



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2016 – 06:27 PM EDT

PDB ID : 5AQD  
Title : Crystal structure of Phormidium Phycoerythrin at pH 8.5  
Authors : Kumar, V.; Sharma, M.; Sonani, R.R.; Gupta, G.D.; Madamwar, D.  
Deposited on : 2015-09-22  
Resolution : 2.12 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027790  
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) : rb-20027790



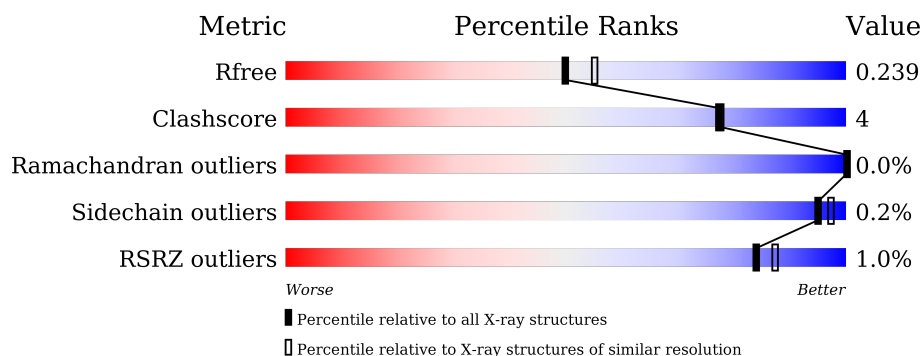
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.12 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))
$R_{free}$	91344	4587 (2.14-2.10)
Clashscore	102246	5132 (2.14-2.10)
Ramachandran outliers	100387	5080 (2.14-2.10)
Sidechain outliers	100360	5081 (2.14-2.10)
RSRZ outliers	91569	4597 (2.14-2.10)

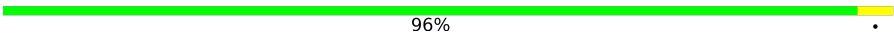
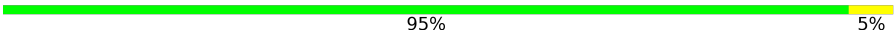
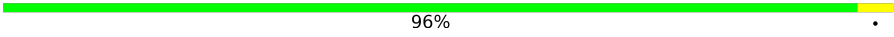
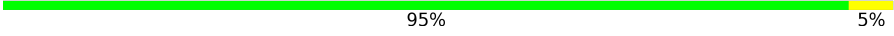
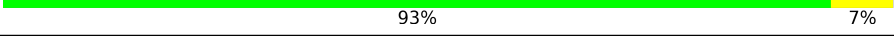
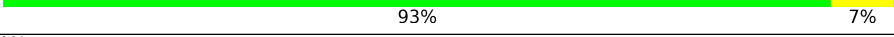
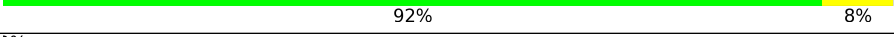
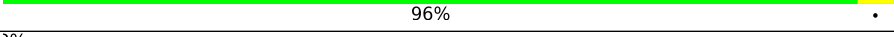
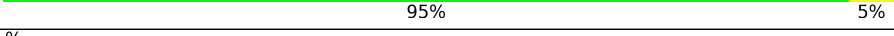
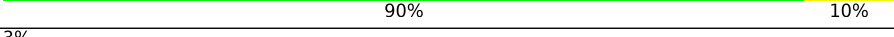
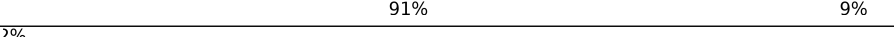
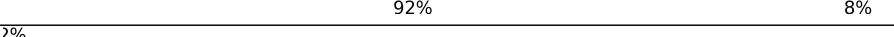
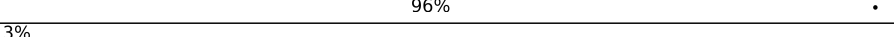
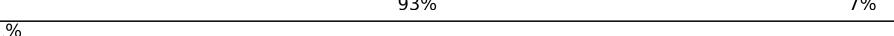


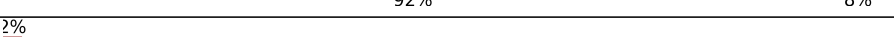
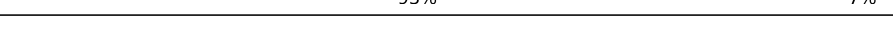
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	164	 96%
1	B	164	 93% 7%
1	C	164	 91% 9%
1	D	164	 98%
1	E	164	 95% 5%
1	F	164	 97%

*Continued on next page...*



Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	164	 96% .
1	H	164	 95% 5%
1	I	164	 96% .
1	J	164	 95% 5%
1	K	164	 93% 7%
1	L	164	 93% 7%
2	M	184	 2% 92% 8%
2	N	184	 2% 96% .
2	O	184	 2% 95% 5%
2	P	184	 % 90% 10%
2	Q	184	 3% 91% 9%
2	R	184	 2% 92% 8%
2	S	184	 2% 96% .
2	T	184	 3% 93% 7%
2	U	184	 % 90% 10%
2	V	184	 3% 91% 9%
2	W	184	 % 92% 8%
2	X	184	 2% 93% 7%

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
3	PEB	C	167	-	-	-	X
3	PEB	D	167	-	-	-	X
4	GOL	A	1165	-	-	-	X
4	GOL	B	1165	-	-	-	X
4	GOL	C	1165	-	-	-	X
4	GOL	D	1165	-	-	-	X
4	GOL	E	1165	-	-	-	X

Continued on next page...



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	H	1165	-	-	-	X
4	GOL	I	1165	-	-	-	X
4	GOL	K	1165	-	-	-	X
5	SO4	E	1200	-	-	-	X
5	SO4	H	1200	-	-	-	X



## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 37483 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 PHYCOERYTHRIN ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1239	771	218	244	6			
1	B	164	Total	C	N	O	S	0	0	0
			1239	771	218	244	6			
1	C	164	Total	C	N	O	S	0	0	0
			1239	771	218	244	6			
1	D	164	Total	C	N	O	S	0	0	0
			1239	771	218	244	6			
1	E	164	Total	C	N	O	S	0	0	0
			1239	771	218	244	6			
1	F	164	Total	C	N	O	S	0	0	0
			1239	771	218	244	6			
1	G	164	Total	C	N	O	S	0	0	0
			1239	771	218	244	6			
1	H	164	Total	C	N	O	S	0	0	0
			1239	771	218	244	6			
1	I	164	Total	C	N	O	S	0	0	0
			1239	771	218	244	6			
1	J	164	Total	C	N	O	S	0	0	0
			1239	771	218	244	6			
1	K	164	Total	C	N	O	S	0	0	0
			1239	771	218	244	6			
1	L	164	Total	C	N	O	S	0	0	0
			1239	771	218	244	6			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
A	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
A	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
A	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
B	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
B	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
B	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
C	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
C	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
C	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
C	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
D	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
D	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
D	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
D	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
E	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
E	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
E	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
E	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
F	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
F	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
F	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
F	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
G	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
G	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
G	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
G	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
H	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
H	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
H	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
H	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
I	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
I	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
I	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
I	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
J	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
J	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
J	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
J	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
K	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
K	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
K	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01
K	164	SER	-	SEE REMARK 999	UNP A0A0E3W01
L	161	ASN	-	SEE REMARK 999	UNP A0A0E3W01
L	162	SER	-	SEE REMARK 999	UNP A0A0E3W01
L	163	LEU	-	SEE REMARK 999	UNP A0A0E3W01

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
L	164	SER	-	SEE REMARK 999	UNP A0A0E3W01

- Molecule 2 is a protein called PHYCOERYTHRIN BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	184	Total	C	N	O	S	0	0	0
			1347	827	244	263	13			
2	N	184	Total	C	N	O	S	0	0	0
			1347	827	244	263	13			
2	O	184	Total	C	N	O	S	0	0	0
			1347	827	244	263	13			
2	P	184	Total	C	N	O	S	0	0	0
			1347	827	244	263	13			
2	Q	184	Total	C	N	O	S	0	0	0
			1347	827	244	263	13			
2	R	184	Total	C	N	O	S	0	0	0
			1347	827	244	263	13			
2	S	184	Total	C	N	O	S	0	0	0
			1347	827	244	263	13			
2	T	184	Total	C	N	O	S	0	0	0
			1347	827	244	263	13			
2	U	184	Total	C	N	O	S	0	0	0
			1347	827	244	263	13			
2	V	184	Total	C	N	O	S	0	0	0
			1347	827	244	263	13			
2	W	184	Total	C	N	O	S	0	0	0
			1347	827	244	263	13			
2	X	184	Total	C	N	O	S	0	0	0
			1347	827	244	263	13			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
M	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45
M	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
M	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
M	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
M	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
M	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
N	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
N	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
N	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
N	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
N	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
N	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
N	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
O	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
O	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45
O	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
O	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
O	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
O	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
O	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
P	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
P	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45
P	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
P	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
P	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
P	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
P	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
Q	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
Q	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45
Q	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
Q	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
Q	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
Q	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
Q	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
R	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
R	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45
R	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
R	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
R	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
R	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
R	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
S	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
S	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45
S	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
S	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
S	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
S	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
S	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
T	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
T	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45

*Continued on next page...*

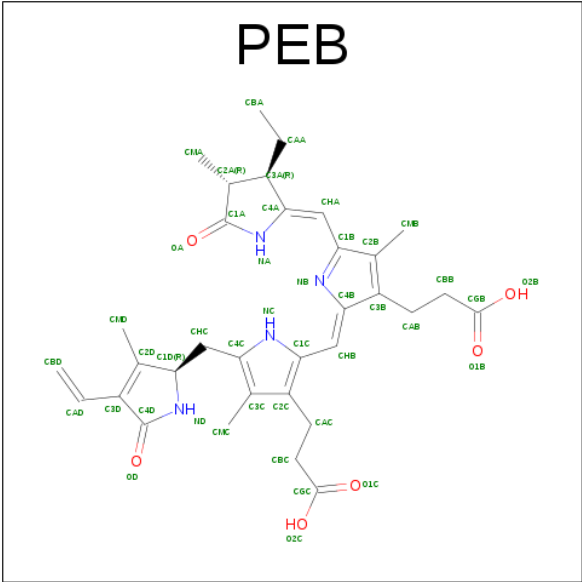


*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
T	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
T	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
T	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
T	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
T	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
U	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
U	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45
U	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
U	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
U	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
U	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
U	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
V	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
V	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45
V	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
V	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
V	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
V	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
V	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
W	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
W	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45
W	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
W	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
W	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
W	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
W	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
X	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
X	2	LEU	-	SEE REMARK 999	UNP A0A0E4G45
X	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
X	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
X	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
X	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
X	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45

- Molecule 3 is PHYCOERYTHROBILIN (three-letter code: PEB) (formula: C<sub>33</sub>H<sub>40</sub>N<sub>4</sub>O<sub>6</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			43	33	4	6		
3	A	1	Total	C	N	O	0	0
			43	33	4	6		
3	B	1	Total	C	N	O	0	0
			43	33	4	6		
3	B	1	Total	C	N	O	0	0
			43	33	4	6		
3	C	1	Total	C	N	O	0	0
			43	33	4	6		
3	C	1	Total	C	N	O	0	0
			43	33	4	6		
3	D	1	Total	C	N	O	0	0
			43	33	4	6		
3	D	1	Total	C	N	O	0	0
			43	33	4	6		
3	E	1	Total	C	N	O	0	0
			43	33	4	6		
3	E	1	Total	C	N	O	0	0
			43	33	4	6		
3	F	1	Total	C	N	O	0	0
			43	33	4	6		
3	F	1	Total	C	N	O	0	0
			43	33	4	6		
3	G	1	Total	C	N	O	0	0
			43	33	4	6		
3	G	1	Total	C	N	O	0	0
			43	33	4	6		

Continued on next page...



*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total 43	C 33	N 4	O 6	0	0
3	H	1	Total 43	C 33	N 4	O 6	0	0
3	I	1	Total 43	C 33	N 4	O 6	0	0
3	I	1	Total 43	C 33	N 4	O 6	0	0
3	J	1	Total 43	C 33	N 4	O 6	0	0
3	J	1	Total 43	C 33	N 4	O 6	0	0
3	K	1	Total 43	C 33	N 4	O 6	0	0
3	K	1	Total 43	C 33	N 4	O 6	0	0
3	L	1	Total 43	C 33	N 4	O 6	0	0
3	L	1	Total 43	C 33	N 4	O 6	0	0
3	M	1	Total 43	C 33	N 4	O 6	0	0
3	M	1	Total 43	C 33	N 4	O 6	0	0
3	M	1	Total 43	C 33	N 4	O 6	0	0
3	N	1	Total 43	C 33	N 4	O 6	0	0
3	N	1	Total 43	C 33	N 4	O 6	0	0
3	N	1	Total 43	C 33	N 4	O 6	0	0
3	O	1	Total 43	C 33	N 4	O 6	0	0
3	O	1	Total 43	C 33	N 4	O 6	0	0
3	O	1	Total 43	C 33	N 4	O 6	0	0
3	P	1	Total 43	C 33	N 4	O 6	0	0
3	P	1	Total 43	C 33	N 4	O 6	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	P	1	Total 43	C 33	N 4	O 6	0	0
3	Q	1	Total 43	C 33	N 4	O 6	0	0
3	Q	1	Total 43	C 33	N 4	O 6	0	0
3	Q	1	Total 43	C 33	N 4	O 6	0	0
3	R	1	Total 43	C 33	N 4	O 6	0	0
3	R	1	Total 43	C 33	N 4	O 6	0	0
3	R	1	Total 43	C 33	N 4	O 6	0	0
3	S	1	Total 43	C 33	N 4	O 6	0	0
3	S	1	Total 43	C 33	N 4	O 6	0	0
3	S	1	Total 43	C 33	N 4	O 6	0	0
3	T	1	Total 43	C 33	N 4	O 6	0	0
3	T	1	Total 43	C 33	N 4	O 6	0	0
3	T	1	Total 43	C 33	N 4	O 6	0	0
3	U	1	Total 43	C 33	N 4	O 6	0	0
3	U	1	Total 43	C 33	N 4	O 6	0	0
3	U	1	Total 43	C 33	N 4	O 6	0	0
3	V	1	Total 43	C 33	N 4	O 6	0	0
3	V	1	Total 43	C 33	N 4	O 6	0	0
3	V	1	Total 43	C 33	N 4	O 6	0	0
3	W	1	Total 43	C 33	N 4	O 6	0	0
3	W	1	Total 43	C 33	N 4	O 6	0	0

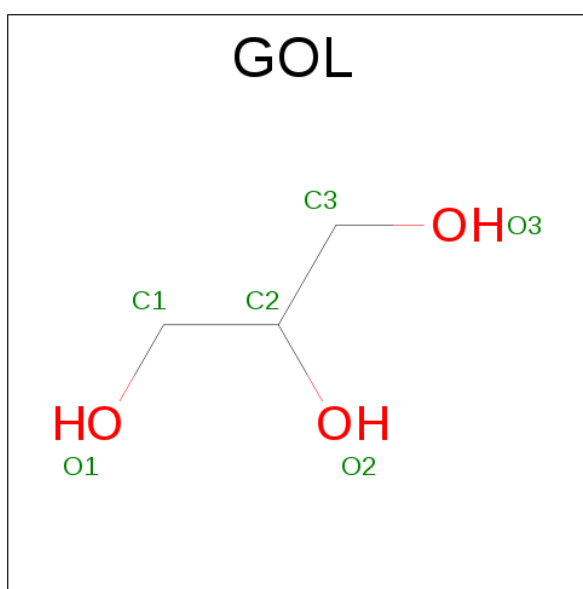
*Continued on next page...*



Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	W	1	Total	C	N	O	0	0
			43	33	4	6		
3	X	1	Total	C	N	O	0	0
			43	33	4	6		
3	X	1	Total	C	N	O	0	0
			43	33	4	6		
3	X	1	Total	C	N	O	0	0
			43	33	4	6		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		

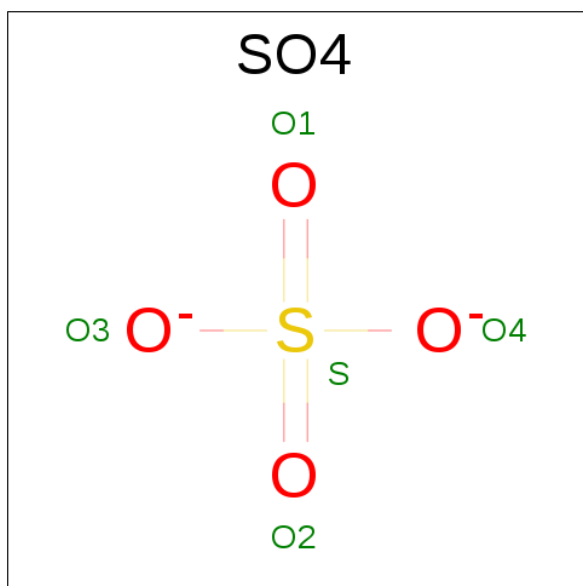
Continued on next page...



Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		
4	J	1	Total	C	O	0	0
			6	3	3		
4	K	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	I	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		

Continued on next page...



*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	M	1	Total	O	S	0	0
			5	4	1		
5	N	1	Total	O	S	0	0
			5	4	1		
5	O	1	Total	O	S	0	0
			5	4	1		
5	P	1	Total	O	S	0	0
			5	4	1		
5	Q	1	Total	O	S	0	0
			5	4	1		
5	R	1	Total	O	S	0	0
			5	4	1		
5	S	1	Total	O	S	0	0
			5	4	1		
5	T	1	Total	O	S	0	0
			5	4	1		
5	U	1	Total	O	S	0	0
			5	4	1		
5	V	1	Total	O	S	0	0
			5	4	1		
5	W	1	Total	O	S	0	0
			5	4	1		
5	X	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	212	Total	O	0	0
			212	212		
6	B	194	Total	O	0	0
			194	194		
6	C	178	Total	O	0	0
			178	178		
6	D	168	Total	O	0	0
			168	168		
6	E	167	Total	O	0	0
			167	167		
6	F	161	Total	O	0	0
			161	161		
6	G	206	Total	O	0	0
			206	206		

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	208	Total 208	O 208	0	0
6	I	188	Total 188	O 188	0	0
6	J	163	Total 163	O 163	0	0
6	K	133	Total 133	O 133	0	0
6	L	148	Total 148	O 148	0	0
6	M	149	Total 149	O 149	0	0
6	N	140	Total 140	O 140	0	0
6	O	121	Total 121	O 121	0	0
6	P	144	Total 144	O 144	0	0
6	Q	134	Total 134	O 134	0	0
6	R	118	Total 118	O 118	0	0
6	S	134	Total 134	O 134	0	0
6	T	107	Total 107	O 107	0	0
6	U	123	Total 123	O 123	0	0
6	V	153	Total 153	O 153	0	0
6	W	134	Total 134	O 134	0	0
6	X	126	Total 126	O 126	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: PHYCOERYTHRIN ALPHA SUBUNIT

Chain A:  96% .



- Molecule 1: PHYCOERYTHRIN ALPHA SUBUNIT

Chain B:  93% 7%



- Molecule 1: PHYCOERYTHRIN ALPHA SUBUNIT

Chain C:  91% 9%



- Molecule 1: PHYCOERYTHRIN ALPHA SUBUNIT

Chain D:  98% .



- Molecule 1: PHYCOERYTHRIN ALPHA SUBUNIT

Chain E:  95% 5%



- Molecule 1: PHYCOERYTHRIN ALPHA SUBUNIT

Chain F:  97% .





- Molecule 1: PHYCOERYTHRIN ALPHA SUBUNIT

Chain G: 96%



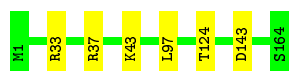
- Molecule 1: PHYCOERYTHRIN ALPHA SUBUNIT

Chain H: 95%



- Molecule 1: PHYCOERYTHRIN ALPHA SUBUNIT

Chain I: 96%



- Molecule 1: PHYCOERYTHRIN ALPHA SUBUNIT

Chain J: 95%



- Molecule 1: PHYCOERYTHRIN ALPHA SUBUNIT

Chain K: 93%



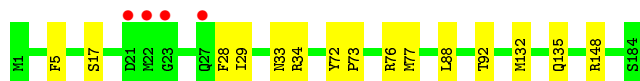
- Molecule 1: PHYCOERYTHRIN ALPHA SUBUNIT

Chain L: 93%



- Molecule 2: PHYCOERYTHRIN BETA SUBUNIT

Chain M: 92%





## ● Molecule 2: PHYCOERYTHRIN BETA SUBUNIT

Chain N:  96% 2% 2%




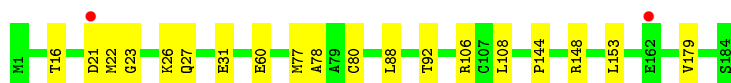
## ● Molecule 2: PHYCOERYTHRIN BETA SUBUNIT

Chain O:  95% 2% 5%



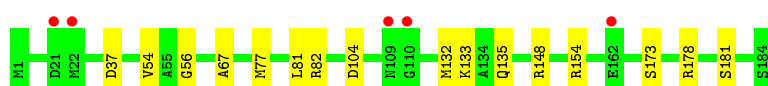
## ● Molecule 2: PHYCOERYTHRIN BETA SUBUNIT

Chain P:  90% 10% 0%



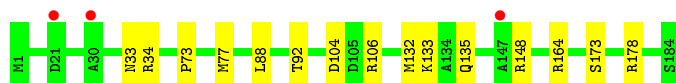
## ● Molecule 2: PHYCOERYTHRIN BETA SUBUNIT

Chain Q:  91% 9% 3%



## ● Molecule 2: PHYCOERYTHRIN BETA SUBUNIT

Chain R:  92% 8% 2%

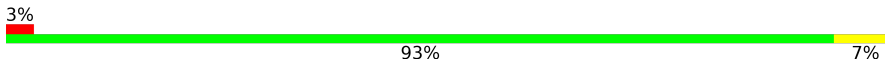


## ● Molecule 2: PHYCOERYTHRIN BETA SUBUNIT

Chain S:  96% 2% 2%



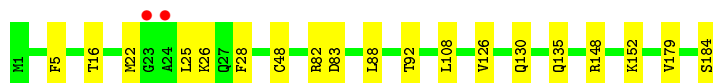
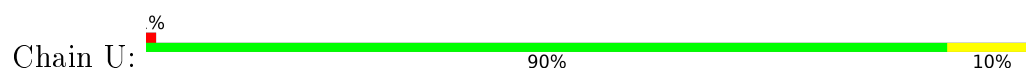
## ● Molecule 2: PHYCOERYTHRIN BETA SUBUNIT

Chain T:  93% 7% 3%

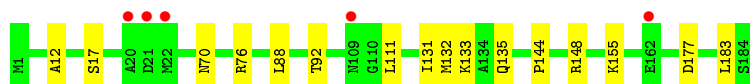
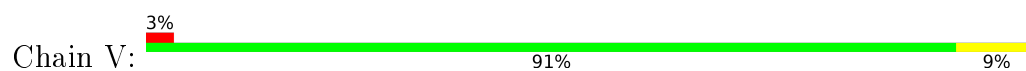


## ● Molecule 2: PHYCOERYTHRIN BETA SUBUNIT

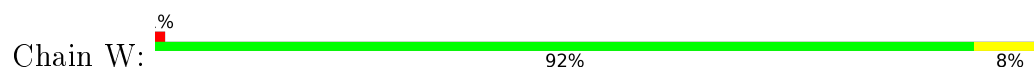




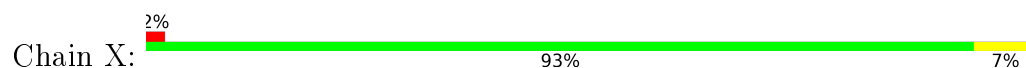
• Molecule 2: PHYCOERYTHRIN BETA SUBUNIT



• Molecule 2: PHYCOERYTHRIN BETA SUBUNIT



• Molecule 2: PHYCOERYTHRIN BETA SUBUNIT





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.30Å 108.36Å 116.59Å 78.94° 82.50° 60.34°	Depositor
Resolution (Å)	29.29 – 2.12 29.29 – 2.12	Depositor EDS
% Data completeness (in resolution range)	96.0 (29.29-2.12) 91.2 (29.29-2.12)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 2.12Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.175 , 0.239 0.176 , 0.239	Depositor DCC
$R_{free}$ test set	12527 reflections (5.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.7	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 57.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.004 for h-k,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	37483	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 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: GOL, MEN, SO4, PEB

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	0.40	0/1259	0.54	0/1706
1	B	0.41	0/1259	0.54	0/1706
1	C	0.39	0/1259	0.52	0/1706
1	D	0.40	0/1259	0.52	0/1706
1	E	0.39	0/1259	0.51	0/1706
1	F	0.41	0/1259	0.51	0/1706
1	G	0.42	0/1259	0.53	0/1706
1	H	0.40	0/1259	0.52	0/1706
1	I	0.38	0/1259	0.52	0/1706
1	J	0.38	0/1259	0.51	0/1706
1	K	0.38	0/1259	0.52	0/1706
1	L	0.39	0/1259	0.53	0/1706
2	M	0.38	0/1349	0.50	0/1820
2	N	0.38	0/1349	0.50	0/1820
2	O	0.37	0/1349	0.50	0/1820
2	P	0.40	0/1349	0.52	0/1820
2	Q	0.36	0/1349	0.51	0/1820
2	R	0.35	0/1349	0.50	0/1820
2	S	0.36	0/1349	0.50	0/1820
2	T	0.33	0/1349	0.49	0/1820
2	U	0.39	0/1349	0.51	0/1820
2	V	0.38	0/1349	0.50	0/1820
2	W	0.36	0/1349	0.48	0/1820
2	X	0.37	0/1349	0.51	0/1820
All	All	0.38	0/31296	0.51	0/42312

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Too-close contacts

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	1239	0	1221	7	0
1	B	1239	0	1221	10	0
1	C	1239	0	1221	10	0
1	D	1239	0	1221	3	0
1	E	1239	0	1221	10	0
1	F	1239	0	1221	5	0
1	G	1239	0	1221	6	0
1	H	1239	0	1221	6	0
1	I	1239	0	1221	5	0
1	J	1239	0	1221	7	0
1	K	1239	0	1221	10	0
1	L	1239	0	1221	8	0
2	M	1347	0	1359	10	0
2	N	1347	0	1359	6	0
2	O	1347	0	1359	7	0
2	P	1347	0	1359	15	0
2	Q	1347	0	1359	12	0
2	R	1347	0	1359	11	0
2	S	1347	0	1359	7	0
2	T	1347	0	1359	12	0
2	U	1347	0	1359	14	0
2	V	1347	0	1359	10	0
2	W	1347	0	1359	9	0
2	X	1347	0	1359	8	0
3	A	86	0	74	2	0
3	B	86	0	74	2	0
3	C	86	0	74	4	0
3	D	86	0	73	2	0
3	E	86	0	74	7	0
3	F	86	0	74	1	0
3	G	86	0	74	3	0
3	H	86	0	74	3	0
3	I	86	0	74	3	0
3	J	86	0	74	4	0
3	K	86	0	74	3	0
3	L	86	0	74	2	0
3	M	129	0	110	5	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	129	0	110	6	0
3	O	129	0	110	6	0
3	P	129	0	110	8	0
3	Q	129	0	110	12	0
3	R	129	0	110	6	0
3	S	129	0	110	7	0
3	T	129	0	110	8	0
3	U	129	0	110	9	0
3	V	129	0	109	6	0
3	W	129	0	110	6	0
3	X	129	0	110	4	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
4	E	6	0	8	1	0
4	F	6	0	8	0	0
4	G	6	0	8	0	0
4	H	6	0	8	1	0
4	I	6	0	8	0	0
4	J	6	0	8	0	0
4	K	6	0	8	0	0
4	L	6	0	8	0	0
5	A	5	0	0	0	0
5	D	5	0	0	0	0
5	E	5	0	0	0	0
5	H	5	0	0	0	0
5	I	5	0	0	1	0
5	L	5	0	0	0	0
5	M	5	0	0	0	0
5	N	5	0	0	0	0
5	O	5	0	0	0	0
5	P	5	0	0	1	0
5	Q	5	0	0	0	0
5	R	5	0	0	1	0
5	S	5	0	0	0	0
5	T	5	0	0	0	0
5	U	5	0	0	0	0
5	V	5	0	0	0	0
5	W	5	0	0	0	0
5	X	5	0	0	0	0
6	A	212	0	0	1	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	194	0	0	1	0
6	C	178	0	0	0	0
6	D	168	0	0	0	0
6	E	167	0	0	1	0
6	F	161	0	0	0	0
6	G	206	0	0	0	0
6	H	208	0	0	1	0
6	I	188	0	0	0	0
6	J	163	0	0	0	0
6	K	133	0	0	2	0
6	L	148	0	0	0	0
6	M	149	0	0	1	0
6	N	140	0	0	0	0
6	O	121	0	0	0	0
6	P	144	0	0	0	0
6	Q	134	0	0	0	0
6	R	118	0	0	1	0
6	S	134	0	0	1	0
6	T	107	0	0	0	0
6	U	123	0	0	0	0
6	V	153	0	0	0	0
6	W	134	0	0	0	0
6	X	126	0	0	0	0
All	All	37483	0	33262	247	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 4.

All (247) 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)
2:P:16:THR:HG23	2:Q:67:ALA:HB2	1.66	0.77
2:T:54:VAL:HG21	2:T:81:LEU:HD23	1.72	0.72
2:X:22:MET:HG2	2:X:25:LEU:HD12	1.72	0.71
2:M:88:LEU:O	2:M:92:THR:HG23	1.98	0.64
3:Q:186:PEB:HNA	3:Q:186:PEB:HMB2	1.63	0.63
2:Q:82:ARG:NH1	3:Q:186:PEB:O2C	2.32	0.62
1:L:37:ARG:NH1	1:L:98:VAL:O	2.34	0.61
2:P:22:MET:HB2	2:P:26:LYS:NZ	2.16	0.60
2:N:104:ASP:OD2	2:N:178:ARG:NH2	2.34	0.60
2:T:133:LYS:HE3	2:T:173:SER:HB3	1.84	0.59

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:ARG:NE	1:F:25:GLU:OE2	2.36	0.59
3:U:186:PEB:HMB2	3:U:186:PEB:HNA	1.68	0.58
3:W:187:PEB:HNA	3:W:187:PEB:HMB2	1.68	0.58
1:A:37:ARG:NH1	1:A:98:VAL:O	2.36	0.58
2:X:88:LEU:O	2:X:92:THR:HG23	2.03	0.58
1:H:25:GLU:OE2	1:K:37:ARG:NE	2.35	0.58
3:K:166:PEB:HBD1	2:X:72:TYR:CE1	2.39	0.57
3:P:186:PEB:HMB2	3:P:186:PEB:HNA	1.69	0.57
2:N:148:ARG:NH1	3:N:188:PEB:HND	2.02	0.57
3:V:186:PEB:HMB2	3:V:186:PEB:HNA	1.70	0.57
2:M:148:ARG:NE	3:M:188:PEB:O2C	2.30	0.57
3:O:186:PEB:HNA	3:O:186:PEB:HMB2	1.70	0.56
3:R:186:PEB:HNA	3:R:186:PEB:HMB2	1.70	0.56
3:S:187:PEB:HMB2	3:S:187:PEB:HNA	1.71	0.56
2:X:82:ARG:NH1	3:X:186:PEB:O2C	2.38	0.56
2:S:148:ARG:NH1	3:S:188:PEB:HND	2.03	0.56
1:G:25:GLU:OE2	1:J:37:ARG:NE	2.36	0.56
3:T:186:PEB:HMB2	3:T:186:PEB:HNA	1.69	0.56
1:H:37:ARG:NE	1:K:25:GLU:OE2	2.30	0.56
1:E:37:ARG:HD2	1:E:97:LEU:O	2.05	0.56
2:R:148:ARG:NH1	3:R:188:PEB:HND	2.03	0.56
1:K:115:GLU:HG3	6:K:2086:HOH:O	2.06	0.55
1:K:37:ARG:HD2	1:K:97:LEU:O	2.07	0.55
2:O:174:SER:O	2:O:178:ARG:HG3	2.07	0.55
2:X:148:ARG:NE	3:X:188:PEB:O2C	2.27	0.54
2:R:88:LEU:O	2:R:92:THR:HG23	2.07	0.54
3:D:166:PEB:HMC2	2:Q:77:MET:HG2	1.90	0.54
2:T:148:ARG:NH1	3:T:188:PEB:HND	2.05	0.54
2:W:148:ARG:NH1	3:W:188:PEB:HND	2.06	0.54
1:E:118:ARG:NH1	6:E:2120:HOH:O	2.41	0.53
2:S:135:GLN:HG2	3:S:188:PEB:C1B	2.38	0.53
3:N:186:PEB:HNA	3:N:186:PEB:HMB2	1.73	0.53
1:B:37:ARG:HD2	1:B:97:LEU:O	2.10	0.52
3:J:166:PEB:HNA	3:J:166:PEB:HMB2	1.73	0.52
3:F:166:PEB:HMC2	2:P:77:MET:HG2	1.92	0.52
3:N:187:PEB:HMB2	3:N:187:PEB:HNA	1.74	0.52
1:I:37:ARG:HD2	1:I:97:LEU:O	2.08	0.52
3:S:186:PEB:HNA	3:S:186:PEB:HMB2	1.75	0.52
2:U:5:PHE:HE1	2:U:28:PHE:CD1	2.28	0.52
2:V:88:LEU:O	2:V:92:THR:HG23	2.10	0.52
3:I:166:PEB:HMC2	2:T:77:MET:HG2	1.93	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:105:LEU:HD21	1:L:159:ALA:HB2	1.93	0.51
3:Q:188:PEB:HMB3	3:Q:188:PEB:HNA	1.75	0.51
3:T:188:PEB:HNA	3:T:188:PEB:HMB3	1.75	0.51
1:I:43:LYS:NZ	1:I:143:ASP:O	2.40	0.51
3:M:187:PEB:HNA	3:M:187:PEB:HMB2	1.75	0.51
3:T:188:PEB:HBB1	3:T:188:PEB:HBB1	1.93	0.51
2:V:70:MEN:HB2	3:V:186:PEB:OA	2.11	0.51
2:P:88:LEU:O	2:P:92:THR:HG23	2.11	0.50
2:P:148:ARG:NH2	2:U:184:SER:OXT	2.44	0.50
2:Q:104:ASP:OD2	2:Q:178:ARG:NH2	2.38	0.50
1:H:114:ARG:NH2	6:H:2143:HOH:O	2.43	0.50
2:R:132:MET:HA	2:R:135:GLN:OE1	2.12	0.50
3:O:188:PEB:HMB3	3:O:188:PEB:HNA	1.76	0.50
3:A:166:PEB:HMC2	2:O:77:MET:HG2	1.94	0.50
1:G:37:ARG:HD2	1:G:97:LEU:O	2.12	0.50
2:P:106:ARG:NE	5:P:189:SO4:O3	2.43	0.50
1:I:124:THR:OG1	5:I:1200:SO4:O1	2.27	0.49
2:Q:135:GLN:HG2	3:Q:188:PEB:C1B	2.43	0.49
2:P:60:GLU:OE1	2:U:130:GLN:NE2	2.46	0.49
2:U:48:CYS:SG	2:U:152:LYS:HD3	2.52	0.49
4:H:1165:GOL:H12	2:T:1:MET:HG2	1.94	0.49
3:C:166:PEB:HMB2	3:C:166:PEB:HNA	1.77	0.49
3:W:186:PEB:HNA	3:W:186:PEB:HMB2	1.77	0.49
2:P:22:MET:HB2	2:P:26:LYS:HZ2	1.77	0.49
3:Q:187:PEB:HBA3	3:Q:187:PEB:HHA1	1.95	0.49
2:S:132:MET:HA	2:S:135:GLN:OE1	2.12	0.49
2:O:131:ILE:O	2:O:135:GLN:HG3	2.12	0.48
3:O:188:PEB:HBB1	3:O:188:PEB:HBB1	1.95	0.48
1:G:25:GLU:OE1	1:J:30:SER:HA	2.13	0.48
2:N:133:LYS:HE3	2:N:173:SER:HB3	1.95	0.48
1:K:1:MET:N	2:W:1:MET:O	2.46	0.48
2:U:26:LYS:HD2	2:U:26:LYS:HA	1.66	0.48
3:M:186:PEB:HNA	3:M:186:PEB:HMB2	1.78	0.48
3:Q:187:PEB:HMB2	3:Q:187:PEB:HNA	1.78	0.48
3:U:186:PEB:CMB	3:U:186:PEB:HNA	2.26	0.47
2:U:148:ARG:NH1	3:U:188:PEB:HND	2.11	0.47
3:C:166:PEB:HMC2	2:N:77:MET:HG2	1.96	0.47
1:C:25:GLU:HG2	1:F:33:ARG:HG2	1.97	0.47
3:U:188:PEB:HNA	3:U:188:PEB:HMB3	1.79	0.47
2:W:125:THR:HG21	2:W:183:LEU:HD13	1.95	0.47
1:E:43:LYS:HG3	3:E:167:PEB:HBD1	1.96	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:148:ARG:NH1	3:P:188:PEB:HND	2.12	0.47
1:C:68:ASN:O	1:C:74:SER:HB3	2.15	0.47
1:I:33:ARG:HG2	1:L:25:GLU:HG2	1.96	0.47
3:P:188:PEB:HBB1	3:P:188:PEB:HBB1	1.97	0.47
2:U:83:ASP:OD1	3:U:186:PEB:H1D1	2.15	0.47
3:E:166:PEB:HNA	3:E:166:PEB:HMB2	1.80	0.47
3:W:188:PEB:HMB3	3:W:188:PEB:HNA	1.79	0.47
1:A:33:ARG:HH12	3:P:187:PEB:HMC1	1.80	0.47
1:L:72:ALA:O	1:L:78:PHE:HB3	2.15	0.47
1:B:37:ARG:NE	1:E:25:GLU:OE2	2.44	0.47
3:N:188:PEB:HNA	3:N:188:PEB:HMB3	1.80	0.47
2:R:104:ASP:OD2	2:R:178:ARG:NH2	2.47	0.47
3:V:188:PEB:HNA	3:V:188:PEB:HMB3	1.80	0.46
3:X:186:PEB:HMB2	3:X:186:PEB:HNA	1.80	0.46
2:R:133:LYS:HE3	2:R:173:SER:HB3	1.97	0.46
1:H:33:ARG:NH1	1:H:147:GLN:OE1	2.40	0.46
2:M:132:MET:HA	2:M:135:GLN:OE1	2.14	0.46
2:Q:132:MET:HA	2:Q:135:GLN:OE1	2.15	0.46
2:T:135:GLN:HG2	3:T:188:PEB:C1B	2.44	0.46
2:U:82:ARG:NH1	3:U:186:PEB:O2C	2.48	0.46
1:G:1:MET:HG3	1:G:103:GLY:HA3	1.96	0.46
1:B:25:GLU:OE2	1:E:37:ARG:NE	2.42	0.46
3:Q:187:PEB:HMB2	3:Q:187:PEB:NA	2.31	0.46
3:C:166:PEB:CMB	3:C:166:PEB:HNA	2.29	0.46
2:W:88:LEU:O	2:W:92:THR:HG23	2.16	0.46
1:H:72:ALA:O	1:H:78:PHE:HB3	2.16	0.46
3:E:166:PEB:HNA	3:E:166:PEB:CMB	2.29	0.46
3:X:187:PEB:HMB2	3:X:187:PEB:HNA	1.80	0.46
2:O:33:ASN:HB3	3:O:187:PEB:C1C	2.46	0.46
1:E:43:LYS:HG3	3:E:167:PEB:CBD	2.45	0.45
3:G:166:PEB:HMB2	3:G:166:PEB:HNA	1.81	0.45
1:C:33:ARG:NH1	1:C:147:GLN:OE1	2.45	0.45
2:S:82:ARG:NH1	3:S:186:PEB:O2C	2.49	0.45
1:J:33:ARG:NH1	1:J:147:GLN:OE1	2.40	0.45
3:B:166:PEB:HMC2	2:M:77:MET:HG2	1.97	0.45
3:P:187:PEB:HMB2	3:P:187:PEB:HNA	1.80	0.45
2:V:12:ALA:HB1	2:V:17:SER:O	2.16	0.45
1:B:21:SER:HB2	6:B:2036:HOH:O	2.17	0.45
1:A:33:ARG:NH2	1:A:147:GLN:OE1	2.40	0.45
1:F:115:GLU:OE1	2:P:78:ALA:HB1	2.17	0.45
3:O:187:PEB:HBA3	3:O:187:PEB:HHA1	1.99	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:166:PEB:HMB2	3:H:166:PEB:HNA	1.82	0.45
2:T:67:ALA:HB2	2:U:16:THR:HG23	1.99	0.45
2:U:88:LEU:O	2:U:92:THR:HG23	2.16	0.45
1:J:37:ARG:HD2	1:J:97:LEU:O	2.17	0.45
3:V:188:PEB:HBB1	3:V:188:PEB:HBB1	1.99	0.45
3:J:166:PEB:HNA	3:J:166:PEB:CMB	2.30	0.44
1:A:25:GLU:HG2	1:D:33:ARG:HG2	1.99	0.44
1:B:72:ALA:O	1:B:78:PHE:HB3	2.16	0.44
1:C:139:CYS:SG	3:C:167:PEB:HHA1	2.58	0.44
2:S:33:ASN:HB3	3:S:187:PEB:C1C	2.47	0.44
3:O:187:PEB:NA	3:O:187:PEB:HMB2	2.33	0.44
3:E:166:PEB:HMC2	2:R:77:MET:HG2	2.00	0.44
3:I:166:PEB:HNA	3:I:166:PEB:HMB2	1.82	0.44
2:S:133:LYS:HE3	2:S:173:SER:HB3	1.98	0.44
2:V:133:LYS:NZ	2:V:177:ASP:OD1	2.50	0.44
6:A:2155:HOH:O	1:F:114:ARG:NH1	2.50	0.44
2:N:135:GLN:HG2	3:N:188:PEB:C1B	2.48	0.44
1:C:19:PRO:HG2	2:O:92:THR:HG22	1.98	0.44
1:B:139:CYS:SG	3:B:167:PEB:HHA1	2.58	0.44
2:U:108:LEU:HD21	2:U:179:VAL:HG22	1.99	0.44
3:R:188:PEB:HBB1	3:R:188:PEB:HBB1	2.00	0.43
2:T:59:CYS:HB2	3:T:188:PEB:HBD2	1.78	0.43
2:M:72:TYR:O	2:M:76:ARG:HD2	2.19	0.43
2:R:33:ASN:HB3	3:R:187:PEB:C1C	2.48	0.43
2:R:34:ARG:HE	3:R:187:PEB:CGB	2.31	0.43
2:W:104:ASP:O	2:W:109:ASN:HB2	2.18	0.43
1:C:123:PRO:O	1:C:126:PRO:HD2	2.18	0.43
2:V:144:PRO:HD2	2:V:155:LYS:NZ	2.33	0.43
3:U:187:PEB:HBA3	3:U:187:PEB:HHA1	1.99	0.43
2:Q:133:LYS:HE3	2:Q:173:SER:HB3	2.00	0.43
3:W:187:PEB:HMB2	3:W:187:PEB:NA	2.34	0.43
1:B:25:GLU:HG2	1:E:33:ARG:HG2	2.01	0.43
2:M:148:ARG:HD3	6:M:2114:HOH:O	2.18	0.43
2:N:104:ASP:CG	2:N:178:ARG:HH21	2.22	0.43
1:A:82:CYS:HA	3:A:166:PEB:HAA1	1.85	0.43
2:M:33:ASN:HB3	3:M:187:PEB:C1C	2.49	0.43
3:T:187:PEB:HNA	3:T:187:PEB:HMB2	1.83	0.43
1:H:25:GLU:HG2	1:K:33:ARG:HG2	2.01	0.43
1:B:34:SER:HA	1:B:37:ARG:HG2	2.00	0.43
1:J:139:CYS:SG	3:J:167:PEB:HHA1	2.59	0.43
1:L:37:ARG:HD2	1:L:97:LEU:O	2.19	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:70:MEN:HE22	2:V:76:ARG:HD3	2.01	0.43
3:J:167:PEB:HNA	3:J:167:PEB:HMB2	1.84	0.42
2:P:80:CYS:HA	3:P:186:PEB:HAA1	1.84	0.42
1:E:1:MET:N	4:E:1165:GOL:H31	2.34	0.42
2:M:34:ARG:HE	3:M:187:PEB:CGB	2.32	0.42
2:P:22:MET:HE3	2:P:26:LYS:HE3	2.02	0.42
3:S:188:PEB:HBB1	3:S:188:PEB:HBB1	2.01	0.42
2:S:75:ARG:NH2	6:S:2063:HOH:O	2.51	0.42
1:D:37:ARG:HD2	1:D:97:LEU:O	2.19	0.42
3:H:167:PEB:HNA	3:H:167:PEB:HMB2	1.83	0.42
1:G:33:ARG:HG2	1:J:25:GLU:HG2	2.00	0.42
1:C:97:LEU:HG	1:C:155:LEU:HD12	2.01	0.42
3:P:187:PEB:HBA3	3:P:187:PEB:HHA1	2.00	0.42
2:W:133:LYS:HE3	2:W:173:SER:HB3	2.00	0.42
1:I:43:LYS:HG3	3:I:167:PEB:HBD1	2.01	0.42
2:T:70:MEN:HB2	3:T:186:PEB:OA	2.20	0.42
1:L:1:MET:HG3	1:L:103:GLY:HA3	2.01	0.42
2:Q:54:VAL:HG21	2:Q:81:LEU:HD23	2.01	0.42
3:Q:187:PEB:OD	3:Q:187:PEB:HBD1	2.19	0.42
2:V:148:ARG:NH1	3:V:188:PEB:HND	2.17	0.42
1:C:33:ARG:NH2	1:C:147:GLN:OE1	2.52	0.42
1:L:139:CYS:SG	3:L:167:PEB:HHA1	2.59	0.42
2:P:27:GLN:OE1	2:P:31:GLU:HG3	2.19	0.42
2:Q:56:GLY:HA3	3:Q:188:PEB:HHC2	2.02	0.42
2:U:135:GLN:HG2	3:U:188:PEB:C1B	2.50	0.42
2:V:131:ILE:O	2:V:135:GLN:HG3	2.19	0.42
2:W:111:LEU:HG	2:W:183:LEU:HD21	2.02	0.42
2:X:127:ARG:HD2	2:X:127:ARG:HA	1.83	0.42
2:X:112:LYS:NZ	2:X:184:SER:O	2.40	0.42
2:M:5:PHE:HE1	2:M:28:PHE:CD1	2.37	0.42
2:O:96:LEU:HD12	2:O:96:LEU:HA	1.87	0.42
2:W:31:GLU:O	2:W:34:ARG:HB2	2.19	0.42
3:Q:186:PEB:CMB	3:Q:186:PEB:HNA	2.30	0.41
2:W:33:ASN:HB3	3:W:187:PEB:C1C	2.50	0.41
1:B:58:ALA:O	1:B:61:GLN:HG2	2.19	0.41
3:H:166:PEB:CMB	3:H:166:PEB:HNA	2.33	0.41
2:U:22:MET:HA	2:U:25:LEU:HD12	2.02	0.41
1:L:82:CYS:HA	3:L:166:PEB:HAA1	1.80	0.41
2:P:144:PRO:HG2	2:P:153:LEU:HD11	2.03	0.41
2:T:81:LEU:HA	2:T:81:LEU:HD23	1.93	0.41
1:F:38:LEU:HA	1:F:38:LEU:HD23	1.90	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:187:PEB:HMB2	3:N:187:PEB:NA	2.36	0.41
1:K:136:ASN:OD1	2:T:154:ARG:NH1	2.53	0.41
1:K:137:ARG:HG3	3:K:167:PEB:HHC1	2.03	0.41
3:P:188:PEB:HNA	3:P:188:PEB:HMB3	1.86	0.41
2:P:108:LEU:HD21	2:P:179:VAL:HG22	2.02	0.41
2:R:106:ARG:NH2	5:R:189:SO4:O3	2.46	0.41
2:V:111:LEU:HG	2:V:183:LEU:HD21	2.01	0.41
1:G:139:CYS:SG	3:G:167:PEB:HHA1	2.61	0.41
1:B:132:SER:OG	2:Q:154:ARG:NH2	2.54	0.41
2:R:164:ARG:NH2	6:R:2089:HOH:O	2.44	0.41
3:R:188:PEB:HMB3	3:R:188:PEB:HNA	1.85	0.41
3:E:167:PEB:NA	3:E:167:PEB:HMB2	2.36	0.41
1:A:38:LEU:HA	1:A:38:LEU:HD23	1.77	0.41
2:X:132:MET:HA	2:X:135:GLN:OE1	2.21	0.41
3:E:167:PEB:HMB2	3:E:167:PEB:HNA	1.86	0.40
3:G:166:PEB:CMB	3:G:166:PEB:HNA	2.34	0.40
2:Q:37:ASP:OD1	3:Q:187:PEB:HHC1	2.21	0.40
1:A:25:GLU:O	1:D:29:GLY:HA3	2.21	0.40
1:C:114:ARG:HD2	1:E:118:ARG:NH1	2.37	0.40
1:J:155:LEU:HD23	1:J:155:LEU:HA	1.94	0.40
2:V:132:MET:HA	2:V:135:GLN:OE1	2.21	0.40
3:V:187:PEB:NA	3:V:187:PEB:HMB2	2.35	0.40
2:T:155:LYS:HD3	2:T:155:LYS:HA	1.72	0.40
3:D:166:PEB:HNA	3:D:166:PEB:HMB2	1.86	0.40
2:M:29:ILE:HD13	2:M:29:ILE:HA	1.92	0.40
2:O:155:LYS:HD3	2:O:155:LYS:HA	1.90	0.40
2:Q:148:ARG:NH1	3:Q:188:PEB:HND	2.18	0.40
3:U:187:PEB:HNA	3:U:187:PEB:HMB2	1.86	0.40
1:K:127:TYR:CE1	3:K:166:PEB:H3A1	2.57	0.40
1:K:64:PRO:HG3	6:K:2059:HOH:O	2.22	0.40
1:E:108:TRP:O	2:R:73:PRO:HB2	2.21	0.40
2:U:126:VAL:O	2:U:130:GLN:HG3	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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



of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	B	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
1	C	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
1	D	162/164 (99%)	160 (99%)	2 (1%)	0	100	100
1	E	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
1	F	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	G	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
1	H	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
1	I	162/164 (99%)	160 (99%)	2 (1%)	0	100	100
1	J	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
1	K	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
1	L	162/164 (99%)	160 (99%)	2 (1%)	0	100	100
2	M	181/184 (98%)	177 (98%)	3 (2%)	1 (1%)	30	24
2	N	181/184 (98%)	180 (99%)	1 (1%)	0	100	100
2	O	181/184 (98%)	178 (98%)	3 (2%)	0	100	100
2	P	181/184 (98%)	175 (97%)	5 (3%)	1 (1%)	30	24
2	Q	181/184 (98%)	175 (97%)	6 (3%)	0	100	100
2	R	181/184 (98%)	173 (96%)	8 (4%)	0	100	100
2	S	181/184 (98%)	176 (97%)	5 (3%)	0	100	100
2	T	181/184 (98%)	176 (97%)	5 (3%)	0	100	100
2	U	181/184 (98%)	174 (96%)	7 (4%)	0	100	100
2	V	181/184 (98%)	177 (98%)	4 (2%)	0	100	100
2	W	181/184 (98%)	177 (98%)	4 (2%)	0	100	100
2	X	181/184 (98%)	176 (97%)	5 (3%)	0	100	100
All	All	4116/4176 (99%)	4018 (98%)	96 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	23	GLY

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	M	73	PRO

### 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	127/127 (100%)	127 (100%)	0	100	100
1	B	127/127 (100%)	127 (100%)	0	100	100
1	C	127/127 (100%)	126 (99%)	1 (1%)	86	90
1	D	127/127 (100%)	127 (100%)	0	100	100
1	E	127/127 (100%)	127 (100%)	0	100	100
1	F	127/127 (100%)	127 (100%)	0	100	100
1	G	127/127 (100%)	127 (100%)	0	100	100
1	H	127/127 (100%)	126 (99%)	1 (1%)	86	90
1	I	127/127 (100%)	127 (100%)	0	100	100
1	J	127/127 (100%)	127 (100%)	0	100	100
1	K	127/127 (100%)	126 (99%)	1 (1%)	86	90
1	L	127/127 (100%)	127 (100%)	0	100	100
2	M	138/138 (100%)	137 (99%)	1 (1%)	88	92
2	N	138/138 (100%)	138 (100%)	0	100	100
2	O	138/138 (100%)	138 (100%)	0	100	100
2	P	138/138 (100%)	137 (99%)	1 (1%)	88	92
2	Q	138/138 (100%)	137 (99%)	1 (1%)	88	92
2	R	138/138 (100%)	138 (100%)	0	100	100
2	S	138/138 (100%)	138 (100%)	0	100	100
2	T	138/138 (100%)	138 (100%)	0	100	100
2	U	138/138 (100%)	138 (100%)	0	100	100
2	V	138/138 (100%)	138 (100%)	0	100	100
2	W	138/138 (100%)	137 (99%)	1 (1%)	88	92

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	X	138/138 (100%)	138 (100%)	0	100	100
All	All	3180/3180 (100%)	3173 (100%)	7 (0%)	95	97

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	30	SER
1	H	30	SER
1	K	61	GLN
2	M	17	SER
2	P	21	ASP
2	Q	181	SER
2	W	26	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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
2	MEN	M	70	2	6,8,9	0.51	0	6,9,11	1.25	1 (16%)
2	MEN	N	70	2	6,8,9	0.44	0	6,9,11	1.25	1 (16%)
2	MEN	O	70	2	6,8,9	0.55	0	6,9,11	1.13	1 (16%)
2	MEN	P	70	2	6,8,9	0.46	0	6,9,11	1.07	1 (16%)
2	MEN	Q	70	2	6,8,9	0.53	0	6,9,11	1.27	1 (16%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MEN	R	70	2	6,8,9	0.46	0	6,9,11	1.16	1 (16%)
2	MEN	S	70	2	6,8,9	0.57	0	6,9,11	1.06	1 (16%)
2	MEN	T	70	2	6,8,9	0.48	0	6,9,11	1.17	1 (16%)
2	MEN	U	70	2	6,8,9	0.53	0	6,9,11	1.08	1 (16%)
2	MEN	V	70	2	6,8,9	0.63	0	6,9,11	1.17	1 (16%)
2	MEN	W	70	2	6,8,9	0.43	0	6,9,11	1.12	1 (16%)
2	MEN	X	70	2	6,8,9	0.44	0	6,9,11	1.16	1 (16%)

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
2	MEN	M	70	2	-	0/6/8/10	0/0/0/0
2	MEN	N	70	2	-	0/6/8/10	0/0/0/0
2	MEN	O	70	2	-	0/6/8/10	0/0/0/0
2	MEN	P	70	2	-	0/6/8/10	0/0/0/0
2	MEN	Q	70	2	-	0/6/8/10	0/0/0/0
2	MEN	R	70	2	-	0/6/8/10	0/0/0/0
2	MEN	S	70	2	-	0/6/8/10	0/0/0/0
2	MEN	T	70	2	-	0/6/8/10	0/0/0/0
2	MEN	U	70	2	-	0/6/8/10	0/0/0/0
2	MEN	V	70	2	-	0/6/8/10	0/0/0/0
2	MEN	W	70	2	-	0/6/8/10	0/0/0/0
2	MEN	X	70	2	-	0/6/8/10	0/0/0/0

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	70	MEN	O-C-CA	-3.03	117.61	125.72
2	N	70	MEN	O-C-CA	-3.00	117.68	125.72
2	M	70	MEN	O-C-CA	-2.98	117.72	125.72
2	R	70	MEN	O-C-CA	-2.83	118.14	125.72
2	T	70	MEN	O-C-CA	-2.77	118.29	125.72
2	W	70	MEN	O-C-CA	-2.65	118.62	125.72
2	X	70	MEN	O-C-CA	-2.64	118.63	125.72
2	O	70	MEN	O-C-CA	-2.60	118.74	125.72
2	V	70	MEN	O-C-CA	-2.53	118.92	125.72

*Continued on next page...*



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	70	MEN	O-C-CA	-2.46	119.12	125.72
2	S	70	MEN	O-C-CA	-2.32	119.49	125.72
2	U	70	MEN	O-C-CA	-2.31	119.52	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	70	MEN	1	0
2	V	70	MEN	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

90 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	GOL	A	1165	-	5,5,5	0.23	0	5,5,5	0.53	0
5	SO4	A	1200	-	4,4,4	0.16	0	6,6,6	0.14	0
3	PEB	A	166	1	37,46,46	3.47	10 (27%)	36,67,67	2.76	19 (52%)
3	PEB	A	167	1	37,46,46	3.35	10 (27%)	36,67,67	2.26	15 (41%)
4	GOL	B	1165	-	5,5,5	0.31	0	5,5,5	0.50	0
3	PEB	B	166	1	37,46,46	3.44	10 (27%)	36,67,67	2.66	17 (47%)
3	PEB	B	167	1	37,46,46	3.38	11 (29%)	36,67,67	2.32	16 (44%)
4	GOL	C	1165	-	5,5,5	0.32	0	5,5,5	0.27	0
3	PEB	C	166	1	37,46,46	3.39	9 (24%)	36,67,67	2.68	19 (52%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PEB	C	167	1	37,46,46	3.35	10 (27%)	36,67,67	2.26	14 (38%)
4	GOL	D	1165	-	5,5,5	0.28	0	5,5,5	0.42	0
5	SO4	D	1200	-	4,4,4	0.29	0	6,6,6	0.11	0
3	PEB	D	166	1	37,46,46	3.47	10 (27%)	36,67,67	2.60	18 (50%)
3	PEB	D	167	1	37,46,46	3.39	11 (29%)	36,67,67	2.67	17 (47%)
4	GOL	E	1165	-	5,5,5	0.25	0	5,5,5	0.43	0
5	SO4	E	1200	-	4,4,4	0.24	0	6,6,6	0.16	0
3	PEB	E	166	1	37,46,46	3.44	10 (27%)	36,67,67	2.58	18 (50%)
3	PEB	E	167	1	37,46,46	3.45	11 (29%)	36,67,67	2.33	16 (44%)
4	GOL	F	1165	-	5,5,5	0.30	0	5,5,5	0.36	0
3	PEB	F	166	1	37,46,46	3.24	9 (24%)	36,67,67	2.74	16 (44%)
3	PEB	F	167	1	37,46,46	3.56	9 (24%)	36,67,67	2.18	13 (36%)
4	GOL	G	1165	-	5,5,5	0.26	0	5,5,5	0.35	0
3	PEB	G	166	1	37,46,46	3.26	9 (24%)	36,67,67	2.73	15 (41%)
3	PEB	G	167	1	37,46,46	3.49	11 (29%)	36,67,67	2.23	14 (38%)
4	GOL	H	1165	-	5,5,5	0.37	0	5,5,5	0.50	0
5	SO4	H	1200	-	4,4,4	0.25	0	6,6,6	0.14	0
3	PEB	H	166	1	37,46,46	3.44	11 (29%)	36,67,67	2.62	17 (47%)
3	PEB	H	167	1	37,46,46	3.38	11 (29%)	36,67,67	2.29	16 (44%)
4	GOL	I	1165	-	5,5,5	0.31	0	5,5,5	0.31	0
5	SO4	I	1200	-	4,4,4	0.19	0	6,6,6	0.25	0
3	PEB	I	166	1	37,46,46	3.48	11 (29%)	36,67,67	2.65	16 (44%)
3	PEB	I	167	1	37,46,46	3.35	11 (29%)	36,67,67	2.65	17 (47%)
4	GOL	J	1165	-	5,5,5	0.33	0	5,5,5	0.40	0
3	PEB	J	166	1	37,46,46	3.54	10 (27%)	36,67,67	2.65	15 (41%)
3	PEB	J	167	1	37,46,46	3.35	10 (27%)	36,67,67	2.26	14 (38%)
4	GOL	K	1165	-	5,5,5	0.33	0	5,5,5	0.34	0
3	PEB	K	166	1	37,46,46	3.35	11 (29%)	36,67,67	2.81	17 (47%)
3	PEB	K	167	1	37,46,46	3.37	12 (32%)	36,67,67	2.33	16 (44%)
4	GOL	L	1165	-	5,5,5	0.33	0	5,5,5	0.31	0
5	SO4	L	1200	-	4,4,4	0.21	0	6,6,6	0.25	0
3	PEB	L	166	1	37,46,46	3.37	9 (24%)	36,67,67	2.74	16 (44%)
3	PEB	L	167	1	37,46,46	3.24	9 (24%)	36,67,67	2.35	15 (41%)
3	PEB	M	186	2	37,46,46	3.48	9 (24%)	36,67,67	2.46	16 (44%)
3	PEB	M	187	2	37,46,46	3.31	9 (24%)	36,67,67	2.41	13 (36%)
3	PEB	M	188	2	37,46,46	3.54	11 (29%)	36,67,67	2.32	16 (44%)
5	SO4	M	189	-	4,4,4	0.17	0	6,6,6	0.18	0
3	PEB	N	186	2	37,46,46	3.48	11 (29%)	36,67,67	2.43	13 (36%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PEB	N	187	2	37,46,46	3.46	10 (27%)	36,67,67	2.25	14 (38%)
3	PEB	N	188	2	37,46,46	3.41	8 (21%)	36,67,67	2.33	14 (38%)
5	SO4	N	189	-	4,4,4	0.11	0	6,6,6	0.14	0
3	PEB	O	186	2	37,46,46	3.44	11 (29%)	36,67,67	2.56	16 (44%)
3	PEB	O	187	2	37,46,46	3.37	10 (27%)	36,67,67	2.15	14 (38%)
3	PEB	O	188	2	37,46,46	3.44	10 (27%)	36,67,67	2.35	16 (44%)
5	SO4	O	189	-	4,4,4	0.11	0	6,6,6	0.25	0
3	PEB	P	186	2	37,46,46	3.50	9 (24%)	36,67,67	2.37	17 (47%)
3	PEB	P	187	2	37,46,46	3.46	9 (24%)	36,67,67	2.23	16 (44%)
3	PEB	P	188	2	37,46,46	3.47	10 (27%)	36,67,67	2.26	16 (44%)
5	SO4	P	189	-	4,4,4	0.11	0	6,6,6	0.15	0
3	PEB	Q	186	2	37,46,46	3.44	10 (27%)	36,67,67	2.46	15 (41%)
3	PEB	Q	187	2	37,46,46	3.61	11 (29%)	36,67,67	2.34	15 (41%)
3	PEB	Q	188	2	37,46,46	3.52	10 (27%)	36,67,67	2.24	13 (36%)
5	SO4	Q	189	-	4,4,4	0.11	0	6,6,6	0.22	0
3	PEB	R	186	2	37,46,46	3.55	10 (27%)	36,67,67	2.31	15 (41%)
3	PEB	R	187	2	37,46,46	3.35	10 (27%)	36,67,67	2.34	14 (38%)
3	PEB	R	188	2	37,46,46	3.49	10 (27%)	36,67,67	2.33	16 (44%)
5	SO4	R	189	-	4,4,4	0.12	0	6,6,6	0.17	0
3	PEB	S	186	2	37,46,46	3.57	9 (24%)	36,67,67	2.40	14 (38%)
3	PEB	S	187	2	37,46,46	3.43	10 (27%)	36,67,67	2.28	16 (44%)
3	PEB	S	188	2	37,46,46	3.54	11 (29%)	36,67,67	2.25	16 (44%)
5	SO4	S	189	-	4,4,4	0.10	0	6,6,6	0.13	0
3	PEB	T	186	2	37,46,46	3.39	10 (27%)	36,67,67	2.66	16 (44%)
3	PEB	T	187	2	37,46,46	3.41	10 (27%)	36,67,67	2.32	16 (44%)
3	PEB	T	188	2	37,46,46	3.57	10 (27%)	36,67,67	2.27	15 (41%)
5	SO4	T	189	-	4,4,4	0.19	0	6,6,6	0.08	0
3	PEB	U	186	2	37,46,46	3.61	10 (27%)	36,67,67	2.53	13 (36%)
3	PEB	U	187	2	37,46,46	3.47	9 (24%)	36,67,67	2.42	16 (44%)
3	PEB	U	188	2	37,46,46	3.47	10 (27%)	36,67,67	2.28	16 (44%)
5	SO4	U	189	-	4,4,4	0.09	0	6,6,6	0.19	0
3	PEB	V	186	2	37,46,46	3.40	11 (29%)	36,67,67	2.64	17 (47%)
3	PEB	V	187	2	37,46,46	3.42	11 (29%)	36,67,67	2.39	16 (44%)
3	PEB	V	188	2	37,46,46	3.50	12 (32%)	36,67,67	2.20	16 (44%)
5	SO4	V	189	-	4,4,4	0.11	0	6,6,6	0.25	0
3	PEB	W	186	2	37,46,46	3.49	9 (24%)	36,67,67	2.35	15 (41%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PEB	W	187	2	37,46,46	3.31	10 (27%)	36,67,67	2.36	15 (41%)
3	PEB	W	188	2	37,46,46	3.49	8 (21%)	36,67,67	2.10	15 (41%)
5	SO4	W	189	-	4,4,4	0.06	0	6,6,6	0.18	0
3	PEB	X	186	2	37,46,46	3.44	9 (24%)	36,67,67	2.47	15 (41%)
3	PEB	X	187	2	37,46,46	3.35	11 (29%)	36,67,67	2.35	15 (41%)
3	PEB	X	188	2	37,46,46	3.56	10 (27%)	36,67,67	2.30	17 (47%)
5	SO4	X	189	-	4,4,4	0.17	0	6,6,6	0.14	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
4	GOL	A	1165	-	-	0/4/4/4	0/0/0/0
5	SO4	A	1200	-	-	0/0/0/0	0/0/0/0
3	PEB	A	166	1	-	2/19/74/74	0/4/4/4
3	PEB	A	167	1	-	2/19/74/74	0/4/4/4
4	GOL	B	1165	-	-	0/4/4/4	0/0/0/0
3	PEB	B	166	1	-	2/19/74/74	0/4/4/4
3	PEB	B	167	1	-	2/19/74/74	0/4/4/4
4	GOL	C	1165	-	-	0/4/4/4	0/0/0/0
3	PEB	C	166	1	-	2/19/74/74	0/4/4/4
3	PEB	C	167	1	-	2/19/74/74	0/4/4/4
4	GOL	D	1165	-	-	0/4/4/4	0/0/0/0
5	SO4	D	1200	-	-	0/0/0/0	0/0/0/0
3	PEB	D	166	1	-	2/19/74/74	0/4/4/4
3	PEB	D	167	1	-	2/19/74/74	0/4/4/4
4	GOL	E	1165	-	-	0/4/4/4	0/0/0/0
5	SO4	E	1200	-	-	0/0/0/0	0/0/0/0
3	PEB	E	166	1	-	2/19/74/74	0/4/4/4
3	PEB	E	167	1	-	2/19/74/74	0/4/4/4
4	GOL	F	1165	-	-	0/4/4/4	0/0/0/0
3	PEB	F	166	1	-	2/19/74/74	0/4/4/4
3	PEB	F	167	1	-	2/19/74/74	0/4/4/4
4	GOL	G	1165	-	-	0/4/4/4	0/0/0/0
3	PEB	G	166	1	-	2/19/74/74	0/4/4/4
3	PEB	G	167	1	-	2/19/74/74	0/4/4/4

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	H	1165	-	-	0/4/4/4	0/0/0/0
5	SO4	H	1200	-	-	0/0/0/0	0/0/0/0
3	PEB	H	166	1	-	2/19/74/74	0/4/4/4
3	PEB	H	167	1	-	2/19/74/74	0/4/4/4
4	GOL	I	1165	-	-	0/4/4/4	0/0/0/0
5	SO4	I	1200	-	-	0/0/0/0	0/0/0/0
3	PEB	I	166	1	-	2/19/74/74	0/4/4/4
3	PEB	I	167	1	-	2/19/74/74	0/4/4/4
4	GOL	J	1165	-	-	0/4/4/4	0/0/0/0
3	PEB	J	166	1	-	2/19/74/74	0/4/4/4
3	PEB	J	167	1	-	2/19/74/74	0/4/4/4
4	GOL	K	1165	-	-	0/4/4/4	0/0/0/0
3	PEB	K	166	1	-	2/19/74/74	0/4/4/4
3	PEB	K	167	1	-	2/19/74/74	0/4/4/4
4	GOL	L	1165	-	-	0/4/4/4	0/0/0/0
5	SO4	L	1200	-	-	0/0/0/0	0/0/0/0
3	PEB	L	166	1	-	2/19/74/74	0/4/4/4
3	PEB	L	167	1	-	2/19/74/74	0/4/4/4
3	PEB	M	186	2	-	2/19/74/74	0/4/4/4
3	PEB	M	187	2	-	2/19/74/74	0/4/4/4
3	PEB	M	188	2	-	2/19/74/74	0/4/4/4
5	SO4	M	189	-	-	0/0/0/0	0/0/0/0
3	PEB	N	186	2	-	2/19/74/74	0/4/4/4
3	PEB	N	187	2	-	2/19/74/74	0/4/4/4
3	PEB	N	188	2	-	2/19/74/74	0/4/4/4
5	SO4	N	189	-	-	0/0/0/0	0/0/0/0
3	PEB	O	186	2	-	2/19/74/74	0/4/4/4
3	PEB	O	187	2	-	2/19/74/74	0/4/4/4
3	PEB	O	188	2	-	2/19/74/74	0/4/4/4
5	SO4	O	189	-	-	0/0/0/0	0/0/0/0
3	PEB	P	186	2	-	2/19/74/74	0/4/4/4
3	PEB	P	187	2	-	2/19/74/74	0/4/4/4
3	PEB	P	188	2	-	2/19/74/74	0/4/4/4
5	SO4	P	189	-	-	0/0/0/0	0/0/0/0
3	PEB	Q	186	2	-	2/19/74/74	0/4/4/4
3	PEB	Q	187	2	-	2/19/74/74	0/4/4/4

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEB	Q	188	2	-	2/19/74/74	0/4/4/4
5	SO4	Q	189	-	-	0/0/0/0	0/0/0/0
3	PEB	R	186	2	-	2/19/74/74	0/4/4/4
3	PEB	R	187	2	-	2/19/74/74	0/4/4/4
3	PEB	R	188	2	-	2/19/74/74	0/4/4/4
5	SO4	R	189	-	-	0/0/0/0	0/0/0/0
3	PEB	S	186	2	-	2/19/74/74	0/4/4/4
3	PEB	S	187	2	-	2/19/74/74	0/4/4/4
3	PEB	S	188	2	-	2/19/74/74	0/4/4/4
5	SO4	S	189	-	-	0/0/0/0	0/0/0/0
3	PEB	T	186	2	-	2/19/74/74	0/4/4/4
3	PEB	T	187	2	-	2/19/74/74	0/4/4/4
3	PEB	T	188	2	-	2/19/74/74	0/4/4/4
5	SO4	T	189	-	-	0/0/0/0	0/0/0/0
3	PEB	U	186	2	-	2/19/74/74	0/4/4/4
3	PEB	U	187	2	-	2/19/74/74	0/4/4/4
3	PEB	U	188	2	-	2/19/74/74	0/4/4/4
5	SO4	U	189	-	-	0/0/0/0	0/0/0/0
3	PEB	V	186	2	-	2/19/74/74	0/4/4/4
3	PEB	V	187	2	-	2/19/74/74	0/4/4/4
3	PEB	V	188	2	-	2/19/74/74	0/4/4/4
5	SO4	V	189	-	-	0/0/0/0	0/0/0/0
3	PEB	W	186	2	-	2/19/74/74	0/4/4/4
3	PEB	W	187	2	-	2/19/74/74	0/4/4/4
3	PEB	W	188	2	-	2/19/74/74	0/4/4/4
5	SO4	W	189	-	-	0/0/0/0	0/0/0/0
3	PEB	X	186	2	-	2/19/74/74	0/4/4/4
3	PEB	X	187	2	-	2/19/74/74	0/4/4/4
3	PEB	X	188	2	-	2/19/74/74	0/4/4/4
5	SO4	X	189	-	-	0/0/0/0	0/0/0/0

All (603) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	166	PEB	C2A-C1A	-4.42	1.47	1.52
3	W	187	PEB	C1A-NA	-3.83	1.32	1.37
3	T	188	PEB	C1A-NA	-3.58	1.33	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	167	PEB	C1A-NA	-3.58	1.33	1.37
3	M	187	PEB	C1A-NA	-3.56	1.33	1.37
3	V	188	PEB	C1A-NA	-3.54	1.33	1.37
3	M	188	PEB	C1A-NA	-3.53	1.33	1.37
3	R	187	PEB	C1A-NA	-3.53	1.33	1.37
3	S	187	PEB	C1A-NA	-3.52	1.33	1.37
3	F	167	PEB	C1A-NA	-3.48	1.33	1.37
3	N	187	PEB	C1A-NA	-3.45	1.33	1.37
3	O	187	PEB	C1A-NA	-3.44	1.33	1.37
3	W	186	PEB	C1A-NA	-3.37	1.33	1.37
3	I	167	PEB	C1A-NA	-3.30	1.33	1.37
3	X	187	PEB	C1A-NA	-3.24	1.33	1.37
3	C	167	PEB	C1A-NA	-3.23	1.33	1.37
3	L	167	PEB	C1A-NA	-3.22	1.33	1.37
3	Q	186	PEB	C1A-NA	-3.21	1.33	1.37
3	W	188	PEB	C1A-NA	-3.19	1.33	1.37
3	R	188	PEB	C1A-NA	-3.19	1.33	1.37
3	C	166	PEB	C2A-C1A	-3.18	1.49	1.52
3	B	167	PEB	C1A-NA	-3.16	1.33	1.37
3	N	188	PEB	C1A-NA	-3.16	1.33	1.37
3	J	167	PEB	C1A-NA	-3.15	1.33	1.37
3	Q	187	PEB	C1A-NA	-3.11	1.33	1.37
3	R	186	PEB	C1A-NA	-3.11	1.33	1.37
3	E	167	PEB	C1A-NA	-3.10	1.33	1.37
3	V	187	PEB	C1A-NA	-3.09	1.33	1.37
3	G	167	PEB	C1A-NA	-3.09	1.33	1.37
3	P	187	PEB	C1A-NA	-3.04	1.33	1.37
3	D	166	PEB	C2A-C1A	-3.03	1.49	1.52
3	G	166	PEB	C1A-NA	-3.00	1.33	1.37
3	H	167	PEB	C1A-NA	-2.97	1.33	1.37
3	O	188	PEB	C1A-NA	-2.96	1.33	1.37
3	X	188	PEB	C1A-NA	-2.95	1.33	1.37
3	X	186	PEB	C1A-NA	-2.95	1.33	1.37
3	U	188	PEB	C1A-NA	-2.95	1.33	1.37
3	P	188	PEB	C1A-NA	-2.94	1.33	1.37
3	I	166	PEB	C2A-C1A	-2.93	1.49	1.52
3	S	186	PEB	C1A-NA	-2.92	1.33	1.37
3	S	188	PEB	C1A-NA	-2.90	1.33	1.37
3	I	166	PEB	C1A-NA	-2.85	1.33	1.37
3	P	186	PEB	C1A-NA	-2.85	1.34	1.37
3	U	187	PEB	C1A-NA	-2.82	1.34	1.37
3	B	166	PEB	C2A-C1A	-2.82	1.49	1.52

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	167	PEB	C1A-NA	-2.82	1.34	1.37
3	M	186	PEB	C1A-NA	-2.80	1.34	1.37
3	N	186	PEB	C1A-NA	-2.77	1.34	1.37
3	A	167	PEB	C1A-NA	-2.75	1.34	1.37
3	D	166	PEB	C1A-NA	-2.72	1.34	1.37
3	V	186	PEB	C1A-NA	-2.72	1.34	1.37
3	W	187	PEB	C2A-C1A	-2.71	1.49	1.52
3	H	166	PEB	C1A-NA	-2.71	1.34	1.37
3	Q	188	PEB	C1A-NA	-2.71	1.34	1.37
3	V	186	PEB	C2A-C1A	-2.68	1.49	1.52
3	A	166	PEB	C1A-NA	-2.67	1.34	1.37
3	T	186	PEB	C1A-NA	-2.64	1.34	1.37
3	J	166	PEB	C1A-NA	-2.63	1.34	1.37
3	K	166	PEB	C1A-NA	-2.62	1.34	1.37
3	O	186	PEB	C2A-C1A	-2.58	1.49	1.52
3	E	166	PEB	C1A-NA	-2.56	1.34	1.37
3	O	186	PEB	C1A-NA	-2.55	1.34	1.37
3	T	187	PEB	C1A-NA	-2.54	1.34	1.37
3	L	166	PEB	C1A-NA	-2.54	1.34	1.37
3	C	166	PEB	C1A-NA	-2.52	1.34	1.37
3	A	166	PEB	C2A-C1A	-2.51	1.49	1.52
3	K	166	PEB	C2A-C1A	-2.48	1.49	1.52
3	V	187	PEB	C2A-C1A	-2.46	1.49	1.52
3	F	166	PEB	C1A-NA	-2.46	1.34	1.37
3	U	186	PEB	C1A-NA	-2.46	1.34	1.37
3	D	167	PEB	C2A-C1A	-2.46	1.49	1.52
3	E	166	PEB	C2A-C1A	-2.34	1.49	1.52
3	H	167	PEB	C2A-C1A	-2.28	1.49	1.52
3	G	166	PEB	C2A-C1A	-2.27	1.49	1.52
3	N	186	PEB	C2A-C1A	-2.25	1.49	1.52
3	H	166	PEB	C2A-C1A	-2.20	1.50	1.52
3	B	166	PEB	C1A-NA	-2.18	1.34	1.37
3	X	187	PEB	C2A-C1A	-2.15	1.50	1.52
3	S	188	PEB	C2A-C1A	-2.13	1.50	1.52
3	F	166	PEB	C2A-C1A	-2.11	1.50	1.52
3	T	186	PEB	C2A-C1A	-2.09	1.50	1.52
3	V	188	PEB	C4A-NA	-2.06	1.32	1.37
3	O	187	PEB	C1D-ND	2.02	1.48	1.45
3	M	187	PEB	C1C-CHB	2.03	1.48	1.40
3	K	167	PEB	C1B-C2B	2.03	1.50	1.45
3	S	187	PEB	C1D-ND	2.03	1.48	1.45
3	B	167	PEB	C1B-C2B	2.03	1.50	1.45

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	167	PEB	C4B-C3B	2.04	1.49	1.45
3	U	186	PEB	C1C-CHB	2.05	1.48	1.40
3	L	166	PEB	C1C-CHB	2.05	1.48	1.40
3	S	188	PEB	C4B-C3B	2.05	1.49	1.45
3	F	166	PEB	C1B-C2B	2.05	1.50	1.45
3	R	187	PEB	C1C-CHB	2.05	1.48	1.40
3	W	187	PEB	C1C-CHB	2.05	1.48	1.40
3	Q	188	PEB	C1B-C2B	2.06	1.50	1.45
3	R	186	PEB	C1D-ND	2.07	1.48	1.45
3	O	187	PEB	C1C-CHB	2.07	1.48	1.40
3	K	167	PEB	C1C-CHB	2.08	1.48	1.40
3	U	186	PEB	C1B-C2B	2.08	1.50	1.45
3	Q	186	PEB	C1B-C2B	2.08	1.50	1.45
3	C	167	PEB	C1C-CHB	2.08	1.48	1.40
3	Q	187	PEB	C4B-C3B	2.09	1.49	1.45
3	K	166	PEB	C1C-CHB	2.09	1.48	1.40
3	B	167	PEB	C1C-CHB	2.10	1.48	1.40
3	Q	186	PEB	C1C-CHB	2.11	1.48	1.40
3	X	186	PEB	C1C-CHB	2.12	1.48	1.40
3	K	167	PEB	C4B-C3B	2.13	1.49	1.45
3	N	187	PEB	C4B-C3B	2.13	1.49	1.45
3	V	187	PEB	C1D-ND	2.13	1.49	1.45
3	M	188	PEB	C1B-C2B	2.13	1.50	1.45
3	O	186	PEB	C1B-C2B	2.14	1.50	1.45
3	X	188	PEB	C4B-C3B	2.14	1.49	1.45
3	W	186	PEB	C1C-CHB	2.15	1.48	1.40
3	B	166	PEB	C1C-CHB	2.15	1.48	1.40
3	R	188	PEB	C4B-C3B	2.15	1.49	1.45
3	N	186	PEB	C1D-ND	2.15	1.49	1.45
3	V	186	PEB	C1C-CHB	2.16	1.48	1.40
3	X	187	PEB	C1D-ND	2.16	1.49	1.45
3	X	187	PEB	C1C-CHB	2.16	1.48	1.40
3	V	188	PEB	C4B-C3B	2.16	1.49	1.45
3	V	186	PEB	C1B-C2B	2.16	1.50	1.45
3	M	186	PEB	C1C-CHB	2.16	1.48	1.40
3	G	167	PEB	C4B-C3B	2.16	1.49	1.45
3	A	166	PEB	C1C-CHB	2.16	1.48	1.40
3	N	186	PEB	C1C-CHB	2.17	1.48	1.40
3	I	167	PEB	C1C-CHB	2.18	1.48	1.40
3	S	187	PEB	C1C-CHB	2.18	1.48	1.40
3	P	187	PEB	C1C-CHB	2.18	1.48	1.40
3	E	167	PEB	C1D-ND	2.18	1.49	1.45

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	188	PEB	C1C-CHB	2.19	1.48	1.40
3	M	188	PEB	C4B-C3B	2.19	1.49	1.45
3	B	167	PEB	C1D-ND	2.20	1.49	1.45
3	J	167	PEB	C1C-CHB	2.20	1.48	1.40
3	U	188	PEB	C1C-CHB	2.20	1.48	1.40
3	A	167	PEB	C1C-CHB	2.20	1.48	1.40
3	I	166	PEB	C1B-C2B	2.20	1.50	1.45
3	T	186	PEB	C1C-CHB	2.21	1.48	1.40
3	Q	187	PEB	C1D-ND	2.21	1.49	1.45
3	I	167	PEB	C1D-ND	2.21	1.49	1.45
3	D	167	PEB	C1C-CHB	2.22	1.48	1.40
3	D	166	PEB	C1C-CHB	2.22	1.48	1.40
3	H	167	PEB	C1D-ND	2.23	1.49	1.45
3	E	167	PEB	C4B-C3B	2.24	1.49	1.45
3	P	188	PEB	C4B-C3B	2.24	1.49	1.45
3	L	167	PEB	C1C-CHB	2.24	1.48	1.40
3	G	167	PEB	C1D-ND	2.25	1.49	1.45
3	G	166	PEB	OD-C4D	2.26	1.27	1.23
3	A	167	PEB	C1D-ND	2.26	1.49	1.45
3	T	187	PEB	C1C-CHB	2.26	1.48	1.40
3	V	188	PEB	C1D-ND	2.27	1.49	1.45
3	H	167	PEB	C1C-CHB	2.28	1.49	1.40
3	I	167	PEB	C4B-C3B	2.28	1.49	1.45
3	V	187	PEB	C1C-CHB	2.28	1.49	1.40
3	T	187	PEB	C1D-ND	2.28	1.49	1.45
3	M	188	PEB	C1C-CHB	2.29	1.49	1.40
3	F	167	PEB	C1C-CHB	2.29	1.49	1.40
3	R	188	PEB	C1C-CHB	2.31	1.49	1.40
3	U	187	PEB	C1C-CHB	2.31	1.49	1.40
3	K	167	PEB	C1D-ND	2.31	1.49	1.45
3	O	186	PEB	C1C-CHB	2.31	1.49	1.40
3	Q	188	PEB	C1C-CHB	2.31	1.49	1.40
3	R	186	PEB	C1C-CHB	2.32	1.49	1.40
3	R	187	PEB	C1D-ND	2.32	1.49	1.45
3	H	166	PEB	C1C-CHB	2.33	1.49	1.40
3	X	188	PEB	C1C-CHB	2.33	1.49	1.40
3	P	188	PEB	C1C-CHB	2.33	1.49	1.40
3	H	166	PEB	C1B-C2B	2.33	1.51	1.45
3	M	187	PEB	C1D-ND	2.36	1.49	1.45
3	E	167	PEB	C1C-CHB	2.36	1.49	1.40
3	O	188	PEB	C4B-C3B	2.36	1.49	1.45
3	G	167	PEB	C1C-CHB	2.37	1.49	1.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	166	PEB	C1C-CHB	2.38	1.49	1.40
3	S	186	PEB	C1C-CHB	2.38	1.49	1.40
3	J	166	PEB	C1C-CHB	2.38	1.49	1.40
3	T	188	PEB	C4B-C3B	2.39	1.49	1.45
3	S	188	PEB	C1C-CHB	2.40	1.49	1.40
3	T	188	PEB	C1C-CHB	2.40	1.49	1.40
3	X	187	PEB	OD-C4D	2.40	1.28	1.23
3	O	186	PEB	OD-C4D	2.40	1.28	1.23
3	W	187	PEB	OD-C4D	2.40	1.28	1.23
3	N	187	PEB	C1C-CHB	2.41	1.49	1.40
3	P	186	PEB	C1C-CHB	2.41	1.49	1.40
3	L	167	PEB	OD-C4D	2.42	1.28	1.23
3	U	188	PEB	C4B-C3B	2.43	1.49	1.45
3	K	166	PEB	C1B-C2B	2.43	1.51	1.45
3	O	188	PEB	C1C-CHB	2.44	1.49	1.40
3	D	167	PEB	C4B-C3B	2.46	1.49	1.45
3	E	166	PEB	C1C-CHB	2.47	1.49	1.40
3	C	167	PEB	C1D-ND	2.47	1.49	1.45
3	Q	187	PEB	C1C-CHB	2.47	1.49	1.40
3	W	186	PEB	OD-C4D	2.49	1.28	1.23
3	U	186	PEB	OD-C4D	2.50	1.28	1.23
3	V	186	PEB	OD-C4D	2.54	1.28	1.23
3	F	167	PEB	OD-C4D	2.59	1.28	1.23
3	B	167	PEB	OD-C4D	2.63	1.28	1.23
3	J	166	PEB	OD-C4D	2.68	1.28	1.23
3	M	188	PEB	OD-C4D	2.68	1.28	1.23
3	T	186	PEB	OD-C4D	2.69	1.28	1.23
3	S	188	PEB	OD-C4D	2.70	1.28	1.23
3	N	186	PEB	OD-C4D	2.72	1.28	1.23
3	X	186	PEB	OD-C4D	2.72	1.28	1.23
3	S	187	PEB	OD-C4D	2.74	1.28	1.23
3	H	167	PEB	OD-C4D	2.75	1.28	1.23
3	R	188	PEB	OD-C4D	2.75	1.28	1.23
3	M	186	PEB	OD-C4D	2.75	1.28	1.23
3	J	167	PEB	OD-C4D	2.77	1.28	1.23
3	N	187	PEB	OD-C4D	2.77	1.28	1.23
3	N	188	PEB	OD-C4D	2.77	1.28	1.23
3	P	186	PEB	OD-C4D	2.78	1.28	1.23
3	T	187	PEB	OD-C4D	2.79	1.28	1.23
3	W	188	PEB	OD-C4D	2.82	1.29	1.23
3	I	166	PEB	OD-C4D	2.83	1.29	1.23
3	G	167	PEB	OD-C4D	2.86	1.29	1.23

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	166	PEB	OD-C4D	2.86	1.29	1.23
3	E	166	PEB	OD-C4D	2.86	1.29	1.23
3	C	166	PEB	CHA-C1B	2.87	1.47	1.40
3	P	188	PEB	OD-C4D	2.89	1.29	1.23
3	C	166	PEB	OD-C4D	2.90	1.29	1.23
3	T	188	PEB	OD-C4D	2.91	1.29	1.23
3	U	188	PEB	OD-C4D	2.92	1.29	1.23
3	O	188	PEB	OD-C4D	2.92	1.29	1.23
3	O	187	PEB	OD-C4D	2.94	1.29	1.23
3	D	167	PEB	OD-C4D	2.95	1.29	1.23
3	Q	187	PEB	OD-C4D	2.96	1.29	1.23
3	V	188	PEB	OD-C4D	2.97	1.29	1.23
3	X	188	PEB	OD-C4D	2.99	1.29	1.23
3	E	167	PEB	OD-C4D	3.00	1.29	1.23
3	U	187	PEB	OD-C4D	3.00	1.29	1.23
3	Q	186	PEB	OD-C4D	3.02	1.29	1.23
3	S	186	PEB	OD-C4D	3.04	1.29	1.23
3	G	166	PEB	CHA-C1B	3.04	1.47	1.40
3	V	187	PEB	OD-C4D	3.05	1.29	1.23
3	D	166	PEB	OD-C4D	3.07	1.29	1.23
3	R	187	PEB	OD-C4D	3.08	1.29	1.23
3	K	166	PEB	OD-C4D	3.08	1.29	1.23
3	A	167	PEB	OD-C4D	3.09	1.29	1.23
3	B	166	PEB	OD-C4D	3.10	1.29	1.23
3	K	167	PEB	OD-C4D	3.12	1.29	1.23
3	L	166	PEB	OD-C4D	3.12	1.29	1.23
3	P	187	PEB	OD-C4D	3.13	1.29	1.23
3	U	187	PEB	C2C-C3C	3.13	1.46	1.37
3	A	167	PEB	CHA-C1B	3.16	1.48	1.40
3	C	167	PEB	OD-C4D	3.17	1.29	1.23
3	Q	188	PEB	OD-C4D	3.17	1.29	1.23
3	D	167	PEB	C2C-C3C	3.19	1.47	1.37
3	F	166	PEB	CHA-C1B	3.22	1.48	1.40
3	U	188	PEB	C2C-C3C	3.22	1.47	1.37
3	S	187	PEB	C2C-C3C	3.23	1.47	1.37
3	X	187	PEB	C2C-C3C	3.24	1.47	1.37
3	A	166	PEB	OD-C4D	3.25	1.29	1.23
3	R	186	PEB	OD-C4D	3.25	1.29	1.23
3	S	188	PEB	C2C-C3C	3.25	1.47	1.37
3	I	167	PEB	OD-C4D	3.26	1.29	1.23
3	B	167	PEB	C2C-C3C	3.27	1.47	1.37
3	J	166	PEB	CHA-C1B	3.28	1.48	1.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	188	PEB	C2C-C3C	3.28	1.47	1.37
3	L	167	PEB	C2C-C3C	3.30	1.47	1.37
3	O	188	PEB	C2C-C3C	3.31	1.47	1.37
3	L	166	PEB	CHA-C1B	3.31	1.48	1.40
3	A	166	PEB	CHA-C1B	3.31	1.48	1.40
3	V	186	PEB	C2C-C3C	3.31	1.47	1.37
3	J	167	PEB	CHA-C1B	3.32	1.48	1.40
3	L	166	PEB	C2C-C3C	3.32	1.47	1.37
3	C	167	PEB	C2C-C3C	3.34	1.47	1.37
3	L	167	PEB	CHA-C1B	3.34	1.48	1.40
3	M	188	PEB	C2C-C3C	3.35	1.47	1.37
3	J	167	PEB	C2C-C3C	3.35	1.47	1.37
3	Q	187	PEB	C2C-C3C	3.36	1.47	1.37
3	S	186	PEB	C2C-C3C	3.36	1.47	1.37
3	T	187	PEB	C2C-C3C	3.37	1.47	1.37
3	R	186	PEB	C2C-C3C	3.37	1.47	1.37
3	R	188	PEB	C2C-C3C	3.39	1.47	1.37
3	P	186	PEB	C2C-C3C	3.39	1.47	1.37
3	H	167	PEB	C2C-C3C	3.39	1.47	1.37
3	X	188	PEB	C2C-C3C	3.39	1.47	1.37
3	K	167	PEB	C2C-C3C	3.41	1.47	1.37
3	N	188	PEB	CHA-C1B	3.42	1.48	1.40
3	D	166	PEB	C2C-C3C	3.42	1.47	1.37
3	R	187	PEB	C2C-C3C	3.43	1.47	1.37
3	I	167	PEB	C2C-C3C	3.43	1.47	1.37
3	P	187	PEB	C2C-C3C	3.43	1.47	1.37
3	I	167	PEB	CHA-C1B	3.43	1.48	1.40
3	A	166	PEB	C2C-C3C	3.43	1.47	1.37
3	G	167	PEB	C2C-C3C	3.44	1.47	1.37
3	F	167	PEB	C2C-C3C	3.44	1.47	1.37
3	F	166	PEB	C2C-C3C	3.44	1.47	1.37
3	G	166	PEB	C2C-C3C	3.45	1.47	1.37
3	P	188	PEB	C2C-C3C	3.45	1.47	1.37
3	E	167	PEB	C2C-C3C	3.45	1.47	1.37
3	E	166	PEB	C2C-C3C	3.45	1.47	1.37
3	O	186	PEB	C2C-C3C	3.46	1.47	1.37
3	M	187	PEB	C2C-C3C	3.46	1.47	1.37
3	C	167	PEB	CHA-C1B	3.47	1.49	1.40
3	T	186	PEB	CHA-C1B	3.48	1.49	1.40
3	Q	188	PEB	C2C-C3C	3.48	1.48	1.37
3	C	166	PEB	C2C-C3C	3.49	1.48	1.37
3	D	166	PEB	CHA-C1B	3.50	1.49	1.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	167	PEB	CHA-C1B	3.50	1.49	1.40
3	F	167	PEB	CHA-C1B	3.50	1.49	1.40
3	G	167	PEB	CHA-C1B	3.51	1.49	1.40
3	V	187	PEB	C2C-C3C	3.51	1.48	1.37
3	X	186	PEB	CHA-C1B	3.52	1.49	1.40
3	Q	187	PEB	CHA-C1B	3.53	1.49	1.40
3	V	187	PEB	CHA-C1B	3.54	1.49	1.40
3	O	187	PEB	C2C-C3C	3.54	1.48	1.37
3	W	188	PEB	C2C-C3C	3.54	1.48	1.37
3	K	166	PEB	C2C-C3C	3.54	1.48	1.37
3	W	187	PEB	C2C-C3C	3.54	1.48	1.37
3	I	166	PEB	C2C-C3C	3.54	1.48	1.37
3	H	167	PEB	CHA-C1B	3.55	1.49	1.40
3	B	166	PEB	C2C-C3C	3.55	1.48	1.37
3	A	167	PEB	C2C-C3C	3.55	1.48	1.37
3	M	186	PEB	C2C-C3C	3.56	1.48	1.37
3	T	188	PEB	C2C-C3C	3.58	1.48	1.37
3	K	167	PEB	CHA-C1B	3.58	1.49	1.40
3	Q	186	PEB	CHA-C1B	3.58	1.49	1.40
3	X	186	PEB	C2C-C3C	3.59	1.48	1.37
3	T	186	PEB	C2C-C3C	3.60	1.48	1.37
3	N	186	PEB	C2C-C3C	3.61	1.48	1.37
3	U	186	PEB	C2C-C3C	3.61	1.48	1.37
3	H	166	PEB	C2C-C3C	3.62	1.48	1.37
3	V	188	PEB	C2C-C3C	3.64	1.48	1.37
3	W	186	PEB	C2C-C3C	3.66	1.48	1.37
3	N	187	PEB	C2C-C3C	3.67	1.48	1.37
3	E	167	PEB	CHA-C1B	3.67	1.49	1.40
3	X	187	PEB	CHA-C1B	3.67	1.49	1.40
3	B	167	PEB	CHA-C1B	3.69	1.49	1.40
3	E	166	PEB	CHA-C1B	3.71	1.49	1.40
3	J	166	PEB	C2C-C3C	3.72	1.48	1.37
3	R	187	PEB	CHA-C1B	3.72	1.49	1.40
3	P	187	PEB	CHA-C1B	3.75	1.49	1.40
3	U	188	PEB	CHA-C1B	3.76	1.49	1.40
3	Q	186	PEB	C2C-C3C	3.76	1.48	1.37
3	T	187	PEB	CHA-C1B	3.76	1.49	1.40
3	U	187	PEB	CHA-C1B	3.77	1.49	1.40
3	P	186	PEB	CHA-C1B	3.77	1.49	1.40
3	O	188	PEB	CHA-C1B	3.78	1.49	1.40
3	M	187	PEB	CHA-C1B	3.78	1.49	1.40
3	S	187	PEB	CHA-C1B	3.80	1.49	1.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	188	PEB	CHA-C1B	3.82	1.49	1.40
3	P	188	PEB	CHA-C1B	3.84	1.49	1.40
3	M	186	PEB	CHA-C1B	3.85	1.49	1.40
3	T	188	PEB	CHA-C1B	3.86	1.49	1.40
3	N	187	PEB	CHA-C1B	3.87	1.50	1.40
3	K	166	PEB	CHA-C1B	3.87	1.50	1.40
3	O	187	PEB	CHA-C1B	3.88	1.50	1.40
3	V	188	PEB	CHA-C1B	3.89	1.50	1.40
3	X	188	PEB	CHA-C1B	3.89	1.50	1.40
3	M	188	PEB	CHA-C1B	3.89	1.50	1.40
3	V	186	PEB	CHA-C1B	3.90	1.50	1.40
3	U	186	PEB	CHA-C1B	3.91	1.50	1.40
3	Q	188	PEB	CHA-C1B	3.92	1.50	1.40
3	H	166	PEB	CHA-C1B	3.93	1.50	1.40
3	I	166	PEB	CHA-C1B	3.95	1.50	1.40
3	W	187	PEB	CHA-C1B	3.97	1.50	1.40
3	S	188	PEB	CHA-C1B	4.00	1.50	1.40
3	B	166	PEB	CHA-C1B	4.01	1.50	1.40
3	W	188	PEB	CHA-C1B	4.01	1.50	1.40
3	O	186	PEB	CHA-C1B	4.05	1.50	1.40
3	N	186	PEB	CHA-C1B	4.08	1.50	1.40
3	W	186	PEB	CHA-C1B	4.10	1.50	1.40
3	R	186	PEB	CHA-C1B	4.10	1.50	1.40
3	S	186	PEB	CHA-C1B	4.49	1.51	1.40
3	O	186	PEB	C3B-C2B	4.66	1.46	1.36
3	T	186	PEB	C3B-C2B	4.67	1.46	1.36
3	O	188	PEB	C3B-C2B	4.70	1.47	1.36
3	R	186	PEB	C3B-C2B	4.85	1.47	1.36
3	H	167	PEB	C3B-C2B	4.88	1.47	1.36
3	C	166	PEB	C3B-C2B	4.90	1.47	1.36
3	T	187	PEB	C3B-C2B	4.91	1.47	1.36
3	Q	186	PEB	C3B-C2B	4.93	1.47	1.36
3	P	186	PEB	C3B-C2B	4.94	1.47	1.36
3	O	187	PEB	C3B-C2B	4.97	1.47	1.36
3	U	186	PEB	C3B-C2B	4.99	1.47	1.36
3	X	188	PEB	C3B-C2B	5.00	1.47	1.36
3	M	186	PEB	C3B-C2B	5.02	1.47	1.36
3	X	187	PEB	C3B-C2B	5.02	1.47	1.36
3	V	186	PEB	C3B-C2B	5.03	1.47	1.36
3	N	186	PEB	C3B-C2B	5.04	1.47	1.36
3	S	187	PEB	C3B-C2B	5.04	1.47	1.36
3	D	167	PEB	C3B-C2B	5.05	1.47	1.36

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	187	PEB	C3B-C2B	5.05	1.47	1.36
3	X	186	PEB	C3B-C2B	5.05	1.47	1.36
3	K	166	PEB	C3B-C2B	5.06	1.47	1.36
3	F	166	PEB	C3B-C2B	5.09	1.47	1.36
3	D	167	PEB	C3C-C4C	5.13	1.49	1.42
3	E	167	PEB	C3B-C2B	5.13	1.47	1.36
3	D	166	PEB	C3B-C2B	5.14	1.47	1.36
3	Q	187	PEB	C3B-C2B	5.14	1.47	1.36
3	W	186	PEB	C3B-C2B	5.16	1.47	1.36
3	L	166	PEB	C3B-C2B	5.17	1.48	1.36
3	I	166	PEB	C3B-C2B	5.18	1.48	1.36
3	B	167	PEB	C3B-C2B	5.19	1.48	1.36
3	I	167	PEB	C3C-C4C	5.19	1.49	1.42
3	P	186	PEB	C3C-C4C	5.19	1.49	1.42
3	M	188	PEB	C3B-C2B	5.19	1.48	1.36
3	V	188	PEB	C3B-C2B	5.20	1.48	1.36
3	K	167	PEB	C3B-C2B	5.20	1.48	1.36
3	W	187	PEB	C3C-C4C	5.20	1.49	1.42
3	E	166	PEB	C3B-C2B	5.22	1.48	1.36
3	S	186	PEB	C3B-C2B	5.22	1.48	1.36
3	M	186	PEB	C3C-C4C	5.22	1.49	1.42
3	M	187	PEB	C3C-C4C	5.23	1.49	1.42
3	A	166	PEB	C3B-C2B	5.24	1.48	1.36
3	M	187	PEB	C3B-C2B	5.25	1.48	1.36
3	G	166	PEB	C3B-C2B	5.26	1.48	1.36
3	A	167	PEB	C3C-C4C	5.27	1.49	1.42
3	J	166	PEB	C3B-C2B	5.28	1.48	1.36
3	U	187	PEB	C3B-C2B	5.28	1.48	1.36
3	W	186	PEB	C3C-C4C	5.29	1.49	1.42
3	R	187	PEB	C3B-C2B	5.29	1.48	1.36
3	C	167	PEB	C3B-C2B	5.30	1.48	1.36
3	J	167	PEB	C3B-C2B	5.31	1.48	1.36
3	I	167	PEB	C3B-C2B	5.31	1.48	1.36
3	T	188	PEB	C3B-C2B	5.32	1.48	1.36
3	A	167	PEB	C3B-C2B	5.32	1.48	1.36
3	U	188	PEB	C3B-C2B	5.32	1.48	1.36
3	H	167	PEB	C3C-C4C	5.32	1.49	1.42
3	L	167	PEB	C3B-C2B	5.33	1.48	1.36
3	S	188	PEB	C3B-C2B	5.34	1.48	1.36
3	B	166	PEB	C3B-C2B	5.34	1.48	1.36
3	Q	188	PEB	C3B-C2B	5.36	1.48	1.36
3	K	167	PEB	C3C-C4C	5.37	1.50	1.42

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	187	PEB	C3C-C4C	5.39	1.50	1.42
3	W	187	PEB	C3B-C2B	5.40	1.48	1.36
3	W	188	PEB	C3B-C2B	5.41	1.48	1.36
3	G	167	PEB	C3C-C4C	5.42	1.50	1.42
3	H	166	PEB	C3B-C2B	5.44	1.48	1.36
3	J	166	PEB	C3C-C4C	5.44	1.50	1.42
3	S	186	PEB	C3C-C4C	5.44	1.50	1.42
3	E	167	PEB	C3C-C4C	5.45	1.50	1.42
3	N	187	PEB	C3B-C2B	5.45	1.48	1.36
3	D	166	PEB	C3C-C4C	5.45	1.50	1.42
3	P	188	PEB	C3C-C4C	5.46	1.50	1.42
3	B	167	PEB	C3C-C4C	5.46	1.50	1.42
3	U	186	PEB	C3C-C4C	5.46	1.50	1.42
3	P	188	PEB	C3B-C2B	5.48	1.48	1.36
3	P	187	PEB	C3B-C2B	5.48	1.48	1.36
3	Q	188	PEB	C3C-C4C	5.50	1.50	1.42
3	R	187	PEB	C3C-C4C	5.51	1.50	1.42
3	T	188	PEB	C3C-C4C	5.52	1.50	1.42
3	J	167	PEB	C3C-C4C	5.52	1.50	1.42
3	G	167	PEB	C3B-C2B	5.54	1.48	1.36
3	L	167	PEB	C3C-C4C	5.55	1.50	1.42
3	N	188	PEB	C3B-C2B	5.55	1.48	1.36
3	L	166	PEB	C3C-C4C	5.57	1.50	1.42
3	R	188	PEB	C3C-C4C	5.57	1.50	1.42
3	R	188	PEB	C3B-C2B	5.58	1.48	1.36
3	X	187	PEB	C3C-C4C	5.58	1.50	1.42
3	N	187	PEB	C3C-C4C	5.59	1.50	1.42
3	N	186	PEB	C3C-C4C	5.59	1.50	1.42
3	F	167	PEB	C3B-C2B	5.60	1.48	1.36
3	U	188	PEB	C3C-C4C	5.61	1.50	1.42
3	G	166	PEB	C3C-C4C	5.63	1.50	1.42
3	O	188	PEB	C3C-C4C	5.65	1.50	1.42
3	X	188	PEB	C3C-C4C	5.66	1.50	1.42
3	A	166	PEB	C3C-C4C	5.68	1.50	1.42
3	O	186	PEB	C3C-C4C	5.71	1.50	1.42
3	S	187	PEB	C3C-C4C	5.74	1.50	1.42
3	V	187	PEB	C3C-C4C	5.75	1.50	1.42
3	W	188	PEB	C3C-C4C	5.76	1.50	1.42
3	I	166	PEB	C3C-C4C	5.79	1.50	1.42
3	U	187	PEB	C3C-C4C	5.79	1.50	1.42
3	M	188	PEB	C3C-C4C	5.81	1.50	1.42
3	F	167	PEB	C3C-C4C	5.82	1.50	1.42

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	186	PEB	C3C-C4C	5.82	1.50	1.42
3	V	188	PEB	C3C-C4C	5.82	1.50	1.42
3	Q	186	PEB	C3C-C4C	5.83	1.50	1.42
3	V	186	PEB	C3C-C4C	5.85	1.50	1.42
3	T	187	PEB	C3C-C4C	5.87	1.50	1.42
3	X	186	PEB	C3C-C4C	5.89	1.50	1.42
3	B	166	PEB	C3C-C4C	5.93	1.50	1.42
3	T	186	PEB	C3C-C4C	5.96	1.50	1.42
3	E	166	PEB	C3C-C4C	6.01	1.50	1.42
3	C	166	PEB	C3C-C4C	6.03	1.50	1.42
3	P	187	PEB	C3C-C4C	6.04	1.50	1.42
3	K	166	PEB	C3C-C4C	6.05	1.51	1.42
3	H	166	PEB	C3C-C4C	6.05	1.51	1.42
3	S	188	PEB	C3C-C4C	6.07	1.51	1.42
3	C	167	PEB	C3C-C4C	6.12	1.51	1.42
3	O	187	PEB	C3C-C4C	6.19	1.51	1.42
3	F	166	PEB	C3C-C4C	6.30	1.51	1.42
3	N	188	PEB	C3C-C4C	6.52	1.51	1.42
3	L	167	PEB	C2D-C3D	8.37	1.45	1.34
3	M	188	PEB	C2D-C3D	8.61	1.45	1.34
3	S	187	PEB	C2D-C3D	8.73	1.46	1.34
3	H	166	PEB	C2D-C3D	8.73	1.46	1.34
3	D	167	PEB	C2D-C3D	8.81	1.46	1.34
3	M	187	PEB	C2D-C3D	8.83	1.46	1.34
3	G	166	PEB	C2D-C3D	8.85	1.46	1.34
3	J	167	PEB	C2D-C3D	8.92	1.46	1.34
3	J	166	PEB	C2D-C3D	8.94	1.46	1.34
3	X	186	PEB	C2D-C3D	8.96	1.46	1.34
3	X	188	PEB	C2D-C3D	8.96	1.46	1.34
3	E	166	PEB	C2D-C3D	8.98	1.46	1.34
3	N	187	PEB	C2D-C3D	9.00	1.46	1.34
3	H	167	PEB	C2D-C3D	9.00	1.46	1.34
3	S	188	PEB	C2D-C3D	9.06	1.46	1.34
3	C	167	PEB	C2D-C3D	9.07	1.46	1.34
3	K	166	PEB	C2D-C3D	9.10	1.46	1.34
3	F	166	PEB	C2D-C3D	9.11	1.46	1.34
3	F	167	PEB	C2D-C3D	9.13	1.46	1.34
3	O	188	PEB	C2D-C3D	9.13	1.46	1.34
3	Q	188	PEB	C2D-C3D	9.13	1.46	1.34
3	B	166	PEB	C2D-C3D	9.14	1.46	1.34
3	U	188	PEB	C2D-C3D	9.14	1.46	1.34
3	V	188	PEB	C2D-C3D	9.17	1.46	1.34

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	186	PEB	C2D-C3D	9.17	1.46	1.34
3	X	187	PEB	C2D-C3D	9.17	1.46	1.34
3	V	187	PEB	C2D-C3D	9.18	1.46	1.34
3	W	187	PEB	C2D-C3D	9.22	1.46	1.34
3	I	167	PEB	C2D-C3D	9.23	1.46	1.34
3	P	188	PEB	C2D-C3D	9.23	1.46	1.34
3	G	167	PEB	C2D-C3D	9.24	1.46	1.34
3	O	187	PEB	C2D-C3D	9.25	1.46	1.34
3	A	167	PEB	C2D-C3D	9.25	1.46	1.34
3	K	167	PEB	C2D-C3D	9.26	1.46	1.34
3	E	167	PEB	C2D-C3D	9.27	1.46	1.34
3	C	166	PEB	C2D-C3D	9.29	1.46	1.34
3	R	187	PEB	C2D-C3D	9.31	1.46	1.34
3	T	188	PEB	C2D-C3D	9.33	1.46	1.34
3	I	166	PEB	C2D-C3D	9.34	1.46	1.34
3	P	187	PEB	C2D-C3D	9.35	1.46	1.34
3	T	186	PEB	C2D-C3D	9.35	1.46	1.34
3	V	186	PEB	C2D-C3D	9.36	1.46	1.34
3	W	186	PEB	C2D-C3D	9.36	1.46	1.34
3	T	187	PEB	C2D-C3D	9.38	1.46	1.34
3	O	186	PEB	C2D-C3D	9.43	1.46	1.34
3	D	166	PEB	C2D-C3D	9.43	1.46	1.34
3	N	188	PEB	C2D-C3D	9.47	1.46	1.34
3	N	186	PEB	C2D-C3D	9.49	1.47	1.34
3	U	187	PEB	C2D-C3D	9.53	1.47	1.34
3	R	186	PEB	C2D-C3D	9.54	1.47	1.34
3	R	188	PEB	C2D-C3D	9.59	1.47	1.34
3	Q	186	PEB	C2D-C3D	9.60	1.47	1.34
3	M	186	PEB	C2D-C3D	9.62	1.47	1.34
3	W	188	PEB	C2D-C3D	9.63	1.47	1.34
3	S	186	PEB	C2D-C3D	9.68	1.47	1.34
3	L	166	PEB	C2D-C3D	9.69	1.47	1.34
3	B	167	PEB	C2D-C3D	9.76	1.47	1.34
3	A	166	PEB	C2D-C3D	9.82	1.47	1.34
3	U	186	PEB	C2D-C3D	9.95	1.47	1.34
3	Q	187	PEB	C2D-C3D	10.27	1.48	1.34
3	F	166	PEB	CHB-C4B	13.43	1.47	1.35
3	W	187	PEB	CHB-C4B	13.57	1.47	1.35
3	C	167	PEB	CHB-C4B	13.86	1.47	1.35
3	G	166	PEB	CHB-C4B	13.91	1.47	1.35
3	R	187	PEB	CHB-C4B	13.93	1.47	1.35
3	K	166	PEB	CHB-C4B	13.95	1.47	1.35

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	167	PEB	CHB-C4B	14.01	1.47	1.35
3	I	167	PEB	CHB-C4B	14.06	1.48	1.35
3	K	167	PEB	CHB-C4B	14.09	1.48	1.35
3	O	187	PEB	CHB-C4B	14.11	1.48	1.35
3	B	167	PEB	CHB-C4B	14.17	1.48	1.35
3	M	187	PEB	CHB-C4B	14.23	1.48	1.35
3	L	166	PEB	CHB-C4B	14.24	1.48	1.35
3	N	188	PEB	CHB-C4B	14.28	1.48	1.35
3	X	187	PEB	CHB-C4B	14.34	1.48	1.35
3	A	167	PEB	CHB-C4B	14.47	1.48	1.35
3	V	186	PEB	CHB-C4B	14.51	1.48	1.35
3	J	167	PEB	CHB-C4B	14.52	1.48	1.35
3	C	166	PEB	CHB-C4B	14.58	1.48	1.35
3	Q	186	PEB	CHB-C4B	14.60	1.48	1.35
3	T	187	PEB	CHB-C4B	14.66	1.48	1.35
3	V	187	PEB	CHB-C4B	14.69	1.48	1.35
3	T	186	PEB	CHB-C4B	14.72	1.48	1.35
3	A	166	PEB	CHB-C4B	14.72	1.48	1.35
3	H	167	PEB	CHB-C4B	14.77	1.48	1.35
3	B	166	PEB	CHB-C4B	14.86	1.48	1.35
3	H	166	PEB	CHB-C4B	14.87	1.48	1.35
3	O	186	PEB	CHB-C4B	14.92	1.48	1.35
3	E	167	PEB	CHB-C4B	14.94	1.48	1.35
3	I	166	PEB	CHB-C4B	14.96	1.48	1.35
3	D	167	PEB	CHB-C4B	14.97	1.48	1.35
3	R	188	PEB	CHB-C4B	14.99	1.48	1.35
3	P	187	PEB	CHB-C4B	14.99	1.48	1.35
3	W	188	PEB	CHB-C4B	15.03	1.48	1.35
3	D	166	PEB	CHB-C4B	15.03	1.48	1.35
3	E	166	PEB	CHB-C4B	15.05	1.48	1.35
3	S	187	PEB	CHB-C4B	15.06	1.48	1.35
3	N	187	PEB	CHB-C4B	15.07	1.48	1.35
3	N	186	PEB	CHB-C4B	15.09	1.48	1.35
3	O	188	PEB	CHB-C4B	15.10	1.48	1.35
3	V	188	PEB	CHB-C4B	15.15	1.49	1.35
3	U	187	PEB	CHB-C4B	15.15	1.49	1.35
3	G	167	PEB	CHB-C4B	15.19	1.49	1.35
3	U	188	PEB	CHB-C4B	15.23	1.49	1.35
3	P	188	PEB	CHB-C4B	15.24	1.49	1.35
3	X	186	PEB	CHB-C4B	15.28	1.49	1.35
3	M	186	PEB	CHB-C4B	15.33	1.49	1.35
3	W	186	PEB	CHB-C4B	15.47	1.49	1.35

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	186	PEB	CHB-C4B	15.56	1.49	1.35
3	S	186	PEB	CHB-C4B	15.65	1.49	1.35
3	S	188	PEB	CHB-C4B	15.70	1.49	1.35
3	Q	188	PEB	CHB-C4B	15.73	1.49	1.35
3	Q	187	PEB	CHB-C4B	15.74	1.49	1.35
3	T	188	PEB	CHB-C4B	15.74	1.49	1.35
3	J	166	PEB	CHB-C4B	15.82	1.49	1.35
3	F	167	PEB	CHB-C4B	15.82	1.49	1.35
3	P	186	PEB	CHB-C4B	15.87	1.49	1.35
3	M	188	PEB	CHB-C4B	15.95	1.49	1.35
3	X	188	PEB	CHB-C4B	16.20	1.49	1.35
3	U	186	PEB	CHB-C4B	16.23	1.49	1.35

All (934) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	166	PEB	OA-C1A-C2A	-7.04	120.64	126.30
3	J	166	PEB	OA-C1A-C2A	-6.89	120.76	126.30
3	F	166	PEB	CHA-C1B-NB	-6.81	112.17	124.89
3	K	166	PEB	CHA-C1B-NB	-6.77	112.25	124.89
3	D	167	PEB	CHC-C4C-C3C	-6.66	121.99	130.95
3	T	186	PEB	OA-C1A-C2A	-6.60	120.99	126.30
3	M	186	PEB	C2D-C3D-C4D	-6.49	99.39	108.25
3	G	166	PEB	CHA-C1B-NB	-6.44	112.85	124.89
3	L	166	PEB	CHA-C1B-NB	-6.42	112.90	124.89
3	A	166	PEB	OA-C1A-C2A	-6.41	121.14	126.30
3	X	186	PEB	C2D-C3D-C4D	-6.40	99.51	108.25
3	V	186	PEB	OA-C1A-C2A	-6.39	121.16	126.30
3	I	167	PEB	CHC-C4C-C3C	-6.36	122.39	130.95
3	W	186	PEB	C2D-C3D-C4D	-6.32	99.63	108.25
3	M	187	PEB	C2D-C3D-C4D	-6.31	99.63	108.25
3	G	166	PEB	C2D-C3D-C4D	-6.30	99.65	108.25
3	V	187	PEB	C2D-C3D-C4D	-6.25	99.71	108.25
3	O	186	PEB	C2D-C3D-C4D	-6.24	99.73	108.25
3	D	167	PEB	C2D-C3D-C4D	-6.21	99.77	108.25
3	X	187	PEB	C2D-C3D-C4D	-6.20	99.78	108.25
3	G	166	PEB	CHC-C4C-C3C	-6.19	122.62	130.95
3	U	186	PEB	C2D-C3D-C4D	-6.18	99.81	108.25
3	A	166	PEB	CHA-C1B-NB	-6.18	113.35	124.89
3	C	166	PEB	OA-C1A-C2A	-6.18	121.33	126.30
3	I	166	PEB	C2D-C3D-C4D	-6.15	99.85	108.25
3	W	187	PEB	C2D-C3D-C4D	-6.14	99.87	108.25

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	166	PEB	OA-C1A-C2A	-6.13	121.37	126.30
3	J	167	PEB	C2D-C3D-C4D	-6.12	99.90	108.25
3	N	187	PEB	C2D-C3D-C4D	-6.11	99.90	108.25
3	K	166	PEB	C2D-C3D-C4D	-6.11	99.91	108.25
3	L	167	PEB	C2D-C3D-C4D	-6.10	99.92	108.25
3	W	188	PEB	C2D-C3D-C4D	-6.09	99.93	108.25
3	T	187	PEB	C2D-C3D-C4D	-6.08	99.95	108.25
3	L	166	PEB	C2D-C3D-C4D	-6.08	99.96	108.25
3	J	166	PEB	C2D-C3D-C4D	-6.05	99.99	108.25
3	F	167	PEB	C2D-C3D-C4D	-6.04	100.00	108.25
3	S	186	PEB	C2D-C3D-C4D	-6.03	100.01	108.25
3	B	166	PEB	CHA-C1B-NB	-6.02	113.65	124.89
3	I	167	PEB	C2D-C3D-C4D	-5.99	100.08	108.25
3	T	186	PEB	C2D-C3D-C4D	-5.98	100.08	108.25
3	C	166	PEB	C2D-C3D-C4D	-5.98	100.09	108.25
3	U	187	PEB	C2D-C3D-C4D	-5.97	100.10	108.25
3	B	167	PEB	C2D-C3D-C4D	-5.97	100.10	108.25
3	K	166	PEB	OA-C1A-C2A	-5.96	121.50	126.30
3	P	187	PEB	C2D-C3D-C4D	-5.96	100.12	108.25
3	T	188	PEB	C2D-C3D-C4D	-5.95	100.12	108.25
3	V	186	PEB	C2D-C3D-C4D	-5.94	100.14	108.25
3	H	166	PEB	CHA-C1B-NB	-5.94	113.79	124.89
3	Q	187	PEB	C2D-C3D-C4D	-5.94	100.14	108.25
3	C	166	PEB	CHA-C1B-NB	-5.93	113.81	124.89
3	H	166	PEB	C2D-C3D-C4D	-5.93	100.16	108.25
3	K	167	PEB	C2D-C3D-C4D	-5.92	100.17	108.25
3	E	167	PEB	C2D-C3D-C4D	-5.91	100.19	108.25
3	A	167	PEB	C2D-C3D-C4D	-5.90	100.19	108.25
3	S	187	PEB	C2D-C3D-C4D	-5.89	100.21	108.25
3	G	167	PEB	C2D-C3D-C4D	-5.86	100.25	108.25
3	O	187	PEB	C2D-C3D-C4D	-5.82	100.31	108.25
3	D	166	PEB	CHA-C1B-NB	-5.81	114.04	124.89
3	Q	186	PEB	C2D-C3D-C4D	-5.80	100.33	108.25
3	N	186	PEB	C2D-C3D-C4D	-5.80	100.33	108.25
3	B	166	PEB	C2D-C3D-C4D	-5.80	100.34	108.25
3	Q	188	PEB	C2D-C3D-C4D	-5.79	100.35	108.25
3	R	188	PEB	C2D-C3D-C4D	-5.78	100.36	108.25
3	P	188	PEB	C2D-C3D-C4D	-5.75	100.40	108.25
3	D	167	PEB	OA-C1A-C2A	-5.74	121.68	126.30
3	N	188	PEB	C2D-C3D-C4D	-5.72	100.44	108.25
3	F	166	PEB	OA-C1A-C2A	-5.71	121.71	126.30
3	R	186	PEB	C2D-C3D-C4D	-5.71	100.46	108.25

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	166	PEB	C2D-C3D-C4D	-5.70	100.47	108.25
3	M	188	PEB	C2D-C3D-C4D	-5.70	100.47	108.25
3	D	166	PEB	OA-C1A-C2A	-5.70	121.72	126.30
3	P	186	PEB	C2D-C3D-C4D	-5.69	100.48	108.25
3	U	188	PEB	C2D-C3D-C4D	-5.69	100.48	108.25
3	D	166	PEB	C2D-C3D-C4D	-5.69	100.48	108.25
3	A	166	PEB	C2D-C3D-C4D	-5.69	100.49	108.25
3	C	167	PEB	C2D-C3D-C4D	-5.67	100.52	108.25
3	E	166	PEB	C2D-C3D-C4D	-5.66	100.53	108.25
3	L	166	PEB	CHC-C4C-C3C	-5.65	123.34	130.95
3	I	166	PEB	CHA-C1B-NB	-5.65	114.34	124.89
3	R	187	PEB	C2D-C3D-C4D	-5.63	100.56	108.25
3	S	188	PEB	C2D-C3D-C4D	-5.62	100.58	108.25
3	E	166	PEB	CHA-C1B-NB	-5.61	114.40	124.89
3	X	188	PEB	C2D-C3D-C4D	-5.60	100.61	108.25
3	H	167	PEB	C2D-C3D-C4D	-5.60	100.61	108.25
3	O	186	PEB	OA-C1A-C2A	-5.58	121.81	126.30
3	E	166	PEB	OA-C1A-C2A	-5.57	121.82	126.30
3	N	186	PEB	CHC-C4C-C3C	-5.53	123.51	130.95
3	U	187	PEB	CAC-CBC-CGC	-5.53	102.03	112.78
3	O	188	PEB	C2D-C3D-C4D	-5.52	100.71	108.25
3	P	188	PEB	CHC-C4C-C3C	-5.51	123.52	130.95
3	E	167	PEB	CHC-C4C-C3C	-5.51	123.53	130.95
3	H	166	PEB	OA-C1A-C2A	-5.44	121.92	126.30
3	M	188	PEB	CHC-C4C-C3C	-5.38	123.70	130.95
3	M	186	PEB	CHC-C4C-C3C	-5.38	123.70	130.95
3	A	166	PEB	CHC-C4C-C3C	-5.38	123.71	130.95
3	T	188	PEB	CHC-C4C-C3C	-5.32	123.79	130.95
3	N	187	PEB	CHC-C4C-C3C	-5.30	123.81	130.95
3	L	166	PEB	OA-C1A-C2A	-5.29	122.04	126.30
3	R	187	PEB	CHC-C4C-C3C	-5.26	123.87	130.95
3	V	188	PEB	C2D-C3D-C4D	-5.23	101.10	108.25
3	A	167	PEB	CHC-C4C-C3C	-5.22	123.92	130.95
3	W	186	PEB	CHC-C4C-C3C	-5.20	123.95	130.95
3	J	166	PEB	CHA-C1B-NB	-5.10	115.36	124.89
3	L	167	PEB	CHC-C4C-C3C	-5.08	124.11	130.95
3	W	187	PEB	CHC-C4C-C3C	-5.08	124.12	130.95
3	R	188	PEB	CHC-C4C-C3C	-5.07	124.13	130.95
3	M	187	PEB	CHC-C4C-C3C	-5.02	124.19	130.95
3	S	186	PEB	CHC-C4C-C3C	-5.02	124.19	130.95
3	V	187	PEB	OA-C1A-C2A	-4.97	122.30	126.30
3	H	167	PEB	CHC-C4C-C3C	-4.96	124.28	130.95

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	166	PEB	CHC-C4C-C3C	-4.95	124.28	130.95
3	X	186	PEB	CHA-C1B-NB	-4.95	115.65	124.89
3	U	187	PEB	CHC-C4C-C3C	-4.94	124.30	130.95
3	Q	186	PEB	CHA-C1B-NB	-4.94	115.67	124.89
3	U	186	PEB	OA-C1A-C2A	-4.91	122.35	126.30
3	O	186	PEB	CHC-C4C-C3C	-4.85	124.41	130.95
3	S	186	PEB	OA-C1A-C2A	-4.85	122.39	126.30
3	U	186	PEB	CHA-C1B-NB	-4.85	115.83	124.89
3	Q	188	PEB	CHC-C4C-C3C	-4.84	124.43	130.95
3	T	186	PEB	CHA-C1B-NB	-4.83	115.86	124.89
3	M	186	PEB	CHA-C1B-NB	-4.82	115.88	124.89
3	V	186	PEB	CHC-C4C-C3C	-4.79	124.50	130.95
3	K	167	PEB	CHC-C4C-C3C	-4.78	124.51	130.95
3	M	188	PEB	OA-C1A-C2A	-4.77	122.47	126.30
3	O	188	PEB	OA-C1A-C2A	-4.75	122.48	126.30
3	X	187	PEB	OA-C1A-C2A	-4.74	122.49	126.30
3	G	167	PEB	CHC-C4C-C3C	-4.73	124.58	130.95
3	N	186	PEB	CHA-C1B-NB	-4.73	116.05	124.89
3	U	188	PEB	CHC-C4C-C3C	-4.71	124.60	130.95
3	X	188	PEB	CHC-C4C-C3C	-4.71	124.61	130.95
3	T	187	PEB	OA-C1A-C2A	-4.69	122.53	126.30
3	V	187	PEB	CHC-C4C-C3C	-4.68	124.65	130.95
3	X	187	PEB	CHC-C4C-C3C	-4.66	124.67	130.95
3	V	186	PEB	CHA-C1B-NB	-4.66	116.19	124.89
3	X	188	PEB	OA-C1A-C2A	-4.65	122.56	126.30
3	T	187	PEB	CHC-C4C-C3C	-4.63	124.72	130.95
3	Q	187	PEB	CHC-C4C-C3C	-4.61	124.74	130.95
3	B	167	PEB	CHC-C4C-C3C	-4.61	124.74	130.95
3	F	167	PEB	CHC-C4C-C3C	-4.61	124.74	130.95
3	N	188	PEB	OA-C1A-C2A	-4.60	122.59	126.30
3	U	188	PEB	OA-C1A-C2A	-4.57	122.62	126.30
3	N	186	PEB	OA-C1A-C2A	-4.57	122.62	126.30
3	S	188	PEB	OA-C1A-C2A	-4.56	122.63	126.30
3	E	167	PEB	OA-C1A-C2A	-4.54	122.65	126.30
3	H	166	PEB	CHC-C4C-C3C	-4.53	124.84	130.95
3	W	186	PEB	CHA-C1B-NB	-4.50	116.48	124.89
3	R	186	PEB	OA-C1A-C2A	-4.49	122.68	126.30
3	O	188	PEB	CHC-C4C-C3C	-4.49	124.90	130.95
3	R	186	PEB	CHA-C1B-NB	-4.47	116.54	124.89
3	P	186	PEB	CHC-C4C-C3C	-4.46	124.94	130.95
3	S	186	PEB	CHA-C1B-NB	-4.45	116.57	124.89
3	I	167	PEB	OA-C1A-C2A	-4.44	122.73	126.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	186	PEB	OA-C1A-C2A	-4.42	122.74	126.30
3	I	167	PEB	CHB-C4B-NB	-4.42	120.89	128.71
3	P	186	PEB	CHA-C1B-NB	-4.41	116.65	124.89
3	O	186	PEB	CHA-C1B-NB	-4.40	116.67	124.89
3	J	167	PEB	CHC-C4C-C3C	-4.34	125.11	130.95
3	A	167	PEB	OA-C1A-C2A	-4.33	122.81	126.30
3	B	166	PEB	CHC-C4C-C3C	-4.30	125.16	130.95
3	F	166	PEB	CHC-C4C-C3C	-4.28	125.19	130.95
3	I	166	PEB	CHC-C4C-C3C	-4.24	125.25	130.95
3	M	186	PEB	OA-C1A-C2A	-4.22	122.90	126.30
3	X	186	PEB	OA-C1A-C2A	-4.21	122.91	126.30
3	G	166	PEB	OA-C1A-C2A	-4.19	122.92	126.30
3	O	187	PEB	CHC-C4C-C3C	-4.17	125.33	130.95
3	E	166	PEB	CHC-C4C-C3C	-4.16	125.35	130.95
3	C	167	PEB	CHC-C4C-C3C	-4.15	125.36	130.95
3	L	166	PEB	CHB-C4B-NB	-4.14	121.37	128.71
3	G	167	PEB	OA-C1A-C2A	-4.09	123.01	126.30
3	R	188	PEB	OA-C1A-C2A	-4.08	123.01	126.30
3	S	187	PEB	CHC-C4C-C3C	-4.08	125.45	130.95
3	D	166	PEB	CHC-C4C-C3C	-4.07	125.47	130.95
3	B	167	PEB	OA-C1A-C2A	-4.07	123.03	126.30
3	C	167	PEB	OA-C1A-C2A	-4.04	123.05	126.30
3	Q	186	PEB	CHC-C4C-C3C	-4.04	125.51	130.95
3	R	186	PEB	CHC-C4C-C3C	-4.03	125.53	130.95
3	H	167	PEB	OA-C1A-C2A	-4.01	123.07	126.30
3	F	167	PEB	OA-C1A-C2A	-4.01	123.07	126.30
3	M	187	PEB	OA-C1A-C2A	-4.00	123.08	126.30
3	C	166	PEB	CHC-C4C-C3C	-4.00	125.57	130.95
3	T	186	PEB	CHC-C4C-C3C	-3.97	125.60	130.95
3	N	187	PEB	OA-C1A-C2A	-3.94	123.13	126.30
3	H	166	PEB	CHB-C4B-NB	-3.92	121.76	128.71
3	A	166	PEB	CHB-C4B-NB	-3.90	121.80	128.71
3	Q	187	PEB	CBC-CAC-C2C	-3.90	105.64	112.49
3	P	186	PEB	OA-C1A-C2A	-3.88	123.18	126.30
3	R	187	PEB	OA-C1A-C2A	-3.88	123.18	126.30
3	K	167	PEB	OA-C1A-C2A	-3.87	123.18	126.30
3	M	187	PEB	C4B-C3B-C2B	-3.85	102.61	106.80
3	S	188	PEB	CHC-C4C-C3C	-3.85	125.77	130.95
3	N	188	PEB	C4B-C3B-C2B	-3.84	102.62	106.80
3	Q	188	PEB	OA-C1A-C2A	-3.83	123.22	126.30
3	W	187	PEB	OA-C1A-C2A	-3.83	123.22	126.30
3	L	167	PEB	OA-C1A-C2A	-3.81	123.23	126.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	166	PEB	CHC-C4C-C3C	-3.79	125.84	130.95
3	D	167	PEB	CHB-C4B-NB	-3.77	122.04	128.71
3	R	187	PEB	CHA-C1B-NB	-3.73	117.93	124.89
3	S	187	PEB	CHA-C1B-NB	-3.72	117.94	124.89
3	E	166	PEB	CHB-C4B-NB	-3.70	122.16	128.71
3	O	188	PEB	OD-C4D-C3D	-3.69	120.87	130.06
3	N	188	PEB	CHC-C4C-C3C	-3.67	126.01	130.95
3	G	166	PEB	C1B-C2B-C3B	-3.67	102.20	106.43
3	M	187	PEB	CHA-C1B-NB	-3.65	118.08	124.89
3	P	187	PEB	OA-C1A-C2A	-3.64	123.37	126.30
3	V	188	PEB	OA-C1A-C2A	-3.63	123.38	126.30
3	W	188	PEB	CHC-C4C-C3C	-3.63	126.06	130.95
3	R	188	PEB	CBC-CAC-C2C	-3.63	106.11	112.49
3	N	187	PEB	C4B-C3B-C2B	-3.61	102.87	106.80
3	J	166	PEB	CMA-C2A-C1A	-3.61	104.66	112.39
3	S	187	PEB	OA-C1A-C2A	-3.60	123.40	126.30
3	U	186	PEB	CAB-CBB-CGB	-3.59	105.79	112.78
3	Q	187	PEB	OA-C1A-C2A	-3.59	123.41	126.30
3	L	167	PEB	C4B-C3B-C2B	-3.58	102.90	106.80
3	I	166	PEB	CHB-C4B-NB	-3.57	122.38	128.71
3	J	167	PEB	C1B-C2B-C3B	-3.57	102.31	106.43
3	U	186	PEB	CHC-C4C-C3C	-3.56	126.16	130.95
3	C	167	PEB	C4B-C3B-C2B	-3.53	102.96	106.80
3	P	187	PEB	CHC-C4C-C3C	-3.52	126.20	130.95
3	W	187	PEB	C4B-C3B-C2B	-3.52	102.97	106.80
3	W	186	PEB	OA-C1A-C2A	-3.51	123.47	126.30
3	V	188	PEB	OD-C4D-C3D	-3.51	121.31	130.06
3	U	187	PEB	OA-C1A-C2A	-3.51	123.47	126.30
3	V	188	PEB	CHC-C4C-C3C	-3.51	126.23	130.95
3	K	167	PEB	CHB-C4B-NB	-3.50	122.50	128.71
3	V	188	PEB	C4B-C3B-C2B	-3.50	102.99	106.80
3	I	167	PEB	CAB-CBB-CGB	-3.50	105.97	112.78
3	J	166	PEB	CHB-C4B-NB	-3.49	122.52	128.71
3	E	167	PEB	CHB-C4B-NB	-3.49	122.52	128.71
3	S	188	PEB	C4B-C3B-C2B	-3.48	103.01	106.80
3	Q	187	PEB	OD-C4D-C3D	-3.46	121.43	130.06
3	P	187	PEB	C4B-C3B-C2B	-3.45	103.04	106.80
3	P	188	PEB	OA-C1A-C2A	-3.41	123.56	126.30
3	X	187	PEB	C4B-C3B-C2B	-3.41	103.09	106.80
3	I	167	PEB	C4B-C3B-C2B	-3.39	103.11	106.80
3	T	188	PEB	CHA-C1B-NB	-3.37	118.59	124.89
3	D	167	PEB	CAB-CBB-CGB	-3.35	106.26	112.78

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	186	PEB	CAB-CBB-CGB	-3.35	106.27	112.78
3	X	186	PEB	CHC-C4C-C3C	-3.33	126.46	130.95
3	J	167	PEB	OA-C1A-C2A	-3.32	123.63	126.30
3	G	166	PEB	CHB-C4B-NB	-3.31	122.85	128.71
3	L	166	PEB	C1B-C2B-C3B	-3.30	102.62	106.43
3	O	187	PEB	C4B-C3B-C2B	-3.29	103.21	106.80
3	I	167	PEB	CHA-C1B-NB	-3.29	118.75	124.89
3	S	188	PEB	OD-C4D-C3D	-3.28	121.88	130.06
3	B	167	PEB	C4B-C3B-C2B	-3.28	103.23	106.80
3	Q	188	PEB	C4B-C3B-C2B	-3.27	103.24	106.80
3	R	188	PEB	C4B-C3B-C2B	-3.27	103.24	106.80
3	P	186	PEB	OD-C4D-C3D	-3.25	121.95	130.06
3	U	188	PEB	CHB-C4B-NB	-3.23	122.99	128.71
3	A	166	PEB	C4B-C3B-C2B	-3.23	103.29	106.80
3	D	166	PEB	CHB-C4B-NB	-3.22	123.00	128.71
3	L	167	PEB	CHA-C1B-NB	-3.22	118.87	124.89
3	C	167	PEB	OD-C4D-C3D	-3.22	122.05	130.06
3	K	167	PEB	C4B-C3B-C2B	-3.21	103.31	106.80
3	B	167	PEB	CHB-C4B-NB	-3.21	123.03	128.71
3	W	187	PEB	CAB-CBB-CGB	-3.21	106.54	112.78
3	F	166	PEB	C1B-C2B-C3B	-3.20	102.73	106.43
3	U	187	PEB	C4B-C3B-C2B	-3.20	103.31	106.80
3	Q	187	PEB	CHB-C4B-NB	-3.20	123.04	128.71
3	M	187	PEB	OD-C4D-C3D	-3.20	122.08	130.06
3	E	166	PEB	OD-C4D-ND	-3.20	120.48	126.06
3	H	166	PEB	C4B-C3B-C2B	-3.20	103.32	106.80
3	T	187	PEB	CHA-C1B-NB	-3.18	118.94	124.89
3	B	167	PEB	OD-C4D-C3D	-3.18	122.13	130.06
3	Q	187	PEB	CHA-C1B-NB	-3.18	118.95	124.89
3	X	187	PEB	OD-C4D-C3D	-3.16	122.19	130.06
3	W	188	PEB	C4B-C3B-C2B	-3.15	103.38	106.80
3	Q	188	PEB	CHA-C1B-NB	-3.14	119.02	124.89
3	R	187	PEB	C4B-C3B-C2B	-3.14	103.38	106.80
3	K	166	PEB	OD-C4D-C3D	-3.14	122.23	130.06
3	C	166	PEB	C4B-C3B-C2B	-3.13	103.39	106.80
3	W	187	PEB	CHA-C1B-NB	-3.13	119.04	124.89
3	U	187	PEB	OD-C4D-C3D	-3.13	122.27	130.06
3	N	188	PEB	OD-C4D-C3D	-3.12	122.28	130.06
3	I	167	PEB	CBC-CAC-C2C	-3.12	107.01	112.49
3	X	186	PEB	OD-C4D-C3D	-3.12	122.29	130.06
3	O	188	PEB	CHB-C4B-NB	-3.11	123.20	128.71
3	D	167	PEB	C4B-C3B-C2B	-3.10	103.42	106.80

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	187	PEB	CHA-C1B-NB	-3.10	119.10	124.89
3	T	188	PEB	OA-C1A-C2A	-3.10	123.80	126.30
3	G	167	PEB	OD-C4D-C3D	-3.10	122.33	130.06
3	F	166	PEB	C4B-C3B-C2B	-3.10	103.43	106.80
3	S	186	PEB	OD-C4D-C3D	-3.10	122.34	130.06
3	V	186	PEB	C1B-C2B-C3B	-3.10	102.86	106.43
3	T	187	PEB	OD-C4D-C3D	-3.09	122.35	130.06
3	W	187	PEB	OD-C4D-C3D	-3.09	122.36	130.06
3	R	188	PEB	CHB-C4B-NB	-3.08	123.25	128.71
3	V	187	PEB	C4B-C3B-C2B	-3.08	103.45	106.80
3	D	167	PEB	CBC-CAC-C2C	-3.07	107.09	112.49
3	T	188	PEB	CHB-C4B-NB	-3.07	123.27	128.71
3	K	166	PEB	CHB-C4B-NB	-3.05	123.30	128.71
3	K	166	PEB	CAC-CBC-CGC	-3.05	106.84	112.78
3	N	186	PEB	OD-C4D-C3D	-3.05	122.46	130.06
3	I	166	PEB	CMA-C2A-C1A	-3.04	105.88	112.39
3	G	167	PEB	C4B-C3B-C2B	-3.03	103.50	106.80
3	U	186	PEB	OD-C4D-C3D	-3.02	122.53	130.06
3	U	188	PEB	OD-C4D-C3D	-3.02	122.53	130.06
3	G	167	PEB	CHA-C1B-NB	-3.02	119.25	124.89
3	M	186	PEB	OD-C4D-C3D	-3.02	122.54	130.06
3	Q	186	PEB	CHB-C4B-NB	-3.01	123.37	128.71
3	V	188	PEB	CHB-C4B-NB	-3.01	123.38	128.71
3	Q	187	PEB	C4B-C3B-C2B	-3.01	103.52	106.80
3	A	166	PEB	CAC-CBC-CGC	-3.01	106.93	112.78
3	W	188	PEB	OA-C1A-C2A	-3.00	123.88	126.30
3	O	187	PEB	OA-C1A-C2A	-3.00	123.88	126.30
3	J	167	PEB	CHB-C4B-NB	-3.00	123.40	128.71
3	L	167	PEB	OD-C4D-ND	-2.99	120.84	126.06
3	S	187	PEB	OD-C4D-C3D	-2.99	122.61	130.06
3	O	186	PEB	OD-C4D-C3D	-2.99	122.62	130.06
3	N	188	PEB	CBC-CAC-C2C	-2.98	107.25	112.49
3	T	187	PEB	C4B-C3B-C2B	-2.98	103.56	106.80
3	K	167	PEB	CAB-CBB-CGB	-2.97	107.00	112.78
3	D	166	PEB	C1B-C2B-C3B	-2.97	103.00	106.43
3	L	167	PEB	CHB-C4B-NB	-2.97	123.45	128.71
3	C	167	PEB	CHA-C1B-NB	-2.97	119.35	124.89
3	F	166	PEB	CHB-C4B-NB	-2.96	123.46	128.71
3	I	167	PEB	C1B-C2B-C3B	-2.96	103.01	106.43
3	T	186	PEB	C1B-C2B-C3B	-2.96	103.01	106.43
3	J	167	PEB	CHA-C1B-NB	-2.96	119.37	124.89
3	A	166	PEB	C1B-C2B-C3B	-2.96	103.02	106.43

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	167	PEB	C4B-C3B-C2B	-2.95	103.59	106.80
3	A	166	PEB	OD-C4D-ND	-2.95	120.92	126.06
3	N	187	PEB	CHA-C1B-NB	-2.95	119.39	124.89
3	N	187	PEB	OD-C4D-C3D	-2.95	122.72	130.06
3	V	187	PEB	OD-C4D-ND	-2.94	120.92	126.06
3	X	186	PEB	C1B-C2B-C3B	-2.94	103.04	106.43
3	H	167	PEB	C4B-C3B-C2B	-2.93	103.61	106.80
3	W	188	PEB	OD-C4D-C3D	-2.93	122.77	130.06
3	O	188	PEB	C4B-C3B-C2B	-2.93	103.62	106.80
3	J	166	PEB	OD-C4D-C3D	-2.92	122.77	130.06
3	J	167	PEB	OD-C4D-C3D	-2.92	122.77	130.06
3	T	186	PEB	CAB-CBB-CGB	-2.92	107.09	112.78
3	U	186	PEB	C1B-C2B-C3B	-2.92	103.06	106.43
3	H	167	PEB	CHB-C4B-NB	-2.92	123.55	128.71
3	C	167	PEB	CHB-C4B-NB	-2.91	123.56	128.71
3	K	167	PEB	OD-C4D-C3D	-2.91	122.82	130.06
3	N	186	PEB	CHB-C4B-NB	-2.90	123.57	128.71
3	P	188	PEB	CHB-C4B-NB	-2.90	123.58	128.71
3	O	187	PEB	OD-C4D-C3D	-2.89	122.86	130.06
3	H	166	PEB	OD-C4D-C3D	-2.89	122.87	130.06
3	Q	188	PEB	OD-C4D-C3D	-2.89	122.87	130.06
3	G	167	PEB	C1B-C2B-C3B	-2.88	103.11	106.43
3	N	186	PEB	C4B-C3B-C2B	-2.88	103.67	106.80
3	P	188	PEB	CAC-CBC-CGC	-2.87	107.19	112.78
3	M	188	PEB	OD-C4D-C3D	-2.86	122.92	130.06
3	N	188	PEB	CHB-C4B-NB	-2.86	123.64	128.71
3	B	167	PEB	CAB-CBB-CGB	-2.86	107.22	112.78
3	E	167	PEB	C1B-C2B-C3B	-2.86	103.13	106.43
3	U	187	PEB	CHA-C1B-NB	-2.86	119.55	124.89
3	F	167	PEB	OD-C4D-C3D	-2.85	122.95	130.06
3	K	167	PEB	C1B-C2B-C3B	-2.85	103.14	106.43
3	T	188	PEB	C4B-C3B-C2B	-2.85	103.69	106.80
3	K	166	PEB	C1B-C2B-C3B	-2.85	103.14	106.43
3	Q	186	PEB	C4B-C3B-C2B	-2.85	103.70	106.80
3	R	187	PEB	OD-C4D-C3D	-2.84	122.97	130.06
3	S	188	PEB	CHB-C4B-NB	-2.84	123.67	128.71
3	V	186	PEB	OD-C4D-C3D	-2.84	122.98	130.06
3	W	186	PEB	C4B-C3B-C2B	-2.84	103.71	106.80
3	X	188	PEB	CAC-CBC-CGC	-2.84	107.26	112.78
3	S	187	PEB	C4B-C3B-C2B	-2.83	103.72	106.80
3	F	167	PEB	C1B-C2B-C3B	-2.82	103.17	106.43
3	P	188	PEB	CHA-C1B-NB	-2.81	119.63	124.89

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	167	PEB	C1B-C2B-C3B	-2.81	103.19	106.43
3	Q	187	PEB	CAB-CBB-CGB	-2.81	107.31	112.78
3	Q	186	PEB	OD-C4D-C3D	-2.81	123.06	130.06
3	Q	186	PEB	C1B-C2B-C3B	-2.81	103.19	106.43
3	P	187	PEB	CHA-C1B-NB	-2.81	119.65	124.89
3	P	188	PEB	C4B-C3B-C2B	-2.80	103.75	106.80
3	R	186	PEB	C1B-C2B-C3B	-2.80	103.20	106.43
3	A	167	PEB	C1B-C2B-C3B	-2.80	103.20	106.43
3	F	166	PEB	OD-C4D-C3D	-2.79	123.10	130.06
3	C	166	PEB	OD-C4D-C3D	-2.78	123.12	130.06
3	V	188	PEB	CBC-CAC-C2C	-2.78	107.60	112.49
3	T	188	PEB	OD-C4D-C3D	-2.78	123.12	130.06
3	I	166	PEB	C1B-C2B-C3B	-2.78	103.22	106.43
3	M	188	PEB	C1B-C2B-C3B	-2.78	103.22	106.43
3	S	186	PEB	CAB-CBB-CGB	-2.78	107.37	112.78
3	D	167	PEB	CHA-C1B-NB	-2.78	119.70	124.89
3	X	187	PEB	CHB-C4B-NB	-2.78	123.79	128.71
3	W	186	PEB	OD-C4D-C3D	-2.77	123.15	130.06
3	G	167	PEB	CHB-C4B-NB	-2.77	123.81	128.71
3	K	167	PEB	CBC-CAC-C2C	-2.77	107.63	112.49
3	A	167	PEB	CHB-C4B-NB	-2.76	123.82	128.71
3	K	166	PEB	C4B-C3B-C2B	-2.76	103.80	106.80
3	O	186	PEB	C1B-C2B-C3B	-2.76	103.25	106.43
3	D	167	PEB	OD-C4D-C3D	-2.75	123.20	130.06
3	G	166	PEB	OD-C4D-C3D	-2.75	123.20	130.06
3	I	166	PEB	OD-C4D-ND	-2.75	121.26	126.06
3	A	167	PEB	C4B-C3B-C2B	-2.75	103.81	106.80
3	F	167	PEB	C4B-C3B-C2B	-2.74	103.82	106.80
3	T	186	PEB	OD-C4D-C3D	-2.74	123.24	130.06
3	S	187	PEB	CHB-C4B-NB	-2.74	123.86	128.71
3	R	188	PEB	OD-C4D-C3D	-2.73	123.26	130.06
3	S	187	PEB	C1B-C2B-C3B	-2.73	103.28	106.43
3	R	187	PEB	CHB-C4B-NB	-2.73	123.88	128.71
3	X	188	PEB	OD-C4D-C3D	-2.72	123.28	130.06
3	E	166	PEB	C1B-C2B-C3B	-2.72	103.30	106.43
3	I	167	PEB	OD-C4D-C3D	-2.71	123.30	130.06
3	D	166	PEB	CMA-C2A-C1A	-2.70	106.60	112.39
3	U	188	PEB	C1B-C2B-C3B	-2.70	103.31	106.43
3	R	187	PEB	CAA-C3A-C2A	-2.70	107.44	114.17
3	P	187	PEB	OD-C4D-C3D	-2.70	123.34	130.06
3	C	166	PEB	CHB-C4B-NB	-2.69	123.94	128.71
3	T	188	PEB	C1B-C2B-C3B	-2.69	103.32	106.43

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	188	PEB	C1B-C2B-C3B	-2.69	103.33	106.43
3	F	166	PEB	CBA-CAA-C3A	-2.69	106.77	113.43
3	X	188	PEB	C1B-C2B-C3B	-2.69	103.33	106.43
3	C	166	PEB	CBA-CAA-C3A	-2.68	106.79	113.43
3	H	167	PEB	CHA-C1B-NB	-2.68	119.88	124.89
3	H	167	PEB	C1B-C2B-C3B	-2.68	103.33	106.43
3	K	167	PEB	CHA-C1B-NB	-2.67	119.90	124.89
3	L	166	PEB	C4B-C3B-C2B	-2.67	103.89	106.80
3	U	188	PEB	C4B-C3B-C2B	-2.67	103.89	106.80
3	R	187	PEB	C1B-C2B-C3B	-2.67	103.35	106.43
3	J	166	PEB	C1B-C2B-C3B	-2.66	103.36	106.43
3	C	166	PEB	C1B-C2B-C3B	-2.66	103.36	106.43
3	B	167	PEB	CBC-CAC-C2C	-2.66	107.81	112.49
3	E	166	PEB	C4B-C3B-C2B	-2.65	103.92	106.80
3	S	188	PEB	CBC-CAC-C2C	-2.65	107.84	112.49
3	H	166	PEB	CMA-C2A-C1A	-2.64	106.73	112.39
3	B	167	PEB	C1B-C2B-C3B	-2.64	103.38	106.43
3	B	166	PEB	C4B-C3B-C2B	-2.64	103.93	106.80
3	U	188	PEB	CHA-C1B-NB	-2.62	120.00	124.89
3	P	187	PEB	CHB-C4B-NB	-2.62	124.08	128.71
3	X	188	PEB	C4B-C3B-C2B	-2.61	103.96	106.80
3	R	186	PEB	OD-C4D-C3D	-2.61	123.56	130.06
3	O	188	PEB	CHA-C1B-NB	-2.60	120.03	124.89
3	O	187	PEB	CAB-CBB-CGB	-2.60	107.72	112.78
3	B	166	PEB	OD-C4D-C3D	-2.60	123.59	130.06
3	C	167	PEB	C1B-C2B-C3B	-2.59	103.44	106.43
3	V	187	PEB	CHA-C1B-NB	-2.59	120.06	124.89
3	M	188	PEB	C4B-C3B-C2B	-2.59	103.99	106.80
3	R	188	PEB	C1B-C2B-C3B	-2.58	103.45	106.43
3	M	187	PEB	CHB-C4B-NB	-2.58	124.14	128.71
3	W	188	PEB	CHB-C4B-NB	-2.58	124.14	128.71
3	T	186	PEB	CHB-C4B-NB	-2.57	124.15	128.71
3	G	166	PEB	OD-C4D-ND	-2.57	121.57	126.06
3	U	187	PEB	CAB-CBB-CGB	-2.57	107.78	112.78
3	V	187	PEB	CHB-C4B-NB	-2.57	124.17	128.71
3	Q	187	PEB	C1B-C2B-C3B	-2.56	103.47	106.43
3	P	186	PEB	C1B-C2B-C3B	-2.56	103.47	106.43
3	H	167	PEB	OD-C4D-C3D	-2.56	123.68	130.06
3	O	187	PEB	CHA-C1B-NB	-2.56	120.11	124.89
3	A	167	PEB	OD-C4D-C3D	-2.56	123.68	130.06
3	T	187	PEB	CHB-C4B-NB	-2.56	124.18	128.71
3	A	167	PEB	OD-C4D-ND	-2.55	121.61	126.06

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	167	PEB	CHA-C1B-NB	-2.55	120.12	124.89
3	U	187	PEB	CHB-C4B-NB	-2.55	124.20	128.71
3	V	187	PEB	CAB-CBB-CGB	-2.55	107.83	112.78
3	A	167	PEB	CHA-C1B-NB	-2.54	120.15	124.89
3	U	188	PEB	CAC-CBC-CGC	-2.54	107.84	112.78
3	L	167	PEB	C1B-C2B-C3B	-2.54	103.50	106.43
3	N	186	PEB	C1B-C2B-C3B	-2.53	103.51	106.43
3	F	166	PEB	OD-C4D-ND	-2.53	121.64	126.06
3	B	166	PEB	C1B-C2B-C3B	-2.53	103.51	106.43
3	E	167	PEB	OD-C4D-C3D	-2.51	123.80	130.06
3	D	166	PEB	OD-C4D-C3D	-2.51	123.80	130.06
3	P	188	PEB	OD-C4D-C3D	-2.51	123.80	130.06
3	T	187	PEB	C1B-C2B-C3B	-2.51	103.54	106.43
3	X	188	PEB	CHB-C4B-NB	-2.50	124.29	128.71
3	M	188	PEB	CHA-C1B-NB	-2.50	120.22	124.89
3	J	166	PEB	C4B-C3B-C2B	-2.49	104.09	106.80
3	V	186	PEB	CBA-CAA-C3A	-2.49	107.26	113.43
3	H	167	PEB	OD-C4D-ND	-2.49	121.71	126.06
3	B	167	PEB	CHA-C1B-NB	-2.49	120.24	124.89
3	M	188	PEB	CHB-C4B-NB	-2.49	124.30	128.71
3	P	186	PEB	C4B-C3B-C2B	-2.49	104.09	106.80
3	W	188	PEB	C1B-C2B-C3B	-2.48	103.57	106.43
3	L	166	PEB	OD-C4D-ND	-2.48	121.73	126.06
3	P	188	PEB	OD-C4D-ND	-2.48	121.74	126.06
3	M	186	PEB	C1B-C2B-C3B	-2.48	103.57	106.43
3	L	167	PEB	OD-C4D-C3D	-2.47	123.90	130.06
3	G	166	PEB	C4B-C3B-C2B	-2.47	104.12	106.80
3	H	166	PEB	C1B-C2B-C3B	-2.46	103.59	106.43
3	S	186	PEB	C4B-C3B-C2B	-2.46	104.12	106.80
3	C	166	PEB	CAC-CBC-CGC	-2.46	108.00	112.78
3	S	186	PEB	CHB-C4B-NB	-2.45	124.36	128.71
3	N	188	PEB	C1B-C2B-C3B	-2.45	103.60	106.43
3	P	187	PEB	CAA-C3A-C2A	-2.45	108.06	114.17
3	W	186	PEB	OD-C4D-ND	-2.45	121.79	126.06
3	L	166	PEB	OD-C4D-C3D	-2.45	123.96	130.06
3	E	166	PEB	CMA-C2A-C1A	-2.44	107.16	112.39
3	N	187	PEB	CHB-C4B-NB	-2.44	124.38	128.71
3	J	167	PEB	C4B-C3B-C2B	-2.44	104.14	106.80
3	O	188	PEB	C1B-C2B-C3B	-2.44	103.62	106.43
3	W	188	PEB	CHA-C1B-NB	-2.44	120.34	124.89
3	W	188	PEB	CBC-CAC-C2C	-2.44	108.21	112.49
3	W	186	PEB	C1B-C2B-C3B	-2.43	103.62	106.43

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	166	PEB	CHB-C4B-NB	-2.43	124.40	128.71
3	V	187	PEB	C1B-C2B-C3B	-2.43	103.63	106.43
3	I	166	PEB	OD-C4D-C3D	-2.43	124.01	130.06
3	Q	188	PEB	CHB-C4B-NB	-2.43	124.41	128.71
3	E	167	PEB	CHA-C1B-NB	-2.40	120.41	124.89
3	P	186	PEB	CAC-CBC-CGC	-2.40	108.12	112.78
3	O	187	PEB	CHB-C4B-NB	-2.39	124.48	128.71
3	A	167	PEB	CBC-CAC-C2C	-2.39	108.30	112.49
3	R	186	PEB	CHB-C4B-NB	-2.39	124.48	128.71
3	V	188	PEB	CHA-C1B-NB	-2.38	120.44	124.89
3	Q	188	PEB	C1B-C2B-C3B	-2.38	103.69	106.43
3	M	186	PEB	C4B-C3B-C2B	-2.38	104.21	106.80
3	R	188	PEB	OD-C4D-ND	-2.37	121.92	126.06
3	R	188	PEB	CHA-C1B-NB	-2.37	120.46	124.89
3	W	187	PEB	CHB-C4B-C3B	-2.37	120.09	125.48
3	D	167	PEB	OD-C4D-ND	-2.36	121.94	126.06
3	O	187	PEB	C1B-C2B-C3B	-2.36	103.70	106.43
3	X	186	PEB	C4B-C3B-C2B	-2.36	104.23	106.80
3	P	187	PEB	CAC-CBC-CGC	-2.36	108.19	112.78
3	S	186	PEB	C1B-C2B-C3B	-2.36	103.71	106.43
3	D	166	PEB	OD-C4D-ND	-2.34	121.97	126.06
3	N	188	PEB	CBD-CAD-C3D	-2.34	115.20	127.70
3	M	187	PEB	OD-C4D-ND	-2.34	121.98	126.06
3	D	166	PEB	CAC-CBC-CGC	-2.33	108.26	112.78
3	P	186	PEB	CHB-C4B-NB	-2.32	124.59	128.71
3	J	166	PEB	CAC-CBC-CGC	-2.32	108.26	112.78
3	D	166	PEB	C4B-C3B-C2B	-2.32	104.28	106.80
3	C	167	PEB	CAB-CBB-CGB	-2.32	108.28	112.78
3	E	167	PEB	OD-C4D-ND	-2.32	122.02	126.06
3	B	166	PEB	OD-C4D-ND	-2.31	122.02	126.06
3	D	166	PEB	CBA-CAA-C3A	-2.31	107.70	113.43
3	M	186	PEB	CAB-CBB-CGB	-2.31	108.28	112.78
3	M	186	PEB	CHB-C4B-NB	-2.31	124.61	128.71
3	U	187	PEB	C1B-C2B-C3B	-2.31	103.77	106.43
3	Q	187	PEB	CAC-CBC-CGC	-2.31	108.30	112.78
3	O	186	PEB	OD-C4D-ND	-2.30	122.04	126.06
3	X	186	PEB	CAB-CBB-CGB	-2.30	108.31	112.78
3	X	187	PEB	C1B-C2B-C3B	-2.29	103.79	106.43
3	V	186	PEB	CHB-C4B-NB	-2.28	124.67	128.71
3	O	186	PEB	CBA-CAA-C3A	-2.28	107.78	113.43
3	V	186	PEB	OD-C4D-ND	-2.27	122.09	126.06
3	T	186	PEB	OD-C4D-ND	-2.27	122.10	126.06

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	166	PEB	OD-C4D-ND	-2.26	122.11	126.06
3	E	167	PEB	CAB-CBB-CGB	-2.26	108.38	112.78
3	F	167	PEB	OD-C4D-ND	-2.25	122.13	126.06
3	P	187	PEB	C1B-C2B-C3B	-2.25	103.84	106.43
3	S	187	PEB	OD-C4D-ND	-2.24	122.15	126.06
3	T	186	PEB	C4B-C3B-C2B	-2.24	104.36	106.80
3	H	166	PEB	OD-C4D-ND	-2.24	122.15	126.06
3	X	188	PEB	CHA-C1B-NB	-2.24	120.71	124.89
3	P	186	PEB	CBC-CAC-C2C	-2.24	108.56	112.49
3	W	187	PEB	CAA-C3A-C2A	-2.23	108.61	114.17
3	I	166	PEB	C4B-C3B-C2B	-2.23	104.38	106.80
3	V	188	PEB	CBD-CAD-C3D	-2.22	115.85	127.70
3	O	188	PEB	CBC-CAC-C2C	-2.22	108.59	112.49
3	O	186	PEB	CHB-C4B-NB	-2.22	124.78	128.71
3	U	186	PEB	OD-C4D-ND	-2.21	122.20	126.06
3	V	186	PEB	CAB-CBB-CGB	-2.21	108.49	112.78
3	A	166	PEB	CMA-C2A-C1A	-2.21	107.67	112.39
3	E	166	PEB	CAC-CBC-CGC	-2.20	108.51	112.78
3	L	166	PEB	CBA-CAA-C3A	-2.20	108.00	113.43
3	O	188	PEB	CBD-CAD-C3D	-2.19	115.98	127.70
3	V	187	PEB	OD-C4D-C3D	-2.19	124.60	130.06
3	V	188	PEB	C1B-C2B-C3B	-2.18	103.91	106.43
3	L	167	PEB	CBC-CAC-C2C	-2.17	108.68	112.49
3	M	186	PEB	OD-C4D-ND	-2.17	122.28	126.06
3	J	167	PEB	OD-C4D-ND	-2.16	122.30	126.06
3	I	167	PEB	OD-C4D-ND	-2.15	122.30	126.06
3	H	167	PEB	CAC-CBC-CGC	-2.14	108.62	112.78
3	Q	186	PEB	OD-C4D-ND	-2.14	122.33	126.06
3	S	188	PEB	CBD-CAD-C3D	-2.13	116.33	127.70
3	R	186	PEB	C4B-C3B-C2B	-2.12	104.49	106.80
3	G	167	PEB	CAB-CBB-CGB	-2.12	108.65	112.78
3	T	188	PEB	OD-C4D-ND	-2.12	122.36	126.06
3	W	188	PEB	OD-C4D-ND	-2.12	122.36	126.06
3	B	166	PEB	CAC-CBC-CGC	-2.12	108.66	112.78
3	W	187	PEB	C1B-C2B-C3B	-2.12	103.99	106.43
3	M	188	PEB	CBD-CAD-C3D	-2.12	116.40	127.70
3	R	186	PEB	OD-C4D-ND	-2.11	122.37	126.06
3	M	188	PEB	OD-C4D-ND	-2.11	122.37	126.06
3	V	187	PEB	CMA-C2A-C1A	-2.10	107.89	112.39
3	N	188	PEB	CHA-C1B-NB	-2.09	120.98	124.89
3	M	188	PEB	CAC-CBC-CGC	-2.09	108.71	112.78
3	N	187	PEB	C1B-C2B-C3B	-2.09	104.02	106.43

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	166	PEB	OD-C4D-C3D	-2.09	124.85	130.06
3	T	187	PEB	CAB-CBB-CGB	-2.09	108.72	112.78
3	C	166	PEB	OD-C4D-ND	-2.09	122.42	126.06
3	W	186	PEB	CHB-C4B-C3B	-2.09	120.73	125.48
3	X	186	PEB	OD-C4D-ND	-2.07	122.44	126.06
3	X	187	PEB	OD-C4D-ND	-2.07	122.44	126.06
3	C	166	PEB	CMA-C2A-C1A	-2.07	107.96	112.39
3	S	187	PEB	CAA-C3A-C2A	-2.06	109.02	114.17
3	K	166	PEB	CMA-C2A-C1A	-2.06	107.99	112.39
3	P	187	PEB	OD-C4D-ND	-2.06	122.47	126.06
3	V	186	PEB	C4B-C3B-C2B	-2.05	104.57	106.80
3	X	188	PEB	CBD-CAD-C3D	-2.05	116.76	127.70
3	U	187	PEB	OD-C4D-ND	-2.05	122.49	126.06
3	I	166	PEB	CBA-CAA-C3A	-2.04	108.37	113.43
3	N	187	PEB	CAA-C3A-C2A	-2.04	109.07	114.17
3	X	187	PEB	CAA-C3A-C2A	-2.04	109.07	114.17
3	S	188	PEB	CHA-C1B-NB	-2.04	121.08	124.89
3	T	187	PEB	OD-C4D-ND	-2.04	122.50	126.06
3	S	188	PEB	CAC-CBC-CGC	-2.02	108.85	112.78
3	X	188	PEB	OD-C4D-ND	-2.01	122.55	126.06
3	O	187	PEB	CHB-C4B-C3B	-2.01	120.90	125.48
3	U	188	PEB	CBD-CAD-C3D	-2.01	116.98	127.70
3	A	166	PEB	CBA-CAA-C3A	-2.01	108.47	113.43
3	E	166	PEB	CMC-C3C-C4C	2.00	129.18	127.13
3	H	166	PEB	C2A-C1A-NA	2.01	110.30	108.31
3	P	188	PEB	CAB-C3B-C4B	2.01	128.53	125.00
3	K	167	PEB	CAB-C3B-C4B	2.02	128.54	125.00
3	S	186	PEB	CAD-C3D-C4D	2.03	129.43	123.58
3	I	166	PEB	C2A-C1A-NA	2.03	110.32	108.31
3	R	186	PEB	C3B-C4B-NB	2.05	113.11	109.98
3	P	186	PEB	CAB-C3B-C4B	2.06	128.61	125.00
3	T	187	PEB	OA-C1A-NA	2.06	127.36	124.84
3	T	188	PEB	CAB-C3B-C4B	2.07	128.62	125.00
3	U	187	PEB	CAD-C3D-C4D	2.07	129.53	123.58
3	G	166	PEB	OA-C1A-NA	2.07	127.37	124.84
3	X	188	PEB	CAB-C3B-C4B	2.07	128.64	125.00
3	S	186	PEB	C3B-C4B-NB	2.08	113.14	109.98
3	B	167	PEB	CAD-C3D-C4D	2.08	129.56	123.58
3	B	167	PEB	CAB-C3B-C4B	2.08	128.66	125.00
3	R	188	PEB	CAB-C3B-C4B	2.09	128.66	125.00
3	F	166	PEB	CAD-C3D-C4D	2.10	129.62	123.58
3	O	186	PEB	C3A-C4A-NA	2.11	109.97	107.94

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	187	PEB	CMB-C2B-C1B	2.11	128.43	125.06
3	C	166	PEB	CAD-C3D-C4D	2.11	129.65	123.58
3	O	186	PEB	C3B-C4B-NB	2.12	113.21	109.98
3	E	166	PEB	C2A-C1A-NA	2.12	110.41	108.31
3	V	186	PEB	C3A-C4A-NA	2.16	110.02	107.94
3	X	188	PEB	C3B-C4B-NB	2.16	113.28	109.98
3	D	166	PEB	C3B-C4B-NB	2.17	113.28	109.98
3	M	186	PEB	C3B-C4B-NB	2.17	113.29	109.98
3	R	187	PEB	CAD-C3D-C4D	2.17	129.84	123.58
3	T	187	PEB	CAB-C3B-C4B	2.18	128.82	125.00
3	T	187	PEB	C3A-C4A-NA	2.19	110.04	107.94
3	F	167	PEB	C3B-C4B-NB	2.19	113.32	109.98
3	B	166	PEB	C3A-C4A-NA	2.19	110.05	107.94
3	G	167	PEB	C3A-C4A-NA	2.21	110.07	107.94
3	E	167	PEB	CAB-C3B-C4B	2.21	128.88	125.00
3	E	166	PEB	C3A-C4A-NA	2.22	110.08	107.94
3	W	186	PEB	C3A-C4A-NA	2.22	110.08	107.94
3	S	187	PEB	CMC-C3C-C4C	2.23	129.41	127.13
3	K	166	PEB	C3A-C4A-NA	2.24	110.09	107.94
3	M	186	PEB	C3A-C4A-NA	2.25	110.10	107.94
3	P	186	PEB	C3B-C4B-NB	2.25	113.41	109.98
3	Q	187	PEB	C3B-C4B-NB	2.25	113.41	109.98
3	R	188	PEB	CAD-C3D-C4D	2.25	130.07	123.58
3	K	166	PEB	CMC-C3C-C4C	2.25	129.43	127.13
3	U	188	PEB	CAD-C3D-C4D	2.26	130.08	123.58
3	C	166	PEB	C2A-C1A-NA	2.26	110.54	108.31
3	T	188	PEB	C3B-C4B-NB	2.26	113.42	109.98
3	K	167	PEB	CAD-C3D-C4D	2.26	130.10	123.58
3	P	186	PEB	CAD-C3D-C4D	2.27	130.13	123.58
3	W	188	PEB	CAD-C3D-C4D	2.28	130.13	123.58
3	E	166	PEB	C3B-C4B-NB	2.28	113.45	109.98
3	U	188	PEB	C3B-C4B-NB	2.30	113.49	109.98
3	M	188	PEB	C3B-C4B-NB	2.30	113.50	109.98
3	V	186	PEB	CAD-C3D-C4D	2.32	130.25	123.58
3	M	188	PEB	CAD-C3D-C4D	2.32	130.26	123.58
3	P	188	PEB	CAD-C3D-C4D	2.32	130.27	123.58
3	S	188	PEB	CAB-C3B-C4B	2.32	129.07	125.00
3	Q	187	PEB	C2A-C1A-NA	2.34	110.62	108.31
3	S	187	PEB	C2A-C1A-NA	2.34	110.62	108.31
3	B	166	PEB	C3B-C4B-NB	2.34	113.55	109.98
3	O	186	PEB	CAD-C3D-C4D	2.35	130.36	123.58
3	T	186	PEB	C3B-C4B-NB	2.35	113.57	109.98

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	188	PEB	C3B-C4B-NB	2.36	113.58	109.98
3	P	186	PEB	CHA-C1B-C2B	2.37	130.37	124.71
3	O	188	PEB	C3B-C4B-NB	2.37	113.60	109.98
3	N	186	PEB	CAD-C3D-C4D	2.38	130.43	123.58
3	B	167	PEB	C3A-C4A-NA	2.38	110.23	107.94
3	P	187	PEB	CAD-C3D-C4D	2.38	130.44	123.58
3	A	166	PEB	OA-C1A-NA	2.38	127.76	124.84
3	T	187	PEB	CAD-C3D-C4D	2.39	130.46	123.58
3	U	188	PEB	CAB-C3B-C4B	2.39	129.19	125.00
3	A	166	PEB	C3A-C4A-NA	2.40	110.24	107.94
3	H	166	PEB	OA-C1A-NA	2.40	127.78	124.84
3	E	166	PEB	OA-C1A-NA	2.40	127.78	124.84
3	V	187	PEB	C2A-C1A-NA	2.40	110.68	108.31
3	X	186	PEB	C3B-C4B-NB	2.40	113.64	109.98
3	O	188	PEB	CMC-C3C-C4C	2.41	129.59	127.13
3	Q	187	PEB	CMC-C3C-C4C	2.41	129.60	127.13
3	D	167	PEB	C3A-C4A-NA	2.42	110.26	107.94
3	X	188	PEB	CAD-C3D-C4D	2.42	130.55	123.58
3	N	187	PEB	CAD-C3D-C4D	2.42	130.55	123.58
3	R	188	PEB	CMB-C2B-C1B	2.42	128.93	125.06
3	G	167	PEB	CAD-C3D-C4D	2.43	130.57	123.58
3	V	186	PEB	C3B-C4B-NB	2.45	113.71	109.98
3	H	167	PEB	C2A-C1A-NA	2.45	110.73	108.31
3	H	167	PEB	CAB-C3B-C4B	2.45	129.30	125.00
3	T	188	PEB	CAD-C3D-C4D	2.46	130.66	123.58
3	C	166	PEB	C3A-C4A-NA	2.46	110.31	107.94
3	U	187	PEB	CMB-C2B-C1B	2.46	129.00	125.06
3	Q	186	PEB	CAD-C3D-C4D	2.46	130.68	123.58
3	H	166	PEB	CAD-C3D-C4D	2.47	130.69	123.58
3	F	167	PEB	CMB-C2B-C1B	2.47	129.01	125.06
3	D	166	PEB	C3A-C4A-NA	2.48	110.32	107.94
3	W	188	PEB	CMB-C2B-C1B	2.48	129.03	125.06
3	Q	188	PEB	CAD-C3D-C4D	2.48	130.73	123.58
3	A	167	PEB	C3A-C4A-NA	2.48	110.33	107.94
3	R	188	PEB	C3B-C4B-NB	2.48	113.77	109.98
3	R	186	PEB	CAD-C3D-C4D	2.49	130.74	123.58
3	A	167	PEB	C3B-C4B-NB	2.49	113.78	109.98
3	M	187	PEB	C3A-C4A-NA	2.49	110.33	107.94
3	U	186	PEB	C3A-C4A-NA	2.49	110.34	107.94
3	T	188	PEB	C2A-C1A-NA	2.50	110.78	108.31
3	I	167	PEB	CAB-C3B-C4B	2.50	129.39	125.00
3	H	166	PEB	C3A-C4A-NA	2.51	110.35	107.94

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	166	PEB	C2A-C1A-NA	2.51	110.79	108.31
3	A	166	PEB	CAD-C3D-C4D	2.51	130.81	123.58
3	N	187	PEB	C3A-C4A-NA	2.51	110.36	107.94
3	B	166	PEB	CAD-C3D-C4D	2.51	130.82	123.58
3	W	186	PEB	CHA-C1B-C2B	2.52	130.73	124.71
3	U	187	PEB	C3B-C4B-NB	2.53	113.83	109.98
3	L	167	PEB	C3A-C4A-NA	2.53	110.37	107.94
3	K	167	PEB	C3A-C4A-NA	2.53	110.37	107.94
3	R	186	PEB	CHA-C1B-C2B	2.54	130.77	124.71
3	G	167	PEB	C3B-C4B-NB	2.54	113.85	109.98
3	O	187	PEB	C3A-C4A-NA	2.54	110.38	107.94
3	E	167	PEB	C3B-C4B-NB	2.54	113.85	109.98
3	S	188	PEB	C3B-C4B-NB	2.54	113.85	109.98
3	H	167	PEB	CAD-C3D-C4D	2.54	130.90	123.58
3	K	166	PEB	CAD-C3D-C4D	2.54	130.90	123.58
3	S	187	PEB	CAD-C3D-C4D	2.55	130.92	123.58
3	F	166	PEB	C3A-C4A-NA	2.56	110.40	107.94
3	R	187	PEB	C2A-C1A-NA	2.56	110.84	108.31
3	S	188	PEB	C3A-C4A-NA	2.56	110.40	107.94
3	X	187	PEB	CAD-C3D-C4D	2.56	130.97	123.58
3	S	188	PEB	CMB-C2B-C1B	2.57	129.17	125.06
3	W	186	PEB	CAD-C3D-C4D	2.57	130.98	123.58
3	N	186	PEB	C3B-C4B-NB	2.57	113.90	109.98
3	D	166	PEB	CAD-C3D-C4D	2.58	131.00	123.58
3	N	187	PEB	C2A-C1A-NA	2.58	110.86	108.31
3	V	187	PEB	C3B-C4B-NB	2.58	113.91	109.98
3	F	167	PEB	CAD-C3D-C4D	2.59	131.03	123.58
3	V	188	PEB	CAB-C3B-C4B	2.59	129.54	125.00
3	B	166	PEB	C2A-C1A-NA	2.60	110.88	108.31
3	X	187	PEB	C3A-C4A-NA	2.60	110.44	107.94
3	E	166	PEB	CAD-C3D-C4D	2.60	131.07	123.58
3	T	186	PEB	CHA-C1B-C2B	2.60	130.93	124.71
3	U	186	PEB	CAD-C3D-C4D	2.60	131.08	123.58
3	H	167	PEB	C3B-C4B-NB	2.61	113.96	109.98
3	J	167	PEB	C3B-C4B-NB	2.61	113.96	109.98
3	W	187	PEB	CAD-C3D-C4D	2.61	131.11	123.58
3	P	187	PEB	CMB-C2B-C1B	2.62	129.26	125.06
3	L	166	PEB	CAD-C3D-C4D	2.62	131.14	123.58
3	L	166	PEB	C3B-C4B-NB	2.63	113.99	109.98
3	Q	186	PEB	CHA-C1B-C2B	2.63	131.00	124.71
3	S	187	PEB	C3B-C4B-NB	2.63	113.99	109.98
3	J	166	PEB	C2A-C1A-NA	2.63	110.91	108.31

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	W	188	PEB	C3B-C4B-NB	2.63	114.00	109.98
3	V	186	PEB	CHA-C1B-C2B	2.63	131.01	124.71
3	O	186	PEB	CHA-C1B-C2B	2.63	131.01	124.71
3	T	187	PEB	C3B-C4B-NB	2.65	114.02	109.98
3	S	187	PEB	C3A-C4A-NA	2.65	110.48	107.94
3	H	167	PEB	C3A-C4A-NA	2.65	110.49	107.94
3	F	166	PEB	OA-C1A-NA	2.66	128.10	124.84
3	P	187	PEB	C3B-C4B-NB	2.67	114.06	109.98
3	W	186	PEB	C3B-C4B-NB	2.67	114.06	109.98
3	N	186	PEB	CHA-C1B-C2B	2.68	131.11	124.71
3	E	167	PEB	CMB-C2B-C1B	2.68	129.34	125.06
3	S	188	PEB	CMC-C3C-C4C	2.68	129.87	127.13
3	F	167	PEB	C3A-C4A-NA	2.68	110.52	107.94
3	T	186	PEB	CAD-C3D-C4D	2.68	131.30	123.58
3	C	166	PEB	OA-C1A-NA	2.68	128.13	124.84
3	O	188	PEB	CAB-C3B-C4B	2.69	129.71	125.00
3	K	167	PEB	C2A-C1A-NA	2.70	110.97	108.31
3	N	186	PEB	C2A-C1A-NA	2.70	110.98	108.31
3	E	167	PEB	C3A-C4A-NA	2.71	110.54	107.94
3	C	167	PEB	CAD-C3D-C4D	2.72	131.40	123.58
3	W	187	PEB	C3A-C4A-NA	2.72	110.56	107.94
3	D	166	PEB	OA-C1A-NA	2.73	128.18	124.84
3	D	167	PEB	C3B-C4B-NB	2.73	114.14	109.98
3	V	187	PEB	CMB-C2B-C1B	2.73	129.42	125.06
3	R	186	PEB	C3A-C4A-NA	2.73	110.56	107.94
3	G	166	PEB	CAD-C3D-C4D	2.73	131.44	123.58
3	G	167	PEB	C2A-C1A-NA	2.73	111.01	108.31
3	W	188	PEB	C2A-C1A-NA	2.74	111.02	108.31
3	Q	188	PEB	C2A-C1A-NA	2.75	111.02	108.31
3	Q	186	PEB	C2A-C1A-NA	2.75	111.03	108.31
3	N	188	PEB	CMC-C3C-C4C	2.75	129.94	127.13
3	X	186	PEB	CHA-C1B-C2B	2.76	131.30	124.71
3	Q	187	PEB	CMB-C2B-C1B	2.76	129.47	125.06
3	X	187	PEB	CMB-C2B-C1B	2.76	129.48	125.06
3	Q	188	PEB	C3B-C4B-NB	2.77	114.21	109.98
3	A	167	PEB	CAD-C3D-C4D	2.77	131.57	123.58
3	W	186	PEB	C2A-C1A-NA	2.78	111.05	108.31
3	N	187	PEB	C3B-C4B-NB	2.78	114.22	109.98
3	V	188	PEB	C3A-C4A-NA	2.78	110.61	107.94
3	U	188	PEB	C3A-C4A-NA	2.78	110.61	107.94
3	M	186	PEB	C2A-C1A-NA	2.79	111.06	108.31
3	H	166	PEB	C3B-C4B-NB	2.79	114.23	109.98

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	187	PEB	CAD-C3D-C4D	2.79	131.61	123.58
3	V	188	PEB	C3B-C4B-NB	2.79	114.23	109.98
3	Q	186	PEB	C3B-C4B-NB	2.80	114.25	109.98
3	D	167	PEB	CAB-C3B-C4B	2.81	129.93	125.00
3	R	187	PEB	C3B-C4B-NB	2.81	114.26	109.98
3	L	167	PEB	C2A-C1A-NA	2.81	111.09	108.31
3	A	166	PEB	C2A-C1A-NA	2.82	111.09	108.31
3	P	188	PEB	C3A-C4A-NA	2.83	110.66	107.94
3	I	166	PEB	OA-C1A-NA	2.83	128.31	124.84
3	W	187	PEB	C2A-C1A-NA	2.84	111.11	108.31
3	O	186	PEB	C2A-C1A-NA	2.84	111.11	108.31
3	V	188	PEB	CMC-C3C-C4C	2.84	130.04	127.13
3	J	166	PEB	OA-C1A-NA	2.85	128.33	124.84
3	U	187	PEB	CMC-C3C-C4C	2.85	130.04	127.13
3	D	167	PEB	CAD-C3D-C4D	2.85	131.80	123.58
3	K	166	PEB	C3B-C4B-NB	2.86	114.33	109.98
3	L	166	PEB	C3A-C4A-NA	2.87	110.70	107.94
3	X	187	PEB	C3B-C4B-NB	2.87	114.36	109.98
3	V	188	PEB	C2A-C1A-NA	2.87	111.14	108.31
3	P	186	PEB	C2A-C1A-NA	2.88	111.16	108.31
3	J	167	PEB	C2A-C1A-NA	2.88	111.16	108.31
3	A	166	PEB	C3B-C4B-NB	2.89	114.38	109.98
3	C	166	PEB	C3B-C4B-NB	2.89	114.39	109.98
3	J	166	PEB	CHA-C1B-C2B	2.90	131.63	124.71
3	U	188	PEB	CMB-C2B-C1B	2.90	129.70	125.06
3	S	186	PEB	CHA-C1B-C2B	2.91	131.66	124.71
3	P	187	PEB	C3A-C4A-NA	2.93	110.75	107.94
3	X	186	PEB	C3A-C4A-NA	2.93	110.75	107.94
3	I	166	PEB	CAD-C3D-C4D	2.93	132.03	123.58
3	T	188	PEB	C3A-C4A-NA	2.95	110.77	107.94
3	L	167	PEB	C3B-C4B-NB	2.95	114.48	109.98
3	W	188	PEB	C3A-C4A-NA	2.95	110.78	107.94
3	W	187	PEB	CMB-C2B-C1B	2.95	129.78	125.06
3	U	188	PEB	C2A-C1A-NA	2.96	111.24	108.31
3	B	166	PEB	OA-C1A-NA	2.96	128.47	124.84
3	C	167	PEB	C3A-C4A-NA	2.96	110.79	107.94
3	M	187	PEB	C2A-C1A-NA	2.97	111.24	108.31
3	C	167	PEB	C2A-C1A-NA	2.97	111.25	108.31
3	M	186	PEB	CAD-C3D-C4D	2.97	132.14	123.58
3	E	167	PEB	CAD-C3D-C4D	2.98	132.16	123.58
3	I	167	PEB	CMB-C2B-C1B	2.99	129.84	125.06
3	A	167	PEB	CMB-C2B-C1B	3.00	129.85	125.06

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	167	PEB	CMB-C2B-C1B	3.00	129.85	125.06
3	P	187	PEB	CMC-C3C-C4C	3.00	130.19	127.13
3	M	188	PEB	C2A-C1A-NA	3.00	111.27	108.31
3	Q	188	PEB	CMB-C2B-C1B	3.00	129.86	125.06
3	G	166	PEB	C3B-C4B-NB	3.01	114.57	109.98
3	P	186	PEB	C3A-C4A-NA	3.01	110.83	107.94
3	U	186	PEB	CHA-C1B-C2B	3.02	131.92	124.71
3	I	167	PEB	CAD-C3D-C4D	3.02	132.26	123.58
3	L	167	PEB	CAD-C3D-C4D	3.02	132.27	123.58
3	T	188	PEB	CMB-C2B-C1B	3.02	129.89	125.06
3	B	167	PEB	C2A-C1A-NA	3.03	111.30	108.31
3	J	167	PEB	CAD-C3D-C4D	3.03	132.30	123.58
3	M	186	PEB	CHA-C1B-C2B	3.03	131.96	124.71
3	B	167	PEB	C3B-C4B-NB	3.04	114.61	109.98
3	C	167	PEB	C3B-C4B-NB	3.04	114.61	109.98
3	K	166	PEB	C2A-C1A-NA	3.04	111.31	108.31
3	G	166	PEB	C3A-C4A-NA	3.04	110.86	107.94
3	O	187	PEB	C3B-C4B-NB	3.04	114.62	109.98
3	K	167	PEB	C3B-C4B-NB	3.04	114.62	109.98
3	L	167	PEB	CMB-C2B-C1B	3.05	129.94	125.06
3	X	186	PEB	C2A-C1A-NA	3.06	111.34	108.31
3	M	188	PEB	C3A-C4A-NA	3.07	110.89	107.94
3	U	187	PEB	C3A-C4A-NA	3.07	110.89	107.94
3	X	187	PEB	C2A-C1A-NA	3.07	111.34	108.31
3	P	188	PEB	CMB-C2B-C1B	3.08	129.98	125.06
3	P	188	PEB	C2A-C1A-NA	3.08	111.35	108.31
3	M	187	PEB	CAD-C3D-C4D	3.09	132.47	123.58
3	V	188	PEB	CMB-C2B-C1B	3.09	130.00	125.06
3	W	187	PEB	C3B-C4B-NB	3.09	114.69	109.98
3	I	167	PEB	C3B-C4B-NB	3.09	114.70	109.98
3	U	186	PEB	C2A-C1A-NA	3.10	111.37	108.31
3	N	188	PEB	C3B-C4B-NB	3.12	114.73	109.98
3	X	186	PEB	CAD-C3D-C4D	3.12	132.56	123.58
3	M	187	PEB	C3B-C4B-NB	3.13	114.76	109.98
3	D	167	PEB	CMB-C2B-C1B	3.14	130.07	125.06
3	Q	188	PEB	C3A-C4A-NA	3.15	110.97	107.94
3	C	167	PEB	CMB-C2B-C1B	3.15	130.11	125.06
3	R	188	PEB	C2A-C1A-NA	3.16	111.43	108.31
3	C	166	PEB	CHA-C1B-C2B	3.16	132.27	124.71
3	O	187	PEB	CMB-C2B-C1B	3.17	130.14	125.06
3	G	167	PEB	CMB-C2B-C1B	3.18	130.15	125.06
3	I	167	PEB	C3A-C4A-NA	3.20	111.02	107.94

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	167	PEB	CMB-C2B-C1B	3.21	130.19	125.06
3	X	188	PEB	CMB-C2B-C1B	3.21	130.20	125.06
3	K	167	PEB	CMB-C2B-C1B	3.22	130.21	125.06
3	O	188	PEB	C2A-C1A-NA	3.25	111.52	108.31
3	M	187	PEB	CMB-C2B-C1B	3.25	130.26	125.06
3	R	187	PEB	CMB-C2B-C1B	3.26	130.27	125.06
3	O	188	PEB	C3A-C4A-NA	3.26	111.07	107.94
3	J	166	PEB	CMB-C2B-C1B	3.26	130.28	125.06
3	F	166	PEB	C3B-C4B-NB	3.27	114.96	109.98
3	E	167	PEB	C2A-C1A-NA	3.27	111.54	108.31
3	E	166	PEB	CHA-C1B-C2B	3.27	132.53	124.71
3	A	166	PEB	CMB-C2B-C1B	3.28	130.31	125.06
3	X	188	PEB	C2A-C1A-NA	3.30	111.57	108.31
3	R	187	PEB	C3A-C4A-NA	3.30	111.11	107.94
3	A	167	PEB	C2A-C1A-NA	3.33	111.60	108.31
3	T	186	PEB	C3A-C4A-NA	3.33	111.14	107.94
3	S	188	PEB	C2A-C1A-NA	3.36	111.63	108.31
3	R	186	PEB	C2A-C1A-NA	3.37	111.64	108.31
3	F	167	PEB	C2A-C1A-NA	3.38	111.65	108.31
3	A	166	PEB	CHA-C1B-C2B	3.41	132.85	124.71
3	R	188	PEB	C3A-C4A-NA	3.42	111.23	107.94
3	J	167	PEB	C3A-C4A-NA	3.42	111.23	107.94
3	D	166	PEB	CHA-C1B-C2B	3.44	132.94	124.71
3	G	166	PEB	CHA-C1B-C2B	3.45	132.95	124.71
3	S	186	PEB	C2A-C1A-NA	3.46	111.72	108.31
3	V	187	PEB	C3A-C4A-NA	3.47	111.28	107.94
3	V	187	PEB	CAD-C3D-C4D	3.50	133.66	123.58
3	O	188	PEB	CMB-C2B-C1B	3.53	130.71	125.06
3	Q	186	PEB	C3A-C4A-NA	3.53	111.34	107.94
3	V	186	PEB	C2A-C1A-NA	3.55	111.82	108.31
3	T	186	PEB	C2A-C1A-NA	3.59	111.85	108.31
3	N	188	PEB	C3A-C4A-NA	3.59	111.39	107.94
3	M	188	PEB	CMB-C2B-C1B	3.61	130.84	125.06
3	I	167	PEB	C2A-C1A-NA	3.62	111.88	108.31
3	I	166	PEB	CHA-C1B-C2B	3.62	133.36	124.71
3	T	187	PEB	CMB-C2B-C1B	3.63	130.87	125.06
3	H	166	PEB	CHA-C1B-C2B	3.67	133.49	124.71
3	N	188	PEB	C2A-C1A-NA	3.69	111.95	108.31
3	L	166	PEB	CHA-C1B-C2B	3.69	133.53	124.71
3	F	166	PEB	CHA-C1B-C2B	3.72	133.60	124.71
3	D	167	PEB	C2A-C1A-NA	3.78	112.04	108.31
3	B	166	PEB	CMB-C2B-C1B	3.80	131.14	125.06

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	188	PEB	C3A-C4A-NA	3.80	111.60	107.94
3	E	166	PEB	CMB-C2B-C1B	3.82	131.16	125.06
3	B	166	PEB	CHA-C1B-C2B	3.91	134.06	124.71
3	H	167	PEB	CMB-C2B-C1B	3.95	131.38	125.06
3	N	186	PEB	CMB-C2B-C1B	3.97	131.41	125.06
3	S	187	PEB	CMB-C2B-C1B	3.97	131.41	125.06
3	L	166	PEB	CMB-C2B-C1B	3.98	131.43	125.06
3	S	186	PEB	CMB-C2B-C1B	4.02	131.50	125.06
3	W	186	PEB	CMB-C2B-C1B	4.04	131.51	125.06
3	H	166	PEB	CMB-C2B-C1B	4.19	131.76	125.06
3	C	166	PEB	CMB-C2B-C1B	4.22	131.81	125.06
3	M	186	PEB	CMB-C2B-C1B	4.23	131.82	125.06
3	D	166	PEB	CMB-C2B-C1B	4.24	131.84	125.06
3	F	166	PEB	CMB-C2B-C1B	4.34	131.99	125.06
3	I	166	PEB	CMB-C2B-C1B	4.36	132.03	125.06
3	R	186	PEB	CMB-C2B-C1B	4.38	132.06	125.06
3	K	166	PEB	CHA-C1B-C2B	4.43	135.29	124.71
3	P	186	PEB	CMB-C2B-C1B	4.51	132.28	125.06
3	Q	186	PEB	CMB-C2B-C1B	4.59	132.40	125.06
3	G	166	PEB	CMB-C2B-C1B	4.63	132.46	125.06
3	K	166	PEB	CMB-C2B-C1B	4.90	132.89	125.06
3	T	186	PEB	CMB-C2B-C1B	5.00	133.06	125.06
3	X	186	PEB	CMB-C2B-C1B	5.01	133.08	125.06
3	O	186	PEB	CMB-C2B-C1B	5.04	133.12	125.06
3	V	186	PEB	CMB-C2B-C1B	5.15	133.29	125.06
3	U	186	PEB	CMB-C2B-C1B	5.79	134.31	125.06

There are no chirality outliers.

All (120) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	167	PEB	C4A-CHA-C1B-C2B
3	L	167	PEB	C4A-CHA-C1B-C2B
3	K	167	PEB	C4A-CHA-C1B-C2B
3	A	167	PEB	C4A-CHA-C1B-C2B
3	J	167	PEB	C4A-CHA-C1B-C2B
3	X	188	PEB	C4A-CHA-C1B-C2B
3	C	167	PEB	C4A-CHA-C1B-C2B
3	B	167	PEB	C4A-CHA-C1B-C2B
3	D	167	PEB	C4A-CHA-C1B-C2B
3	F	167	PEB	C4A-CHA-C1B-C2B
3	E	167	PEB	C4A-CHA-C1B-C2B

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	R	188	PEB	C4A-CHA-C1B-C2B
3	R	187	PEB	C4A-CHA-C1B-C2B
3	G	167	PEB	C4A-CHA-C1B-C2B
3	N	188	PEB	C4A-CHA-C1B-C2B
3	S	188	PEB	C4A-CHA-C1B-C2B
3	V	187	PEB	C4A-CHA-C1B-C2B
3	P	188	PEB	C4A-CHA-C1B-C2B
3	O	187	PEB	C4A-CHA-C1B-C2B
3	M	188	PEB	C4A-CHA-C1B-C2B
3	U	187	PEB	C4A-CHA-C1B-C2B
3	H	167	PEB	C4A-CHA-C1B-C2B
3	W	188	PEB	C4A-CHA-C1B-C2B
3	U	188	PEB	C4A-CHA-C1B-C2B
3	V	188	PEB	C4A-CHA-C1B-C2B
3	T	187	PEB	C4A-CHA-C1B-C2B
3	T	188	PEB	C4A-CHA-C1B-C2B
3	Q	187	PEB	C4A-CHA-C1B-C2B
3	P	187	PEB	C4A-CHA-C1B-C2B
3	X	187	PEB	C4A-CHA-C1B-C2B
3	M	187	PEB	C4A-CHA-C1B-C2B
3	Q	188	PEB	C4A-CHA-C1B-C2B
3	O	188	PEB	C4A-CHA-C1B-C2B
3	N	187	PEB	C4A-CHA-C1B-C2B
3	W	187	PEB	C4A-CHA-C1B-C2B
3	S	187	PEB	C4A-CHA-C1B-C2B
3	I	167	PEB	C4A-CHA-C1B-NB
3	L	167	PEB	C4A-CHA-C1B-NB
3	J	167	PEB	C4A-CHA-C1B-NB
3	K	167	PEB	C4A-CHA-C1B-NB
3	R	187	PEB	C4A-CHA-C1B-NB
3	A	167	PEB	C4A-CHA-C1B-NB
3	D	167	PEB	C4A-CHA-C1B-NB
3	E	167	PEB	C4A-CHA-C1B-NB
3	C	167	PEB	C4A-CHA-C1B-NB
3	B	167	PEB	C4A-CHA-C1B-NB
3	N	186	PEB	C4A-CHA-C1B-C2B
3	G	167	PEB	C4A-CHA-C1B-NB
3	X	186	PEB	C4A-CHA-C1B-C2B
3	T	186	PEB	C4A-CHA-C1B-C2B
3	O	187	PEB	C4A-CHA-C1B-NB
3	T	187	PEB	C4A-CHA-C1B-NB
3	F	167	PEB	C4A-CHA-C1B-NB

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	R	186	PEB	C4A-CHA-C1B-C2B
3	U	187	PEB	C4A-CHA-C1B-NB
3	M	186	PEB	C4A-CHA-C1B-C2B
3	Q	187	PEB	C4A-CHA-C1B-NB
3	V	187	PEB	C4A-CHA-C1B-NB
3	P	186	PEB	C4A-CHA-C1B-C2B
3	R	188	PEB	C4A-CHA-C1B-NB
3	W	186	PEB	C4A-CHA-C1B-C2B
3	M	187	PEB	C4A-CHA-C1B-NB
3	V	186	PEB	C4A-CHA-C1B-C2B
3	H	167	PEB	C4A-CHA-C1B-NB
3	X	187	PEB	C4A-CHA-C1B-NB
3	N	188	PEB	C4A-CHA-C1B-NB
3	X	188	PEB	C4A-CHA-C1B-NB
3	Q	186	PEB	C4A-CHA-C1B-C2B
3	P	188	PEB	C4A-CHA-C1B-NB
3	P	187	PEB	C4A-CHA-C1B-NB
3	M	188	PEB	C4A-CHA-C1B-NB
3	W	188	PEB	C4A-CHA-C1B-NB
3	S	188	PEB	C4A-CHA-C1B-NB
3	N	187	PEB	C4A-CHA-C1B-NB
3	V	188	PEB	C4A-CHA-C1B-NB
3	O	186	PEB	C4A-CHA-C1B-C2B
3	S	186	PEB	C4A-CHA-C1B-C2B
3	U	188	PEB	C4A-CHA-C1B-NB
3	T	188	PEB	C4A-CHA-C1B-NB
3	Q	188	PEB	C4A-CHA-C1B-NB
3	S	187	PEB	C4A-CHA-C1B-NB
3	W	187	PEB	C4A-CHA-C1B-NB
3	O	188	PEB	C4A-CHA-C1B-NB
3	U	186	PEB	C4A-CHA-C1B-C2B
3	N	186	PEB	C4A-CHA-C1B-NB
3	M	186	PEB	C4A-CHA-C1B-NB
3	T	186	PEB	C4A-CHA-C1B-NB
3	X	186	PEB	C4A-CHA-C1B-NB
3	R	186	PEB	C4A-CHA-C1B-NB
3	V	186	PEB	C4A-CHA-C1B-NB
3	W	186	PEB	C4A-CHA-C1B-NB
3	P	186	PEB	C4A-CHA-C1B-NB
3	I	166	PEB	C4A-CHA-C1B-C2B
3	Q	186	PEB	C4A-CHA-C1B-NB
3	O	186	PEB	C4A-CHA-C1B-NB

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	J	166	PEB	C4A-CHA-C1B-C2B
3	K	166	PEB	C4A-CHA-C1B-C2B
3	B	166	PEB	C4A-CHA-C1B-C2B
3	D	166	PEB	C4A-CHA-C1B-C2B
3	S	186	PEB	C4A-CHA-C1B-NB
3	H	166	PEB	C4A-CHA-C1B-C2B
3	C	166	PEB	C4A-CHA-C1B-C2B
3	U	186	PEB	C4A-CHA-C1B-NB
3	G	166	PEB	C4A-CHA-C1B-C2B
3	G	166	PEB	C4A-CHA-C1B-NB
3	F	166	PEB	C4A-CHA-C1B-C2B
3	J	166	PEB	C4A-CHA-C1B-NB
3	E	166	PEB	C4A-CHA-C1B-C2B
3	I	166	PEB	C4A-CHA-C1B-NB
3	K	166	PEB	C4A-CHA-C1B-NB
3	F	166	PEB	C4A-CHA-C1B-NB
3	B	166	PEB	C4A-CHA-C1B-NB
3	H	166	PEB	C4A-CHA-C1B-NB
3	C	166	PEB	C4A-CHA-C1B-NB
3	E	166	PEB	C4A-CHA-C1B-NB
3	D	166	PEB	C4A-CHA-C1B-NB
3	A	166	PEB	C4A-CHA-C1B-C2B
3	L	166	PEB	C4A-CHA-C1B-C2B
3	A	166	PEB	C4A-CHA-C1B-NB
3	L	166	PEB	C4A-CHA-C1B-NB

There are no ring outliers.

62 monomers are involved in 124 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	166	PEB	2	0
3	B	166	PEB	1	0
3	B	167	PEB	1	0
3	C	166	PEB	3	0
3	C	167	PEB	1	0
3	D	166	PEB	2	0
4	E	1165	GOL	1	0
3	E	166	PEB	3	0
3	E	167	PEB	4	0
3	F	166	PEB	1	0
3	G	166	PEB	2	0
3	G	167	PEB	1	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1165	GOL	1	0
3	H	166	PEB	2	0
3	H	167	PEB	1	0
5	I	1200	SO4	1	0
3	I	166	PEB	2	0
3	I	167	PEB	1	0
3	J	166	PEB	2	0
3	J	167	PEB	2	0
3	K	166	PEB	2	0
3	K	167	PEB	1	0
3	L	166	PEB	1	0
3	L	167	PEB	1	0
3	M	186	PEB	1	0
3	M	187	PEB	3	0
3	M	188	PEB	1	0
3	N	186	PEB	1	0
3	N	187	PEB	2	0
3	N	188	PEB	3	0
3	O	186	PEB	1	0
3	O	187	PEB	3	0
3	O	188	PEB	2	0
3	P	186	PEB	2	0
3	P	187	PEB	3	0
3	P	188	PEB	3	0
5	P	189	SO4	1	0
3	Q	186	PEB	3	0
3	Q	187	PEB	5	0
3	Q	188	PEB	4	0
3	R	186	PEB	1	0
3	R	187	PEB	2	0
3	R	188	PEB	3	0
5	R	189	SO4	1	0
3	S	186	PEB	2	0
3	S	187	PEB	2	0
3	S	188	PEB	3	0
3	T	186	PEB	2	0
3	T	187	PEB	1	0
3	T	188	PEB	5	0
3	U	186	PEB	4	0
3	U	187	PEB	2	0
3	U	188	PEB	3	0
3	V	186	PEB	2	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	V	187	PEB	1	0
3	V	188	PEB	3	0
3	W	186	PEB	1	0
3	W	187	PEB	3	0
3	W	188	PEB	2	0
3	X	186	PEB	2	0
3	X	187	PEB	1	0
3	X	188	PEB	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 ⓘ

### 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	164/164 (100%)	-0.41	0	100	100	8, 13, 20, 27	0
1	B	164/164 (100%)	-0.45	0	100	100	8, 14, 22, 27	0
1	C	164/164 (100%)	-0.45	0	100	100	10, 16, 23, 31	0
1	D	164/164 (100%)	-0.39	0	100	100	8, 14, 24, 30	0
1	E	164/164 (100%)	-0.44	0	100	100	9, 14, 23, 29	0
1	F	164/164 (100%)	-0.40	0	100	100	10, 15, 22, 33	0
1	G	164/164 (100%)	-0.44	0	100	100	9, 14, 21, 29	0
1	H	164/164 (100%)	-0.49	0	100	100	9, 14, 21, 28	0
1	I	164/164 (100%)	-0.38	0	100	100	9, 15, 26, 33	0
1	J	164/164 (100%)	-0.47	0	100	100	11, 15, 23, 29	0
1	K	164/164 (100%)	-0.41	0	100	100	10, 16, 25, 30	0
1	L	164/164 (100%)	-0.37	0	100	100	9, 14, 23, 28	0
2	M	183/184 (99%)	-0.39	4 (2%)	65	71	8, 14, 29, 53	0
2	N	183/184 (99%)	-0.31	3 (1%)	74	79	9, 16, 29, 41	0
2	O	183/184 (99%)	-0.25	3 (1%)	74	79	10, 18, 30, 42	0
2	P	183/184 (99%)	-0.31	2 (1%)	82	86	6, 14, 29, 52	0
2	Q	183/184 (99%)	-0.22	5 (2%)	58	65	9, 17, 30, 47	0
2	R	183/184 (99%)	-0.24	3 (1%)	74	79	12, 19, 34, 54	0
2	S	183/184 (99%)	-0.24	4 (2%)	65	71	10, 16, 30, 55	0
2	T	183/184 (99%)	-0.10	5 (2%)	58	65	13, 21, 36, 49	0
2	U	183/184 (99%)	-0.33	2 (1%)	82	86	8, 14, 28, 42	0
2	V	183/184 (99%)	-0.34	5 (2%)	58	65	9, 15, 29, 48	0
2	W	183/184 (99%)	-0.29	1 (0%)	91	93	10, 17, 31, 50	0
2	X	183/184 (99%)	-0.34	3 (1%)	74	79	9, 15, 28, 47	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	4164/4176 (99%)	-0.35	40 (0%) 84 87	6, 15, 27, 55	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	S	21	ASP	3.6
2	W	23	GLY	3.6
2	M	21	ASP	3.5
2	P	21	ASP	3.4
2	M	23	GLY	3.2
2	N	23	GLY	3.2
2	X	24	ALA	3.2
2	O	162	GLU	3.1
2	T	21	ASP	3.1
2	X	23	GLY	3.0
2	R	21	ASP	3.0
2	Q	109	ASN	3.0
2	X	22	MET	3.0
2	M	22	MET	2.9
2	Q	21	ASP	2.8
2	V	162	GLU	2.8
2	S	23	GLY	2.8
2	S	24	ALA	2.7
2	T	162	GLU	2.6
2	O	20	ALA	2.6
2	V	22	MET	2.5
2	V	109	ASN	2.4
2	R	30	ALA	2.3
2	U	23	GLY	2.3
2	N	162	GLU	2.3
2	U	24	ALA	2.3
2	T	24	ALA	2.3
2	O	22	MET	2.2
2	N	22	MET	2.2
2	V	20	ALA	2.2
2	V	21	ASP	2.2
2	Q	110	GLY	2.2
2	T	109	ASN	2.1
2	S	117	ALA	2.1
2	P	162	GLU	2.1
2	M	27	GLN	2.1
2	T	23	GLY	2.1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	Q	162	GLU	2.0
2	Q	22	MET	2.0
2	R	147	ALA	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
2	MEN	R	70	9/10	0.97	0.06	-	16,17,19,23	0
2	MEN	T	70	9/10	0.98	0.07	-	18,21,23,24	0
2	MEN	W	70	9/10	0.96	0.09	-	8,11,14,16	0
2	MEN	V	70	9/10	0.98	0.07	-	13,14,17,18	0
2	MEN	Q	70	9/10	0.97	0.09	-	14,17,20,21	0
2	MEN	X	70	9/10	0.98	0.09	-	8,13,16,16	0
2	MEN	M	70	9/10	0.98	0.09	-	10,12,13,16	0
2	MEN	U	70	9/10	0.97	0.07	-	9,11,13,15	0
2	MEN	O	70	9/10	0.96	0.07	-	12,16,17,20	0
2	MEN	N	70	9/10	0.96	0.09	-	10,13,17,18	0
2	MEN	P	70	9/10	0.96	0.07	-	8,11,17,17	0
2	MEN	S	70	9/10	0.95	0.08	-	9,14,17,17	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [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( $\text{\AA}^2$ )	Q<0.9
4	GOL	K	1165	6/6	0.93	0.14	6.75	15,25,26,29	0
4	GOL	E	1165	6/6	0.87	0.22	4.88	25,30,33,37	0
4	GOL	I	1165	6/6	0.85	0.20	4.51	24,28,28,33	0
4	GOL	A	1165	6/6	0.95	0.16	4.22	21,23,25,30	0
3	PEB	C	167	43/43	0.92	0.13	4.00	11,19,26,27	0
5	SO4	H	1200	5/5	0.97	0.14	3.77	21,26,33,36	0
4	GOL	H	1165	6/6	0.86	0.18	3.69	25,28,33,36	0
4	GOL	D	1165	6/6	0.84	0.17	3.25	23,28,31,35	0
4	GOL	C	1165	6/6	0.87	0.15	2.68	25,27,32,34	0
5	SO4	E	1200	5/5	0.97	0.13	2.20	18,18,30,38	0
4	GOL	B	1165	6/6	0.89	0.13	2.02	16,23,31,33	0
3	PEB	D	167	43/43	0.90	0.13	2.00	12,18,26,35	0
4	GOL	F	1165	6/6	0.90	0.14	2.00	27,29,31,37	0
4	GOL	G	1165	6/6	0.82	0.13	1.95	27,30,31,37	0
3	PEB	B	167	43/43	0.94	0.13	1.84	10,18,28,31	0
3	PEB	J	167	43/43	0.91	0.13	1.62	10,21,29,32	0
3	PEB	X	186	43/43	0.92	0.13	1.58	8,14,24,41	0
4	GOL	L	1165	6/6	0.89	0.14	1.55	22,28,33,34	0
4	GOL	J	1165	6/6	0.92	0.10	1.45	18,24,27,27	0
3	PEB	I	167	43/43	0.89	0.14	1.36	12,18,23,26	0
3	PEB	K	167	43/43	0.90	0.15	1.32	15,24,29,32	0
3	PEB	N	186	43/43	0.93	0.13	1.15	7,15,23,35	0
3	PEB	M	186	43/43	0.92	0.11	1.06	8,14,23,45	0
5	SO4	I	1200	5/5	0.97	0.11	1.03	24,31,37,38	0
3	PEB	K	166	43/43	0.94	0.10	1.02	8,12,17,21	0
3	PEB	U	186	43/43	0.92	0.13	1.01	9,13,24,33	0
3	PEB	C	166	43/43	0.94	0.10	0.97	7,13,17,28	0
3	PEB	P	186	43/43	0.91	0.13	0.96	9,14,24,34	0
5	SO4	D	1200	5/5	0.98	0.11	0.91	20,26,34,34	0
3	PEB	R	186	43/43	0.92	0.11	0.90	9,17,25,32	0
3	PEB	V	186	43/43	0.89	0.12	0.88	8,17,28,36	0
3	PEB	A	167	43/43	0.93	0.11	0.84	8,15,21,28	0
5	SO4	L	1200	5/5	0.96	0.10	0.83	20,24,32,35	0
3	PEB	G	166	43/43	0.94	0.10	0.75	7,10,15,19	0
3	PEB	W	186	43/43	0.93	0.12	0.73	8,15,23,39	0
3	PEB	Q	186	43/43	0.90	0.13	0.70	12,17,25,38	0
3	PEB	O	186	43/43	0.90	0.11	0.69	7,17,27,37	0
3	PEB	T	186	43/43	0.91	0.13	0.65	14,22,29,37	0
3	PEB	R	187	43/43	0.88	0.15	0.65	12,20,31,40	0
3	PEB	A	166	43/43	0.95	0.10	0.64	8,12,16,20	0
3	PEB	B	166	43/43	0.95	0.09	0.64	6,10,14,18	0
3	PEB	H	166	43/43	0.93	0.11	0.63	9,14,20,25	0
3	PEB	S	186	43/43	0.91	0.12	0.59	10,16,27,38	0

Continued on next page...



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PEB	E	166	43/43	0.94	0.11	0.58	8,15,19,30	0
3	PEB	P	187	43/43	0.89	0.13	0.49	9,15,27,31	0
3	PEB	S	187	43/43	0.91	0.14	0.48	11,17,26,30	0
3	PEB	G	167	43/43	0.95	0.09	0.48	8,15,20,27	0
3	PEB	U	187	43/43	0.91	0.12	0.42	7,15,25,38	0
3	PEB	L	167	43/43	0.92	0.12	0.40	10,16,25,32	0
3	PEB	F	166	43/43	0.94	0.10	0.40	6,12,15,18	0
3	PEB	W	187	43/43	0.93	0.12	0.39	8,16,25,38	0
3	PEB	Q	187	43/43	0.91	0.13	0.38	7,16,34,39	0
3	PEB	N	188	43/43	0.94	0.10	0.34	9,15,22,25	0
3	PEB	X	187	43/43	0.91	0.12	0.32	8,16,23,34	0
3	PEB	S	188	43/43	0.95	0.10	0.24	9,14,20,25	0
3	PEB	T	187	43/43	0.90	0.13	0.19	11,20,31,35	0
3	PEB	X	188	43/43	0.95	0.10	0.18	10,13,22,24	0
3	PEB	L	166	43/43	0.95	0.09	0.12	7,12,17,18	0
3	PEB	O	188	43/43	0.94	0.11	0.08	10,16,24,31	0
3	PEB	U	188	43/43	0.94	0.10	0.08	8,11,16,28	0
3	PEB	W	188	43/43	0.94	0.10	0.07	9,16,23,24	0
3	PEB	Q	188	43/43	0.94	0.10	0.07	9,16,25,31	0
3	PEB	N	187	43/43	0.92	0.11	0.05	10,15,22,24	0
3	PEB	J	166	43/43	0.95	0.09	0.02	9,13,19,24	0
3	PEB	F	167	43/43	0.95	0.10	-0.04	10,15,19,25	0
3	PEB	I	166	43/43	0.94	0.10	-0.05	11,17,25,28	0
3	PEB	T	188	43/43	0.92	0.11	-0.08	13,22,30,40	0
3	PEB	M	187	43/43	0.92	0.10	-0.09	9,14,20,36	0
3	PEB	E	167	43/43	0.95	0.09	-0.13	11,15,20,24	0
3	PEB	O	187	43/43	0.90	0.12	-0.15	12,20,26,31	0
3	PEB	D	166	43/43	0.94	0.09	-0.16	9,15,22,31	0
3	PEB	V	187	43/43	0.92	0.11	-0.19	13,17,23,25	0
3	PEB	P	188	43/43	0.93	0.10	-0.20	6,12,16,19	0
3	PEB	R	188	43/43	0.93	0.10	-0.28	11,17,21,35	0
3	PEB	V	188	43/43	0.94	0.09	-0.46	8,14,19,23	0
3	PEB	M	188	43/43	0.96	0.08	-0.52	10,13,19,20	0
3	PEB	H	167	43/43	0.96	0.08	-0.56	8,14,17,21	0
5	SO4	A	1200	5/5	0.97	0.08	-0.96	23,24,34,40	0
5	SO4	S	189	5/5	0.92	0.28	-	32,38,53,56	0
5	SO4	Q	189	5/5	0.87	0.23	-	32,46,54,57	0
5	SO4	W	189	5/5	0.88	0.22	-	25,37,52,54	0
5	SO4	V	189	5/5	0.91	0.27	-	27,31,51,54	0
5	SO4	U	189	5/5	0.81	0.21	-	40,41,51,63	0
5	SO4	N	189	5/5	0.92	0.21	-	28,34,47,52	0
5	SO4	R	189	5/5	0.89	0.23	-	35,51,58,64	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SO4	X	189	5/5	0.96	0.15	-	30,33,43,52	0
5	SO4	T	189	5/5	0.96	0.32	-	42,46,49,60	0
5	SO4	P	189	5/5	0.93	0.20	-	28,35,56,56	0
5	SO4	M	189	5/5	0.92	0.18	-	26,31,38,46	0
5	SO4	O	189	5/5	0.91	0.26	-	30,41,48,58	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.