A:145:ILE:HG22	1.88	0.54
1:A:23:TYR:HE2	1:A:51:PHE:CE2	2.25	0.54
1:A:104:ASN:H	1:A:104:ASN:HD22	1.54	0.54
1:E:11:GLY:HA2	1:E:83:THR:CG2	2.36	0.54
1:E:60:LEU:H	1:E:60:LEU:HD22	1.72	0.54
1:H:101:PHE:N	1:H:101:PHE:CD1	2.74	0.54
1:G:18:TRP:CZ3	1:G:136:THR:OG1	2.54	0.54
1:F:1:AYA:HM3	2:H:153:HOH:O	2.07	0.54
1:H:28:GLN:HB2	1:H:68:GLU:HA	1.89	0.53
1:A:23:TYR:CE2	1:A:51:PHE:CD2	2.95	0.53
1:G:139:LEU:HD23	1:G:139:LEU:H	1.74	0.53
1:C:11:GLY:HA3	1:C:142:ALA:HA	1.90	0.53
1:G:104:ASN:HD22	1:G:104:ASN:N	2.05	0.53
1:B:92:PRO:HD3	2:B:245:HOH:O	2.07	0.53
1:E:114:ASP:O	1:E:116:GLU:N	2.42	0.53
1:F:74:GLU:HG3	1:F:105:LYS:HG2	1.91	0.53
1:D:40:PHE:O	1:D:56:HIS:HB2	2.09	0.53
1:D:96:VAL:HG12	1:D:140:LEU:O	2.09	0.53
1:H:18:TRP:HH2	1:H:140:LEU:CD1	2.22	0.53
1:F:104:ASN:HD22	1:F:104:ASN:N	2.07	0.53
1:A:89:LEU:HG	1:A:139:LEU:HD21	1.91	0.53
1:C:18:TRP:CZ3	1:C:136:THR:OG1	2.55	0.53
1:A:60:LEU:N	1:A:60:LEU:HD22	2.23	0.52
1:H:18:TRP:CD1	1:H:18:TRP:C	2.81	0.52
1:B:97:ARG:O	1:B:113:GLY:HA3	2.09	0.52
1:G:125:GLU:OE2	1:H:133:LYS:HE3	2.09	0.52
1:D:89:LEU:CD1	1:D:139:LEU:HD22	2.39	0.52
1:C:35:GLU:HG3	1:C:86:PHE:HZ	1.74	0.52
1:H:11:GLY:HA3	1:H:142:ALA:HA	1.91	0.52
1:C:31:LEU:HA	1:C:39:SER:O	2.10	0.52
1:D:14:GLY:O	1:D:135:ARG:CG	2.53	0.52
1:B:23:TYR:CE2	1:B:51:PHE:CE2	2.98	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:ARG:HD2	2:B:268:HOH:O	2.08	0.52
1:E:11:GLY:HA2	1:E:83:THR:HG23	1.91	0.52
1:E:60:LEU:HD11	1:E:89:LEU:CD1	2.30	0.52
1:D:100:THR:HG22	1:D:111:PRO:HA	1.92	0.52
1:A:5:ILE:HG13	1:B:149:LEU:HD13	1.92	0.52
1:D:20:GLU:OE1	1:D:44:TYR:OH	2.27	0.52
1:G:83:THR:HG22	1:G:118:THR:CG2	2.40	0.52
1:D:132:PHE:CE1	1:D:145:ILE:CD1	2.93	0.52
1:F:58:SER:HB2	1:F:138:ASP:O	2.11	0.51
1:A:28:GLN:NE2	1:A:43:ILE:HD12	2.25	0.51
1:F:32:SER:HA	1:F:63:LYS:O	2.10	0.51
1:G:130:VAL:HG21	1:G:148:SER:HB3	1.93	0.51
1:D:86:PHE:CD2	1:D:89:LEU:HG	2.46	0.51
1:D:33:TYR:CD1	1:D:33:TYR:N	2.79	0.51
1:D:60:LEU:HD11	1:D:89:LEU:CD1	2.41	0.51
1:D:86:PHE:HD2	1:D:89:LEU:HG	1.75	0.50
1:G:36:ALA:HA	1:G:97:ARG:HA	1.93	0.50
1:H:35:GLU:HA	1:H:114:ASP:OD2	2.11	0.50
1:H:31:LEU:HA	1:H:39:SER:O	2.11	0.50
1:G:33:TYR:O	1:G:62:TYR:HB3	2.12	0.50
1:B:18:TRP:CZ3	1:B:136:THR:OG1	2.63	0.50
1:D:18:TRP:C	1:D:18:TRP:CD1	2.85	0.50
1:C:22:SER:C	1:C:23:TYR:CD1	2.85	0.50
1:H:135:ARG:HG3	1:H:142:ALA:HB3	1.93	0.50
1:F:41:SER:HB3	1:F:55:LYS:HA	1.94	0.50
1:F:100:THR:HG22	2:F:202:HOH:O	2.10	0.50
1:F:47:ASN:ND2	1:H:22:SER:H	2.09	0.50
1:C:60:LEU:HD11	1:C:89:LEU:CD1	2.35	0.49
1:F:27:ARG:HB2	1:F:43:ILE:HG22	1.93	0.49
1:C:22:SER:O	1:C:23:TYR:CD1	2.65	0.49
1:C:75:PHE:H	1:C:104:ASN:ND2	2.10	0.49
1:E:42:VAL:HG13	1:E:44:TYR:CE2	2.47	0.49
1:B:89:LEU:HD11	1:B:139:LEU:CD2	2.43	0.49
1:F:106:GLY:HA2	2:F:209:HOH:O	2.11	0.49
1:E:62:TYR:CD1	1:E:62:TYR:N	2.80	0.49
1:B:18:TRP:HH2	1:B:140:LEU:CD1	2.26	0.49
1:H:12:GLY:HA2	1:H:94:PRO:HG2	1.94	0.49
1:D:71:PHE:HE2	2:D:177:HOH:O	1.96	0.49
1:C:18:TRP:HH2	1:C:140:LEU:HD13	1.78	0.49
1:F:47:ASN:HD21	1:H:22:SER:H	1.61	0.49
1:E:60:LEU:CG	1:E:89:LEU:HD11	2.43	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:63:LYS:CB	2:G:246:HOH:O	2.61	0.49
1:B:96:VAL:HG13	1:B:140:LEU:O	2.13	0.49
1:B:18:TRP:CD1	1:B:56:HIS:NE2	2.81	0.49
1:H:83:THR:HG22	1:H:118:THR:O	2.12	0.49
1:H:74:GLU:OE1	1:H:107:ARG:NH1	2.45	0.48
1:F:89:LEU:HD11	1:F:139:LEU:HD11	1.95	0.48
1:F:18:TRP:CG	1:F:56:HIS:CE1	3.01	0.48
1:C:97:ARG:NH1	1:C:116:GLU:HG3	2.27	0.48
1:E:84:GLY:O	1:E:95:VAL:HG12	2.14	0.48
1:D:36:ALA:HB3	1:D:139:LEU:CD2	2.43	0.48
1:D:94:PRO:HD2	2:D:236:HOH:O	2.12	0.48
1:G:102:LYS:HD3	1:G:108:THR:HB	1.95	0.48
1:A:3:GLN:HG3	1:B:126:ASN:ND2	2.28	0.48
1:G:8:GLY:N	1:H:123:PRO:O	2.46	0.48
1:F:21:GLY:O	1:F:131:GLY:HA3	2.14	0.48
1:E:18:TRP:CG	1:E:56:HIS:CE1	3.02	0.48
1:A:89:LEU:O	1:A:90:ALA:C	2.51	0.48
1:H:67:ILE:HG12	1:H:109:PHE:CD2	2.48	0.48
1:A:60:LEU:H	1:A:60:LEU:CD2	2.25	0.48
1:D:18:TRP:CH2	1:D:140:LEU:HD11	2.49	0.47
1:C:13:PRO:HD2	1:C:93:THR:OG1	2.14	0.47
1:B:44:TYR:CE1	1:B:131:GLY:HA2	2.49	0.47
1:H:71:PHE:CE1	1:H:72:PRO:HB3	2.50	0.47
1:E:18:TRP:CD1	1:E:18:TRP:C	2.87	0.47
1:F:17:GLY:HA2	1:F:135:ARG:HG2	1.96	0.47
1:D:7:VAL:CG1	1:D:8:GLY:N	2.77	0.47
1:E:5:ILE:HG13	1:F:149:LEU:HD13	1.96	0.47
1:G:95:VAL:HG13	1:G:140:LEU:O	2.14	0.47
1:H:27:ARG:HH21	1:H:50:PRO:N	2.11	0.47
1:B:34:LYS:NZ	2:B:170:HOH:O	2.26	0.47
1:B:18:TRP:CH2	1:B:140:LEU:CD1	2.98	0.47
1:F:33:TYR:HD2	1:F:113:GLY:H	1.62	0.47
1:A:4:THR:HG21	1:A:22:SER:OG	2.14	0.47
1:E:1:AYA:OT	1:G:71:PHE:CE2	2.68	0.47
1:A:23:TYR:HE2	1:A:51:PHE:CD2	2.32	0.47
1:G:71:PHE:C	1:G:71:PHE:CD1	2.88	0.47
1:F:31:LEU:C	1:F:31:LEU:HD12	2.35	0.47
1:G:75:PHE:H	1:G:104:ASN:ND2	2.13	0.47
1:G:11:GLY:HA2	1:G:83:THR:OG1	2.15	0.47
1:A:132:PHE:CE1	1:A:145:ILE:CD1	2.98	0.47
1:G:35:GLU:HB3	1:G:97:ARG:HH21	1.79	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:SER:HA	1:B:5:ILE:HD11	1.97	0.47
1:H:27:ARG:HH21	1:H:49:ASP:C	2.18	0.47
1:H:58:SER:OG	1:H:60:LEU:HB2	2.15	0.47
1:H:40:PHE:O	1:H:56:HIS:HB2	2.15	0.47
1:D:99:LEU:HA	1:D:99:LEU:HD12	1.78	0.46
1:C:58:SER:OG	1:C:60:LEU:HD12	2.15	0.46
1:E:24:THR:O	1:G:2:SER:OG	2.33	0.46
1:F:60:LEU:CD2	1:F:60:LEU:H	2.24	0.46
1:D:74:GLU:HA	1:D:104:ASN:ND2	2.16	0.46
1:F:110:GLY:HA2	2:F:210:HOH:O	2.14	0.46
1:C:74:GLU:CA	1:C:104:ASN:HD21	2.19	0.46
1:A:58:SER:HB2	1:A:138:ASP:O	2.16	0.46
1:A:67:ILE:HG23	1:A:109:PHE:CE2	2.51	0.46
1:D:31:LEU:C	1:D:31:LEU:HD12	2.36	0.46
1:B:93:THR:HG22	2:B:195:HOH:O	2.15	0.46
1:A:28:GLN:NE2	1:A:66:LYS:HE2	2.30	0.46
1:A:67:ILE:HG23	1:A:109:PHE:CD2	2.51	0.46
1:G:17:GLY:HA2	1:G:135:ARG:HG2	1.97	0.46
1:C:46:LEU:HD23	1:C:46:LEU:HA	1.86	0.46
1:F:98:SER:HA	1:F:112:TYR:O	2.15	0.46
1:B:18:TRP:C	1:B:18:TRP:CD1	2.89	0.46
1:G:139:LEU:CD2	1:G:139:LEU:N	2.78	0.46
1:H:27:ARG:NH2	1:H:50:PRO:N	2.64	0.46
1:B:135:ARG:HG3	1:B:142:ALA:HB3	1.98	0.46
1:D:7:VAL:HG13	1:D:8:GLY:N	2.31	0.46
1:H:16:ASN:O	1:H:135:ARG:HA	2.15	0.45
1:F:71:PHE:HE1	1:H:1:AYA:HM3	1.81	0.45
1:H:99:LEU:O	1:H:100:THR:HG22	2.16	0.45
1:G:4:THR:HG21	1:G:146:HIS:ND1	2.31	0.45
1:C:64:ASN:HB3	2:C:172:HOH:O	2.17	0.45
1:F:76:LEU:HD11	1:F:101:PHE:HB3	1.99	0.45
1:F:75:PHE:H	1:F:104:ASN:HD21	1.57	0.45
1:H:18:TRP:CH2	1:H:140:LEU:CD1	3.00	0.45
1:B:109:PHE:HB3	1:B:112:TYR:OH	2.16	0.45
1:H:96:VAL:HG12	1:H:140:LEU:O	2.16	0.45
1:F:90:ALA:HA	2:F:248:HOH:O	2.16	0.45
1:F:58:SER:HB2	1:F:60:LEU:HD23	1.98	0.45
1:A:28:GLN:HB3	1:A:43:ILE:HB	1.98	0.45
1:E:62:TYR:HD1	1:E:62:TYR:N	2.14	0.45
1:B:23:TYR:O	1:B:130:VAL:HG22	2.16	0.45
1:A:74:GLU:HG3	1:A:105:LYS:HB2	1.99	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:44:TYR:O	1:F:51:PHE:N	2.45	0.45
1:G:130:VAL:O	1:G:130:VAL:CG1	2.64	0.45
1:C:97:ARG:HH12	1:C:116:GLU:CD	2.20	0.45
1:E:37:ILE:HG21	1:E:140:LEU:HD23	1.99	0.45
1:G:24:THR:O	1:G:24:THR:HG22	2.17	0.45
1:D:18:TRP:CZ3	1:D:136:THR:CG2	2.77	0.45
1:F:18:TRP:CD1	1:F:18:TRP:C	2.89	0.45
1:A:104:ASN:HD22	1:A:104:ASN:N	2.15	0.45
1:H:37:ILE:HD12	1:H:99:LEU:HD22	1.99	0.45
1:G:26:ILE:HG22	1:G:69:LEU:HD12	1.98	0.44
1:A:89:LEU:CG	1:A:139:LEU:HD21	2.47	0.44
1:A:89:LEU:HA	1:A:89:LEU:HD22	1.63	0.44
1:F:34:LYS:HB2	1:F:62:TYR:CG	2.52	0.44
1:A:18:TRP:CD1	1:A:18:TRP:C	2.91	0.44
1:D:54:PRO:HG2	2:D:164:HOH:O	2.16	0.44
1:E:18:TRP:CD1	1:E:56:HIS:CE1	3.05	0.44
1:A:116:GLU:HG3	2:A:208:HOH:O	2.17	0.44
1:C:71:PHE:CD1	1:C:71:PHE:C	2.91	0.44
1:H:84:GLY:HA2	2:H:202:HOH:O	2.17	0.44
1:E:87:SER:O	1:E:90:ALA:N	2.44	0.44
1:B:18:TRP:HZ3	1:B:136:THR:OG1	1.99	0.44
1:C:18:TRP:HZ3	1:C:136:THR:N	2.16	0.44
1:B:32:SER:HB3	1:B:64:ASN:ND2	2.33	0.44
1:H:97:ARG:O	1:H:113:GLY:HA3	2.17	0.44
1:B:104:ASN:OD1	1:B:104:ASN:N	2.51	0.44
1:A:110:GLY:HA3	2:A:203:HOH:O	2.18	0.44
1:E:60:LEU:HD21	1:E:89:LEU:HD11	2.00	0.44
1:F:68:GLU:HB3	2:F:154:HOH:O	2.18	0.44
1:G:31:LEU:HD12	1:G:31:LEU:C	2.38	0.44
1:A:30:GLU:HG2	1:A:66:LYS:HG3	2.00	0.43
1:B:67:ILE:HG22	1:B:69:LEU:HD22	1.99	0.43
1:A:96:VAL:HG22	1:A:140:LEU:O	2.17	0.43
1:D:103:THR:HG23	1:D:105:LYS:H	1.84	0.43
1:F:74:GLU:OE2	1:F:107:ARG:HD3	2.17	0.43
1:C:87:SER:O	1:C:88:ALA:C	2.56	0.43
1:B:89:LEU:HD11	1:B:139:LEU:HD22	2.00	0.43
1:E:134:GLY:O	1:E:135:ARG:HG3	2.18	0.43
1:C:8:GLY:O	1:C:9:SER:HB2	2.18	0.43
1:E:34:LYS:HB2	1:E:62:TYR:CD1	2.53	0.43
1:C:97:ARG:NH1	1:C:116:GLU:CG	2.82	0.43
1:G:18:TRP:CH2	1:G:140:LEU:CD1	3.02	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:71:PHE:O	2:F:182:HOH:O	2.21	0.43
1:F:18:TRP:CH2	1:F:140:LEU:HD11	2.54	0.43
1:D:86:PHE:CZ	1:D:88:ALA:HB3	2.53	0.43
1:B:39:SER:HB3	1:B:57:THR:CA	2.47	0.43
1:C:5:ILE:HG13	1:D:149:LEU:HD13	2.00	0.43
1:D:67:ILE:HG23	1:D:109:PHE:CE2	2.54	0.43
1:A:77:GLU:O	1:A:77:GLU:HG2	2.17	0.43
1:F:24:THR:HG22	1:F:24:THR:O	2.19	0.43
1:E:33:TYR:HE1	1:E:65:VAL:HG22	1.84	0.43
1:C:105:LYS:HB3	1:C:105:LYS:HE2	1.62	0.43
1:D:43:ILE:HG12	1:D:52:SER:HB3	2.01	0.43
1:B:31:LEU:HA	1:B:39:SER:O	2.19	0.43
1:A:132:PHE:HE1	1:A:145:ILE:HD11	1.82	0.43
1:G:59:LYS:O	1:G:60:LEU:C	2.57	0.43
1:D:139:LEU:HD12	1:D:139:LEU:HA	1.78	0.42
1:B:1:AYA:HM2	1:D:128:LEU:HD21	2.01	0.42
1:B:34:LYS:HG2	1:B:35:GLU:CD	2.39	0.42
1:A:75:PHE:H	1:A:104:ASN:ND2	2.16	0.42
1:D:18:TRP:HH2	1:D:140:LEU:CD1	2.33	0.42
1:C:104:ASN:HD22	1:C:104:ASN:N	2.17	0.42
1:A:20:GLU:CG	1:A:54:PRO:HD2	2.47	0.42
1:E:75:PHE:H	1:E:104:ASN:HD21	1.66	0.42
1:D:69:LEU:HA	1:D:69:LEU:HD12	1.79	0.42
1:B:32:SER:HA	1:B:63:LYS:O	2.19	0.42
1:C:50:PRO:HG2	1:C:50:PRO:O	2.19	0.42
1:H:122:LEU:HA	1:H:122:LEU:HD12	1.77	0.42
1:G:100:THR:HG21	2:G:224:HOH:O	2.18	0.42
1:F:46:LEU:HD12	1:F:46:LEU:HA	1.70	0.42
1:H:96:VAL:CG1	1:H:140:LEU:O	2.67	0.42
1:B:121:ASN:ND2	1:B:123:PRO:HG3	2.35	0.42
1:B:13:PRO:HB2	2:B:160:HOH:O	2.20	0.42
1:G:20:GLU:HG2	1:G:54:PRO:HD2	2.00	0.42
1:E:81:GLY:O	1:E:82:TYR:HB2	2.20	0.42
1:B:23:TYR:N	1:B:23:TYR:CD1	2.87	0.42
1:B:93:THR:HA	1:B:94:PRO:HD3	1.99	0.42
1:G:8:GLY:HA2	1:H:123:PRO:CB	2.36	0.42
1:D:37:ILE:HA	1:D:37:ILE:HD13	1.87	0.42
1:H:27:ARG:CZ	1:H:50:PRO:HG3	2.50	0.42
1:F:34:LYS:HD3	1:F:62:TYR:HA	2.02	0.42
1:C:93:THR:HG23	2:C:200:HOH:O	2.20	0.42
1:H:74:GLU:HA	1:H:104:ASN:ND2	2.21	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ASN:OD1	1:C:23:TYR:CE1	2.73	0.42
1:C:59:LYS:NZ	2:C:188:HOH:O	2.51	0.42
1:G:140:LEU:HD11	1:G:142:ALA:O	2.20	0.42
1:H:27:ARG:NH2	1:H:45:ASP:OD1	2.53	0.42
1:H:60:LEU:HA	1:H:60:LEU:HD12	1.70	0.42
1:A:23:TYR:CE2	1:A:51:PHE:CE2	3.06	0.42
1:G:20:GLU:OE1	1:G:44:TYR:OH	2.25	0.42
1:A:32:SER:HA	1:A:64:ASN:HA	2.02	0.42
1:B:82:TYR:HE1	1:B:115:GLU:OE1	2.02	0.42
1:C:33:TYR:O	1:C:62:TYR:HB3	2.20	0.42
1:C:104:ASN:HD22	1:C:104:ASN:H	1.66	0.42
1:F:29:ILE:HB	1:F:67:ILE:HD12	2.01	0.42
1:D:65:VAL:HG21	1:D:112:TYR:CE1	2.55	0.42
1:H:26:ILE:HG23	1:H:42:VAL:CG2	2.49	0.42
1:E:60:LEU:HD23	1:E:139:LEU:HD12	2.01	0.41
1:A:18:TRP:CE2	1:A:56:HIS:CD2	3.07	0.41
1:H:46:LEU:O	1:H:47:ASN:C	2.59	0.41
1:B:49:ASP:HB3	2:B:230:HOH:O	2.20	0.41
1:F:58:SER:HB2	1:F:60:LEU:CD2	2.50	0.41
1:H:67:ILE:HG23	1:H:109:PHE:CE2	2.55	0.41
1:B:1:AYA:H	1:D:128:LEU:CD2	2.30	0.41
1:A:74:GLU:OE2	1:A:107:ARG:HD3	2.20	0.41
1:E:42:VAL:CG1	1:E:44:TYR:CZ	3.03	0.41
1:D:45:ASP:CG	1:D:71:PHE:CZ	2.93	0.41
1:F:121:ASN:O	1:F:123:PRO:HD3	2.20	0.41
1:G:96:VAL:HG22	1:G:140:LEU:HD23	2.02	0.41
1:F:35:GLU:O	1:F:97:ARG:NE	2.53	0.41
1:H:130:VAL:HG21	1:H:148:SER:HB3	2.02	0.41
1:D:89:LEU:HD11	1:D:139:LEU:HD13	2.02	0.41
1:C:135:ARG:HG3	1:C:142:ALA:CB	2.49	0.41
1:D:109:PHE:N	1:D:109:PHE:CD1	2.88	0.41
1:H:12:GLY:CA	1:H:94:PRO:HG2	2.49	0.41
1:D:129:ILE:HG12	1:D:145:ILE:HG12	2.03	0.41
1:E:34:LYS:HB2	1:E:62:TYR:CG	2.55	0.41
1:A:31:LEU:HD12	1:A:65:VAL:HG12	2.03	0.41
1:F:129:ILE:HG21	1:F:129:ILE:HD13	1.81	0.41
1:D:74:GLU:CG	1:D:105:LYS:HG2	2.51	0.41
1:H:7:VAL:HG13	1:H:8:GLY:N	2.35	0.41
1:F:36:ALA:HA	1:F:97:ARG:HA	2.01	0.41
1:B:58:SER:OG	1:B:60:LEU:HB2	2.21	0.41
1:A:96:VAL:HG21	1:A:140:LEU:HD23	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:TYR:C	1:C:62:TYR:HB3	2.41	0.41
1:F:82:TYR:CD1	1:F:115:GLU:HG2	2.56	0.41
1:C:29:ILE:HG12	1:C:42:VAL:HG13	2.02	0.41
1:H:71:PHE:CD1	1:H:72:PRO:CA	3.02	0.41
1:A:128:LEU:HD21	1:C:1:AYA:CT	2.51	0.41
1:E:89:LEU:O	1:E:90:ALA:HB3	2.21	0.41
1:G:119:TYR:CE2	1:G:121:ASN:HB2	2.56	0.41
1:F:71:PHE:CE1	1:H:1:AYA:HM3	2.55	0.41
1:H:29:ILE:HD11	1:H:76:LEU:HD21	2.02	0.41
1:B:4:THR:HG23	1:B:5:ILE:O	2.21	0.41
1:E:37:ILE:HG23	1:E:37:ILE:HD12	1.82	0.41
1:F:60:LEU:HB3	1:F:61:PRO:HD2	2.02	0.40
1:A:87:SER:O	1:A:90:ALA:HA	2.21	0.40
1:C:123:PRO:HD2	1:D:8:GLY:HA2	2.03	0.40
1:E:125:GLU:HG3	2:E:226:HOH:O	2.20	0.40
1:D:6:THR:HG23	1:D:146:HIS:ND1	2.36	0.40
1:G:104:ASN:ND2	1:G:104:ASN:N	2.70	0.40
1:E:82:TYR:CD2	1:E:115:GLU:HG2	2.55	0.40
1:H:25:GLY:HA2	2:H:153:HOH:O	2.22	0.40
1:A:64:ASN:ND2	2:A:244:HOH:O	2.53	0.40
1:C:132:PHE:CE1	1:C:145:ILE:HD11	2.57	0.40
1:D:129:ILE:HG22	1:D:130:VAL:N	2.36	0.40
1:A:47:ASN:HD21	1:C:22:SER:H	1.67	0.40
1:E:18:TRP:CD1	1:E:19:ASP:N	2.90	0.40
1:H:100:THR:CG2	2:H:196:HOH:O	2.69	0.40
1:E:89:LEU:HD22	1:E:89:LEU:HA	1.68	0.40
1:G:95:VAL:HG11	1:G:139:LEU:HG	2.04	0.40
1:F:121:ASN:C	1:F:123:PRO:HD3	2.41	0.40
1:A:31:LEU:HD12	1:A:31:LEU:C	2.42	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	A	147/149 (99%)	133 (90%)	12 (8%)	2 (1%)	14	19
1	B	147/149 (99%)	136 (92%)	8 (5%)	3 (2%)	9	11
1	C	147/149 (99%)	131 (89%)	11 (8%)	5 (3%)	5	4
1	D	147/149 (99%)	132 (90%)	12 (8%)	3 (2%)	9	11
1	E	147/149 (99%)	131 (89%)	12 (8%)	4 (3%)	6	6
1	F	147/149 (99%)	135 (92%)	11 (8%)	1 (1%)	26	38
1	G	147/149 (99%)	139 (95%)	6 (4%)	2 (1%)	14	19
1	H	147/149 (99%)	128 (87%)	17 (12%)	2 (1%)	14	19
All	All	1176/1192 (99%)	1065 (91%)	89 (8%)	22 (2%)	10	12

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	110	GLY
1	B	9	SER
1	B	110	GLY
1	C	9	SER
1	C	110	GLY
1	D	110	GLY
1	E	110	GLY
1	F	9	SER
1	H	110	GLY
1	C	70	LYS
1	D	130	VAL
1	G	90	ALA
1	B	34	LYS
1	C	106	GLY
1	E	34	LYS
1	E	81	GLY
1	D	34	LYS
1	H	34	LYS
1	G	34	LYS
1	E	13	PRO
1	C	137	GLY

### 5.3.2 Protein sidechains ⓘ

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	A	120/122 (98%)	95 (79%)	25 (21%)	1	1
1	B	120/122 (98%)	93 (78%)	27 (22%)	1	1
1	C	120/122 (98%)	95 (79%)	25 (21%)	1	1
1	D	120/122 (98%)	93 (78%)	27 (22%)	1	1
1	E	119/122 (98%)	95 (80%)	24 (20%)	1	1
1	F	119/122 (98%)	95 (80%)	24 (20%)	1	1
1	G	120/122 (98%)	96 (80%)	24 (20%)	1	1
1	H	120/122 (98%)	90 (75%)	30 (25%)	1	1
All	All	958/976 (98%)	752 (78%)	206 (22%)	1	1

All (206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	7	VAL
1	A	9	SER
1	A	18	TRP
1	A	42	VAL
1	A	58	SER
1	A	59	LYS
1	A	64	ASN
1	A	69	LEU
1	A	72	PRO
1	A	76	LEU
1	A	83	THR
1	A	86	PHE
1	A	89	LEU
1	A	91	THR
1	A	95	VAL
1	A	100	THR
1	A	104	ASN
1	A	108	THR
1	A	116	GLU
1	A	118	THR
1	A	130	VAL
1	A	143	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	145	ILE
1	A	149	LEU
1	B	4	THR
1	B	7	VAL
1	B	18	TRP
1	B	24	THR
1	B	28	GLN
1	B	34	LYS
1	B	39	SER
1	B	42	VAL
1	B	49	ASP
1	B	55	LYS
1	B	59	LYS
1	B	60	LEU
1	B	66	LYS
1	B	76	LEU
1	B	83	THR
1	B	86	PHE
1	B	91	THR
1	B	93	THR
1	B	95	VAL
1	B	96	VAL
1	B	102	LYS
1	B	108	THR
1	B	116	GLU
1	B	130	VAL
1	B	139	LEU
1	B	145	ILE
1	B	149	LEU
1	C	2	SER
1	C	4	THR
1	C	5	ILE
1	C	13	PRO
1	C	22	SER
1	C	35	GLU
1	C	46	LEU
1	C	52	SER
1	C	69	LEU
1	C	76	LEU
1	C	83	THR
1	C	98	SER
1	C	100	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	102	LYS
1	C	104	ASN
1	C	105	LYS
1	C	108	THR
1	C	111	PRO
1	C	118	THR
1	C	130	VAL
1	C	133	LYS
1	C	135	ARG
1	C	139	LEU
1	C	143	ILE
1	C	145	ILE
1	D	7	VAL
1	D	16	ASN
1	D	18	TRP
1	D	22	SER
1	D	34	LYS
1	D	42	VAL
1	D	49	ASP
1	D	69	LEU
1	D	76	LEU
1	D	80	SER
1	D	93	THR
1	D	95	VAL
1	D	96	VAL
1	D	98	SER
1	D	100	THR
1	D	103	THR
1	D	104	ASN
1	D	108	THR
1	D	118	THR
1	D	120	PHE
1	D	130	VAL
1	D	135	ARG
1	D	138	ASP
1	D	143	ILE
1	D	145	ILE
1	D	148	SER
1	D	149	LEU
1	E	5	ILE
1	E	7	VAL
1	E	13	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	18	TRP
1	E	24	THR
1	E	49	ASP
1	E	57	THR
1	E	69	LEU
1	E	76	LEU
1	E	89	LEU
1	E	93	THR
1	E	95	VAL
1	E	103	THR
1	E	104	ASN
1	E	108	THR
1	E	115	GLU
1	E	118	THR
1	E	125	GLU
1	E	130	VAL
1	E	138	ASP
1	E	141	ASP
1	E	143	ILE
1	E	148	SER
1	E	149	LEU
1	F	7	VAL
1	F	18	TRP
1	F	28	GLN
1	F	34	LYS
1	F	42	VAL
1	F	43	ILE
1	F	57	THR
1	F	60	LEU
1	F	70	LYS
1	F	72	PRO
1	F	76	LEU
1	F	80	SER
1	F	87	SER
1	F	89	LEU
1	F	94	PRO
1	F	95	VAL
1	F	102	LYS
1	F	104	ASN
1	F	130	VAL
1	F	133	LYS
1	F	141	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	145	ILE
1	F	148	SER
1	F	149	LEU
1	G	2	SER
1	G	4	THR
1	G	9	SER
1	G	18	TRP
1	G	34	LYS
1	G	49	ASP
1	G	70	LYS
1	G	72	PRO
1	G	76	LEU
1	G	83	THR
1	G	86	PHE
1	G	89	LEU
1	G	96	VAL
1	G	100	THR
1	G	102	LYS
1	G	104	ASN
1	G	105	LYS
1	G	108	THR
1	G	120	PHE
1	G	125	GLU
1	G	130	VAL
1	G	133	LYS
1	G	139	LEU
1	G	145	ILE
1	H	7	VAL
1	H	18	TRP
1	H	22	SER
1	H	28	GLN
1	H	34	LYS
1	H	37	ILE
1	H	42	VAL
1	H	49	ASP
1	H	58	SER
1	H	60	LEU
1	H	68	GLU
1	H	69	LEU
1	H	76	LEU
1	H	77	GLU
1	H	80	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	87	SER
1	H	89	LEU
1	H	91	THR
1	H	95	VAL
1	H	96	VAL
1	H	98	SER
1	H	100	THR
1	H	101	PHE
1	H	104	ASN
1	H	108	THR
1	H	118	THR
1	H	128	LEU
1	H	135	ARG
1	H	143	ILE
1	H	145	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	28	GLN
1	A	47	ASN
1	A	104	ASN
1	B	16	ASN
1	B	47	ASN
1	B	64	ASN
1	B	126	ASN
1	C	16	ASN
1	C	28	GLN
1	C	47	ASN
1	C	104	ASN
1	D	28	GLN
1	D	104	ASN
1	E	47	ASN
1	E	56	HIS
1	E	104	ASN
1	F	47	ASN
1	F	64	ASN
1	F	104	ASN
1	G	47	ASN
1	G	104	ASN
1	H	47	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	104	ASN
1	H	121	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	AYA	A	1	1	6,7,8	1.05	0	7,8,10	10.92	6 (85%)
1	AYA	B	1	1	6,7,8	1.63	2 (33%)	7,8,10	10.44	7 (100%)
1	AYA	C	1	1	6,7,8	1.25	1 (16%)	7,8,10	11.17	6 (85%)
1	AYA	D	1	1	6,7,8	1.80	1 (16%)	7,8,10	11.44	4 (57%)
1	AYA	E	1	1	6,7,8	0.75	0	7,8,10	10.52	4 (57%)
1	AYA	F	1	1	6,7,8	1.59	1 (16%)	7,8,10	10.84	7 (100%)
1	AYA	G	1	1	6,7,8	2.43	1 (16%)	7,8,10	10.55	4 (57%)
1	AYA	H	1	1	6,7,8	1.40	1 (16%)	7,8,10	10.88	7 (100%)

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
1	AYA	A	1	1	1/1/2/4	0/4/6/8	0/0/0/0
1	AYA	B	1	1	1/1/2/4	0/4/6/8	0/0/0/0
1	AYA	C	1	1	1/1/2/4	1/4/6/8	0/0/0/0
1	AYA	D	1	1	-	0/4/6/8	0/0/0/0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	AYA	E	1	1	1/1/2/4	0/4/6/8	0/0/0/0
1	AYA	F	1	1	-	0/4/6/8	0/0/0/0
1	AYA	G	1	1	1/1/2/4	0/4/6/8	0/0/0/0
1	AYA	H	1	1	1/1/2/4	0/4/6/8	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	1	AYA	CA-N	-5.55	1.40	1.46
1	B	1	AYA	CA-N	-2.89	1.43	1.46
1	B	1	AYA	CM-CT	2.46	1.55	1.50
1	C	1	AYA	CM-CT	2.60	1.55	1.50
1	H	1	AYA	OT-CT	2.81	1.29	1.23
1	F	1	AYA	CA-N	3.20	1.50	1.46
1	D	1	AYA	CA-N	3.60	1.50	1.46

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	1	AYA	C-CA-N	-14.41	80.36	110.64
1	D	1	AYA	C-CA-N	-14.03	81.16	110.64
1	F	1	AYA	C-CA-N	-13.48	82.31	110.64
1	C	1	AYA	C-CA-N	-13.05	83.21	110.64
1	B	1	AYA	C-CA-N	-12.95	83.42	110.64
1	A	1	AYA	C-CA-N	-12.94	83.44	110.64
1	E	1	AYA	C-CA-N	-12.69	83.96	110.64
1	G	1	AYA	C-CA-N	-12.40	84.58	110.64
1	F	1	AYA	O-C-CA	-7.17	102.84	124.64
1	B	1	AYA	O-C-CA	-6.93	103.57	124.64
1	C	1	AYA	O-C-CA	-6.60	104.58	124.64
1	H	1	AYA	O-C-CA	-6.48	104.93	124.64
1	G	1	AYA	O-C-CA	-6.32	105.41	124.64
1	E	1	AYA	O-C-CA	-6.19	105.82	124.64
1	A	1	AYA	O-C-CA	-6.12	106.03	124.64
1	D	1	AYA	O-C-CA	-5.96	106.53	124.64
1	B	1	AYA	OT-CT-N	-5.90	109.83	121.86
1	C	1	AYA	OT-CT-CM	-2.91	116.72	122.06
1	H	1	AYA	OT-CT-N	-2.87	116.01	121.86
1	B	1	AYA	OT-CT-CM	-2.74	117.03	122.06
1	F	1	AYA	OT-CT-N	-2.48	116.82	121.86
1	F	1	AYA	OT-CT-CM	-2.35	117.75	122.06
1	A	1	AYA	OT-CT-CM	-2.27	117.89	122.06

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	1	AYA	OT-CT-CM	-2.13	118.16	122.06
1	H	1	AYA	CM-CT-N	2.15	120.22	116.11
1	A	1	AYA	CM-CT-N	2.21	120.33	116.11
1	C	1	AYA	CM-CT-N	2.65	121.18	116.11
1	F	1	AYA	CM-CT-N	3.94	123.65	116.11
1	B	1	AYA	CM-CT-N	4.36	124.45	116.11
1	B	1	AYA	CA-N-CT	7.19	132.60	121.46
1	G	1	AYA	CA-N-CT	8.48	134.61	121.46
1	C	1	AYA	CA-N-CT	10.55	137.80	121.46
1	A	1	AYA	CA-N-CT	10.87	138.30	121.46
1	E	1	AYA	CA-N-CT	11.19	138.80	121.46
1	H	1	AYA	CA-N-CT	11.40	139.12	121.46
1	F	1	AYA	CA-N-CT	11.59	139.41	121.46
1	D	1	AYA	CA-N-CT	12.03	140.09	121.46
1	F	1	AYA	CB-CA-N	20.67	133.68	109.61
1	H	1	AYA	CB-CA-N	20.78	133.81	109.61
1	B	1	AYA	CB-CA-N	20.84	133.88	109.61
1	E	1	AYA	CB-CA-N	21.08	134.16	109.61
1	A	1	AYA	CB-CA-N	22.37	135.66	109.61
1	G	1	AYA	CB-CA-N	22.57	135.89	109.61
1	C	1	AYA	CB-CA-N	23.05	136.45	109.61
1	D	1	AYA	CB-CA-N	23.18	136.60	109.61

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	G	1	AYA	CA
1	A	1	AYA	CA
1	C	1	AYA	CA
1	H	1	AYA	CA
1	B	1	AYA	CA
1	E	1	AYA	CA

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	1	AYA	OT-CT-N-CA

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	AYA	1	0
1	B	1	AYA	4	0
1	C	1	AYA	1	0
1	D	1	AYA	1	0
1	E	1	AYA	1	0
1	F	1	AYA	2	0
1	H	1	AYA	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	148/149 (99%)	-0.70	2 (1%) 78 77	7, 20, 37, 60	0
1	B	148/149 (99%)	-0.58	0 100 100	11, 24, 37, 46	0
1	C	148/149 (99%)	-0.69	1 (0%) 89 88	7, 22, 34, 57	0
1	D	148/149 (99%)	-0.35	4 (2%) 58 57	11, 26, 44, 66	0
1	E	148/149 (99%)	-0.58	2 (1%) 78 77	8, 23, 47, 61	0
1	F	148/149 (99%)	-0.43	4 (2%) 58 57	9, 26, 44, 63	0
1	G	148/149 (99%)	-0.75	1 (0%) 89 88	10, 21, 33, 52	0
1	H	148/149 (99%)	-0.44	2 (1%) 78 77	11, 26, 40, 60	0
All	All	1184/1192 (99%)	-0.57	16 (1%) 78 77	7, 24, 43, 66	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	91	THR	7.8
1	A	88	ALA	4.6
1	F	91	THR	4.3
1	D	91	THR	4.3
1	F	89	LEU	4.3
1	D	89	LEU	4.1
1	A	91	THR	3.8
1	E	91	THR	3.7
1	H	88	ALA	3.6
1	C	23	TYR	3.4
1	F	88	ALA	3.2
1	D	90	ALA	2.9
1	E	88	ALA	2.7
1	F	90	ALA	2.1
1	G	88	ALA	2.0
1	D	103	THR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	AYA	D	1	8/9	0.96	0.12	-	22,28,32,34	0
1	AYA	G	1	8/9	0.95	0.11	-	22,26,31,31	0
1	AYA	A	1	8/9	0.93	0.13	-	24,26,31,35	0
1	AYA	C	1	8/9	0.96	0.12	-	18,23,29,34	0
1	AYA	H	1	8/9	0.97	0.09	-	23,25,30,32	0
1	AYA	F	1	8/9	0.94	0.10	-	17,23,32,32	0
1	AYA	B	1	8/9	0.94	0.12	-	30,33,37,38	0
1	AYA	E	1	8/9	0.94	0.11	-	12,20,22,22	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.