



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2016 – 03:49 PM EDT

PDB ID : 5FVB
Title : CRYSTAL STRUCTURE OF PHORMIDIUM C-PHYCOERYTHRIN AT PH 5.0
Authors : Kumar, V.; Sonani, R.R.; Sharma, M.; Gupta, G.D.; Madamwar, D.
Deposited on : 2016-02-05
Resolution : 1.93 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<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

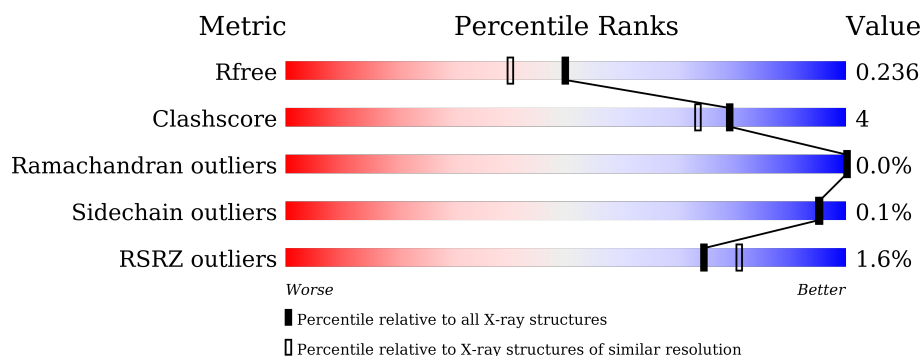
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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.



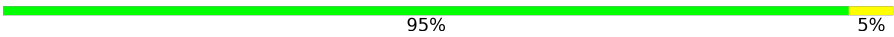
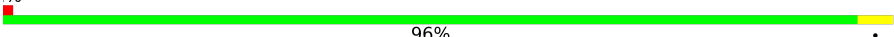

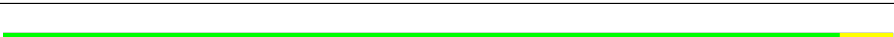
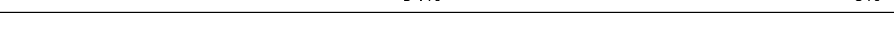
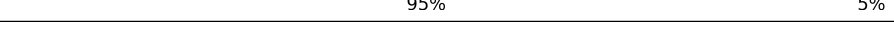

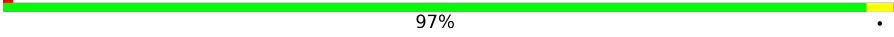
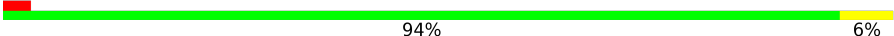
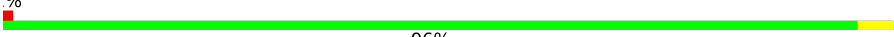

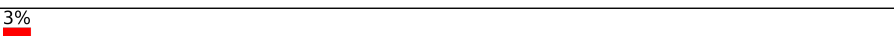
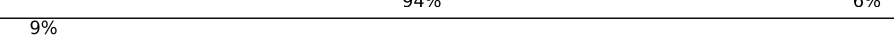
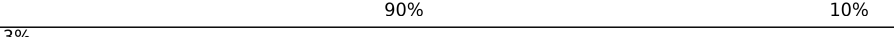
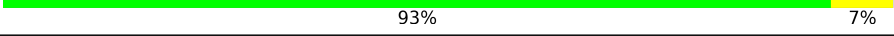
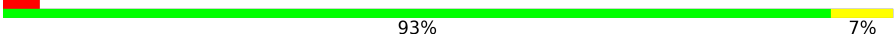
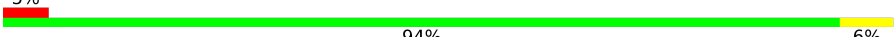

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2910 (1.96-1.92)
Clashscore	102246	3095 (1.96-1.92)
Ramachandran outliers	100387	3062 (1.96-1.92)
Sidechain outliers	100360	3062 (1.96-1.92)
RSRZ outliers	91569	2915 (1.96-1.92)

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 ≥ 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	
1	B	164	
1	C	164	
1	D	164	
1	E	164	
1	F	164	

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Mol	Chain	Length	Quality of chain
1	G	164	
1	H	164	
1	I	164	
1	J	164	
1	K	164	
1	L	164	
2	M	184	
2	N	184	
2	O	184	
2	P	184	
2	Q	184	
2	R	184	
2	S	184	
2	T	184	
2	U	184	
2	V	184	
2	W	184	
2	X	184	

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	J	1166	-	-	-	X
4	GOL	A	1167	-	-	-	X
4	GOL	E	1167	-	-	-	X
4	GOL	H	1167	-	-	-	X
4	GOL	J	1167	-	-	-	X
4	GOL	K	1167	-	-	-	X
4	GOL	O	1188	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 38800 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 C-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

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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

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

- Molecule 2 is a protein called C-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

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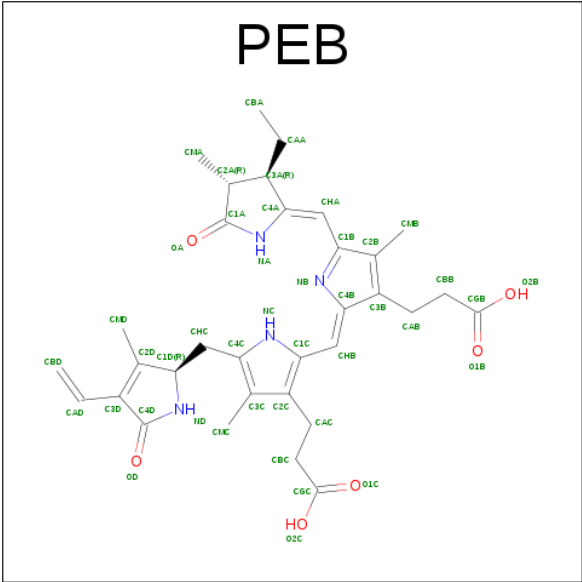
Chain	Residue	Modelled	Actual	Comment	Reference
N	3	ASP	-	SEE REMARK 999	UNP A0A0E4G45
N	4	ALA	-	SEE REMARK 999	UNP A0A0E4G45
N	5	PHE	-	SEE REMARK 999	UNP A0A0E4G45
N	6	SER	-	SEE REMARK 999	UNP A0A0E4G45
N	7	ARG	-	SEE REMARK 999	UNP A0A0E4G45
O	1	MET	-	SEE REMARK 999	UNP A0A0E4G45
O	2	LEU	-	SEE REMARK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

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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: $C_{33}H_{40}N_4O_6$).



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		

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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

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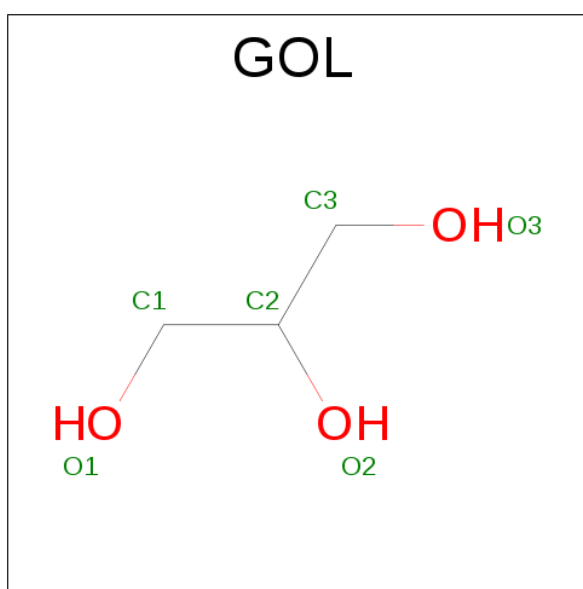
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	P	1	Total 43	C 33	N 4	O 6	0	0
3	Q	1	Total 43	C 33	N 4	O 6	0	0
3	Q	1	Total 43	C 33	N 4	O 6	0	0
3	Q	1	Total 43	C 33	N 4	O 6	0	0
3	R	1	Total 43	C 33	N 4	O 6	0	0
3	R	1	Total 43	C 33	N 4	O 6	0	0
3	R	1	Total 43	C 33	N 4	O 6	0	0
3	S	1	Total 43	C 33	N 4	O 6	0	0
3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

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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	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		
4	O	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	280	Total	O	0	0
			280	280		
5	B	263	Total	O	0	0
			263	263		
5	C	257	Total	O	0	0
			257	257		
5	D	191	Total	O	0	0
			191	191		
5	E	190	Total	O	0	0
			190	190		
5	F	191	Total	O	0	0
			191	191		
5	G	256	Total	O	0	0
			256	256		
5	H	222	Total	O	0	0
			222	222		
5	I	220	Total	O	0	0
			220	220		
5	J	244	Total	O	0	0
			244	244		
5	K	235	Total	O	0	0
			235	235		
5	L	230	Total	O	0	0
			230	230		
5	M	232	Total	O	0	0
			232	232		
5	N	204	Total	O	0	0
			204	204		
5	O	229	Total	O	0	0
			229	229		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	188	Total 188	O 188	0	0
5	Q	184	Total 184	O 184	0	0
5	R	151	Total 151	O 151	0	0
5	S	172	Total 172	O 172	0	0
5	T	183	Total 183	O 183	0	0
5	U	162	Total 162	O 162	0	0
5	V	239	Total 239	O 239	0	0
5	W	192	Total 192	O 192	0	0
5	X	207	Total 207	O 207	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: C-PHYCOERYTHRIN ALPHA SUBUNIT

Chain A:  93% 7%



- Molecule 1: C-PHYCOERYTHRIN ALPHA SUBUNIT

Chain B:  94% 6%



- Molecule 1: C-PHYCOERYTHRIN ALPHA SUBUNIT

Chain C:  94% 6%



- Molecule 1: C-PHYCOERYTHRIN ALPHA SUBUNIT

Chain D:  93% 7%



- Molecule 1: C-PHYCOERYTHRIN ALPHA SUBUNIT

Chain E:  94% 6% 2%



- Molecule 1: C-PHYCOERYTHRIN ALPHA SUBUNIT

Chain F:  95% 5%



- Molecule 1: C-PHYCOERYTHRIN ALPHA SUBUNIT

Chain G: 95% 5%



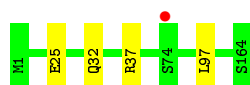
- Molecule 1: C-PHYCOERYTHRIN ALPHA SUBUNIT

Chain H: 96% .



- Molecule 1: C-PHYCOERYTHRIN ALPHA SUBUNIT

Chain I: 98% .



- Molecule 1: C-PHYCOERYTHRIN ALPHA SUBUNIT

Chain J: 94% 6%



- Molecule 1: C-PHYCOERYTHRIN ALPHA SUBUNIT

Chain K: 95% 5%



- Molecule 1: C-PHYCOERYTHRIN ALPHA SUBUNIT

Chain L: 91% 9%

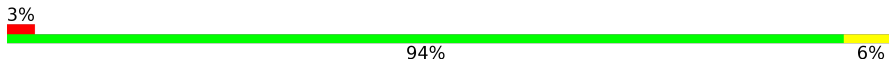


- Molecule 2: C-PHYCOERYTHRIN BETA SUBUNIT

Chain M: 97% ..



- Molecule 2: C-PHYCOERYTHRIN BETA SUBUNIT

Chain N: 



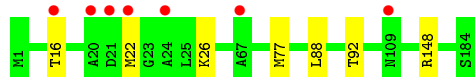
- Molecule 2: C-PHYCOERYTHRIN BETA SUBUNIT

Chain O: 

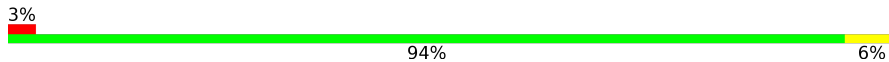


- Molecule 2: C-PHYCOERYTHRIN BETA SUBUNIT

Chain P: 

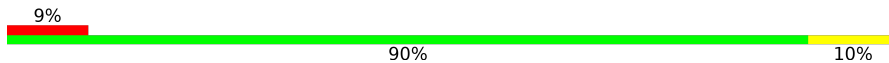


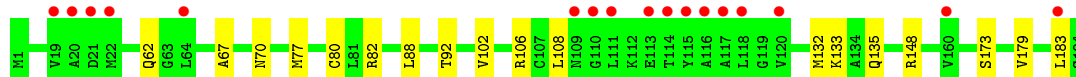
- Molecule 2: C-PHYCOERYTHRIN BETA SUBUNIT

Chain Q: 

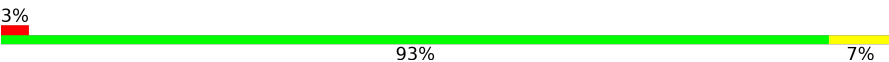


- Molecule 2: C-PHYCOERYTHRIN BETA SUBUNIT

Chain R: 

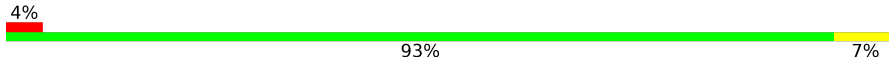


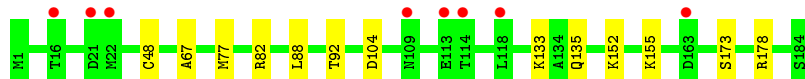
- Molecule 2: C-PHYCOERYTHRIN BETA SUBUNIT

Chain S: 

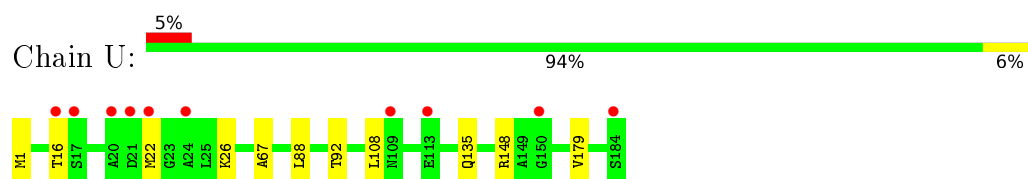


- Molecule 2: C-PHYCOERYTHRIN BETA SUBUNIT

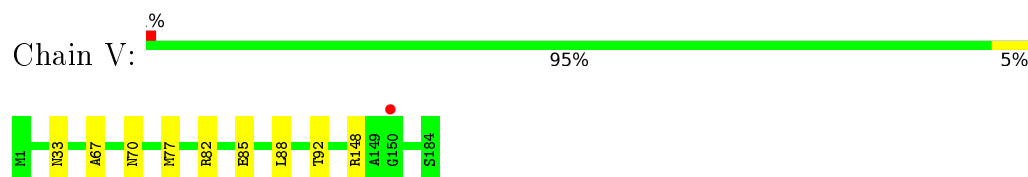
Chain T: 



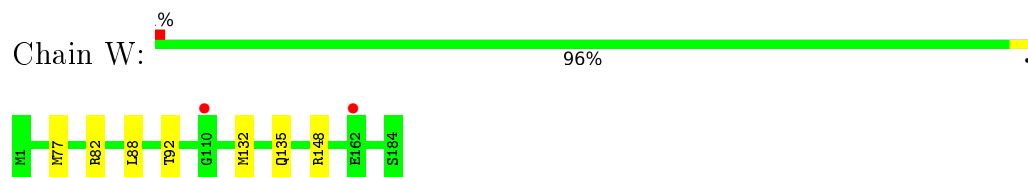
- Molecule 2: C-PHYCOERYTHRIN BETA SUBUNIT



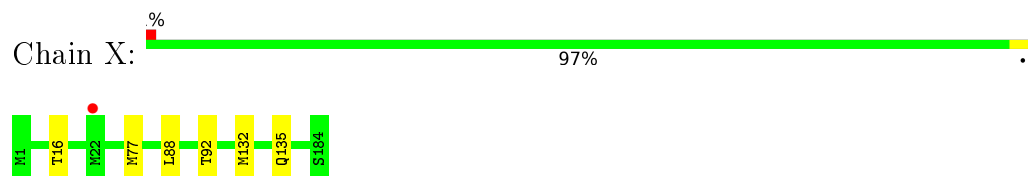
- Molecule 2: C-PHYCOERYTHRIN BETA SUBUNIT



- Molecule 2: C-PHYCOERYTHRIN BETA SUBUNIT



- Molecule 2: C-PHYCOERYTHRIN BETA SUBUNIT



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	109.17Å 109.15Å 117.68Å 78.71° 82.30° 61.55°	Depositor
Resolution (Å)	38.89 – 1.93 38.89 – 1.93	Depositor EDS
% Data completeness (in resolution range)	96.2 (38.89-1.93) 91.2 (38.89-1.93)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 1.94Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.183 , 0.239 0.182 , 0.236	Depositor DCC
R_{free} test set	17281 reflections (5.11%)	DCC
Wilson B-factor (Å ²)	18.6	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	38800	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, 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	0.42	0/1259	0.54	0/1706
1	B	0.39	0/1259	0.54	0/1706
1	C	0.37	0/1259	0.50	0/1706
1	D	0.37	0/1259	0.51	0/1706
1	E	0.36	0/1259	0.50	0/1706
1	F	0.35	0/1259	0.49	0/1706
1	G	0.37	0/1259	0.50	0/1706
1	H	0.36	0/1259	0.50	0/1706
1	I	0.35	0/1259	0.50	0/1706
1	J	0.39	0/1259	0.52	0/1706
1	K	0.40	0/1259	0.51	0/1706
1	L	0.43	0/1259	0.56	0/1706
2	M	0.39	0/1349	0.51	0/1820
2	N	0.35	0/1349	0.48	0/1820
2	O	0.38	0/1349	0.49	0/1820
2	P	0.36	0/1349	0.48	0/1820
2	Q	0.35	0/1349	0.48	0/1820
2	R	0.32	0/1349	0.45	0/1820
2	S	0.34	0/1349	0.47	0/1820
2	T	0.33	0/1349	0.46	0/1820
2	U	0.37	0/1349	0.49	0/1820
2	V	0.40	0/1349	0.52	0/1820
2	W	0.35	0/1349	0.47	0/1820
2	X	0.38	0/1349	0.50	0/1820
All	All	0.37	0/31296	0.50	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	10	0
1	B	1239	0	1221	9	0
1	C	1239	0	1221	8	0
1	D	1239	0	1221	11	0
1	E	1239	0	1221	11	0
1	F	1239	0	1221	9	0
1	G	1239	0	1221	8	0
1	H	1239	0	1221	6	0
1	I	1239	0	1221	3	0
1	J	1239	0	1221	8	0
1	K	1239	0	1221	8	0
1	L	1239	0	1221	10	0
2	M	1347	0	1359	6	0
2	N	1347	0	1359	9	0
2	O	1347	0	1359	7	0
2	P	1347	0	1359	5	0
2	Q	1347	0	1359	9	0
2	R	1347	0	1359	14	0
2	S	1347	0	1359	10	0
2	T	1347	0	1359	9	0
2	U	1347	0	1359	8	0
2	V	1347	0	1359	9	0
2	W	1347	0	1359	6	0
2	X	1347	0	1359	5	0
3	A	86	0	74	3	0
3	B	86	0	74	3	0
3	C	86	0	74	1	0
3	D	86	0	73	1	0
3	E	86	0	74	3	0
3	F	86	0	73	4	0
3	G	86	0	74	3	0
3	H	86	0	73	3	0
3	I	86	0	73	3	0
3	J	86	0	74	5	0
3	K	86	0	74	3	0
3	L	86	0	74	2	0
3	M	129	0	110	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	129	0	110	7	0
3	O	129	0	110	6	0
3	P	129	0	110	5	0
3	Q	129	0	110	7	0
3	R	129	0	110	9	0
3	S	129	0	110	10	0
3	T	129	0	110	5	0
3	U	129	0	110	8	0
3	V	129	0	110	9	0
3	W	129	0	110	7	0
3	X	129	0	110	6	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	D	6	0	8	0	0
4	E	6	0	8	1	0
4	G	6	0	8	0	0
4	H	6	0	8	0	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
4	O	6	0	8	1	0
5	A	280	0	0	1	0
5	B	263	0	0	1	0
5	C	257	0	0	1	0
5	D	191	0	0	1	0
5	E	190	0	0	1	0
5	F	191	0	0	3	0
5	G	256	0	0	4	0
5	H	222	0	0	1	0
5	I	220	0	0	2	0
5	J	244	0	0	0	0
5	K	235	0	0	1	0
5	L	230	0	0	2	0
5	M	232	0	0	1	0
5	N	204	0	0	1	0
5	O	229	0	0	0	0
5	P	188	0	0	0	0
5	Q	184	0	0	0	0
5	R	151	0	0	1	0
5	S	172	0	0	1	0
5	T	183	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	U	162	0	0	0	0
5	V	239	0	0	1	0
5	W	192	0	0	0	0
5	X	207	0	0	0	0
All	All	38800	0	33252	234	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 (234) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:32:GLN:HG3	1:L:32:GLN:HG3	1.39	1.04
1:A:32:GLN:HG3	1:D:32:GLN:HG3	1.40	1.03
1:B:32:GLN:HG3	1:E:32:GLN:HG3	1.49	0.94
1:H:32:GLN:HG3	1:K:32:GLN:HG3	1.48	0.94
1:C:32:GLN:HG3	1:F:32:GLN:HG3	1.53	0.90
2:V:82:ARG:NH1	3:V:1185:PEB:O2C	2.22	0.72
2:V:85:GLU:HG2	5:V:2141:HOH:O	1.91	0.68
2:O:2:LEU:HG	4:O:1188:GOL:H32	1.76	0.68
3:U:1185:PEB:HMB2	3:U:1185:PEB:HNA	1.60	0.66
3:U:1186:PEB:HNA	3:U:1186:PEB:HMB2	1.63	0.64
2:P:148:ARG:NH1	3:P:1187:PEB:HND	1.96	0.62
2:Q:16:THR:HG23	2:R:67:ALA:HB2	1.81	0.62
2:V:67:ALA:HB2	2:X:16:THR:HG23	1.80	0.62
2:T:135:GLN:HG2	3:T:1187:PEB:C1B	2.29	0.62
3:Q:1185:PEB:HNA	3:Q:1185:PEB:HMB2	1.66	0.61
3:M:1185:PEB:HNA	3:M:1185:PEB:HMB2	1.66	0.60
2:P:16:THR:HG23	2:Q:67:ALA:HB2	1.83	0.60
2:T:133:LYS:HE3	2:T:173:SER:HB3	1.83	0.60
2:X:88:LEU:O	2:X:92:THR:HG23	2.01	0.60
1:A:21:SER:HB3	5:A:2021:HOH:O	2.00	0.59
2:U:148:ARG:NH1	3:U:1187:PEB:HND	1.99	0.59
3:T:1185:PEB:HMB2	3:T:1185:PEB:HNA	1.67	0.59
1:B:37:ARG:NE	1:E:25:GLU:OE2	2.29	0.59
2:S:135:GLN:HG2	3:S:1187:PEB:C1B	2.33	0.59
3:N:1185:PEB:HNA	3:N:1185:PEB:HMB2	1.68	0.59
3:P:1185:PEB:HNA	3:P:1185:PEB:HMB2	1.68	0.58
2:T:67:ALA:HB2	2:U:16:THR:HG23	1.86	0.58
1:H:37:ARG:NE	1:K:25:GLU:OE2	2.36	0.56
3:M:1186:PEB:HMB2	3:M:1186:PEB:HNA	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1186:PEB:HNA	3:N:1186:PEB:HMB2	1.70	0.56
2:Q:135:GLN:HG2	3:Q:1187:PEB:C1B	2.36	0.55
3:T:1186:PEB:HBA3	3:T:1186:PEB:HHA1	1.87	0.55
3:S:1186:PEB:HHA1	3:S:1186:PEB:HBA3	1.89	0.55
2:N:148:ARG:NH1	3:N:1187:PEB:HND	2.05	0.54
2:P:88:LEU:O	2:P:92:THR:HG23	2.08	0.54
2:O:88:LEU:O	2:O:92:THR:HG23	2.08	0.54
3:R:1186:PEB:HNA	3:R:1186:PEB:HMB2	1.72	0.54
3:S:1185:PEB:HNA	3:S:1185:PEB:HMB2	1.73	0.54
3:R:1185:PEB:HMB2	3:R:1185:PEB:HNA	1.73	0.54
2:M:85:GLU:HG2	5:M:2130:HOH:O	2.07	0.53
2:S:88:LEU:O	2:S:92:THR:HG23	2.09	0.53
3:Q:1186:PEB:HMB2	3:Q:1186:PEB:HNA	1.73	0.53
1:E:43:LYS:HD2	5:E:2066:HOH:O	2.08	0.53
5:I:2104:HOH:O	1:L:21:SER:HB3	2.08	0.53
3:P:1186:PEB:HNA	3:P:1186:PEB:HMB2	1.74	0.52
2:W:135:GLN:HG2	3:W:1187:PEB:C1B	2.39	0.52
2:V:148:ARG:NH1	3:V:1187:PEB:HND	2.07	0.52
3:H:1165:PEB:HNA	3:H:1165:PEB:HMB2	1.75	0.52
3:Q:1186:PEB:HBA3	3:Q:1186:PEB:HHA1	1.91	0.52
3:A:1165:PEB:HMC2	2:O:77:MET:HG2	1.92	0.52
3:V:1185:PEB:HNA	3:V:1185:PEB:HMB2	1.75	0.52
3:E:1165:PEB:HMB2	3:E:1165:PEB:HNA	1.75	0.51
3:I:1165:PEB:HMB2	3:I:1165:PEB:HNA	1.75	0.51
3:V:1186:PEB:HMB2	3:V:1186:PEB:HNA	1.74	0.51
1:B:25:GLU:OE2	1:E:37:ARG:NE	2.42	0.51
1:F:114:ARG:NH2	5:F:2129:HOH:O	2.44	0.51
2:V:88:LEU:O	2:V:92:THR:HG23	2.11	0.51
5:G:2233:HOH:O	1:J:21:SER:HB3	2.10	0.51
3:E:1165:PEB:CMB	3:E:1165:PEB:HNA	2.24	0.51
2:R:135:GLN:HG2	3:R:1187:PEB:C1B	2.41	0.51
3:U:1185:PEB:CMB	3:U:1185:PEB:HNA	2.24	0.51
1:H:25:GLU:OE2	1:K:37:ARG:NE	2.41	0.51
3:G:1166:PEB:HMB2	3:G:1166:PEB:HNA	1.76	0.51
2:P:22:MET:O	2:P:26:LYS:HG2	2.10	0.51
2:R:133:LYS:HE3	2:R:173:SER:HB3	1.94	0.51
2:M:135:GLN:HG2	3:M:1187:PEB:C1B	2.41	0.50
2:R:108:LEU:HD21	2:R:179:VAL:HG22	1.93	0.50
2:R:88:LEU:O	2:R:92:THR:HG23	2.12	0.50
3:W:1185:PEB:HNA	3:W:1185:PEB:HMB2	1.77	0.50
3:X:1185:PEB:HMB2	3:X:1185:PEB:HNA	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:88:LEU:O	2:U:92:THR:HG23	2.11	0.50
2:U:22:MET:O	2:U:26:LYS:HG2	2.12	0.50
2:T:88:LEU:O	2:T:92:THR:HG23	2.12	0.50
2:V:70:MEN:HB2	3:V:1185:PEB:OA	2.12	0.50
2:T:82:ARG:NH1	3:T:1185:PEB:O2C	2.44	0.49
3:X:1187:PEB:HBB1	3:X:1187:PEB:HBB1	1.93	0.49
1:E:37:ARG:HD2	1:E:97:LEU:O	2.12	0.49
3:S:1186:PEB:HMB2	3:S:1186:PEB:HNA	1.78	0.49
1:K:139:CYS:SG	3:K:1166:PEB:HHA1	2.52	0.49
2:R:82:ARG:NH2	3:R:1185:PEB:O2C	2.41	0.49
3:W:1186:PEB:HBA3	3:W:1186:PEB:HHA1	1.95	0.49
2:N:123:THR:HG23	5:N:2141:HOH:O	2.12	0.49
3:N:1187:PEB:HMB3	3:N:1187:PEB:HNA	1.77	0.49
3:U:1187:PEB:HMB3	3:U:1187:PEB:HNA	1.78	0.49
1:I:37:ARG:HD2	1:I:97:LEU:O	2.13	0.48
2:S:16:THR:HG23	2:U:67:ALA:HB2	1.95	0.48
3:O:1185:PEB:HNA	3:O:1185:PEB:HMB2	1.78	0.48
1:I:25:GLU:OE2	1:L:37:ARG:NE	2.44	0.48
2:N:88:LEU:O	2:N:92:THR:HG23	2.13	0.48
2:W:148:ARG:NH1	3:W:1187:PEB:HND	2.11	0.48
3:P:1187:PEB:HNA	3:P:1187:PEB:HMB3	1.78	0.48
3:W:1187:PEB:HMB3	3:W:1187:PEB:HNA	1.78	0.48
1:B:87:LYS:NZ	5:B:2110:HOH:O	2.47	0.48
3:X:1186:PEB:HNA	3:X:1186:PEB:HMB2	1.78	0.47
1:J:27:VAL:O	1:J:30:SER:HB2	2.14	0.47
3:B:1166:PEB:HMB2	3:B:1166:PEB:HNA	1.80	0.47
1:H:72:ALA:O	1:H:78:PHE:HB3	2.13	0.47
2:X:135:GLN:HG2	3:X:1187:PEB:C1B	2.44	0.47
1:F:32:GLN:HB3	5:F:2046:HOH:O	2.14	0.47
2:O:82:ARG:NH1	3:O:1185:PEB:O2C	2.38	0.47
3:D:1165:PEB:HMB2	3:D:1165:PEB:HNA	1.80	0.47
2:S:85:GLU:HG2	5:S:2090:HOH:O	2.13	0.47
1:D:37:ARG:HD2	1:D:97:LEU:O	2.15	0.47
3:Q:1187:PEB:HNA	3:Q:1187:PEB:HMB3	1.80	0.47
1:G:21:SER:HB3	5:G:2020:HOH:O	2.15	0.47
3:E:1165:PEB:HMC2	2:R:77:MET:HG2	1.97	0.47
3:U:1186:PEB:NA	3:U:1186:PEB:HMB2	2.30	0.47
1:A:25:GLU:OE2	1:D:37:ARG:NE	2.47	0.46
1:C:114:ARG:HD3	1:E:118:ARG:NH1	2.29	0.46
3:H:1165:PEB:HNA	3:H:1165:PEB:CMB	2.29	0.46
3:J:1165:PEB:HMC2	2:W:77:MET:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:34:SER:O	1:E:38:LEU:HG	2.16	0.46
3:R:1186:PEB:HHA1	3:R:1186:PEB:HBA3	1.98	0.46
3:G:1166:PEB:HMB2	3:G:1166:PEB:NA	2.31	0.46
1:C:147:GLN:HG3	5:C:2033:HOH:O	2.16	0.45
2:U:135:GLN:HG2	3:U:1187:PEB:C1B	2.46	0.45
2:N:82:ARG:NH1	3:N:1185:PEB:O2C	2.44	0.45
3:S:1187:PEB:HBB1	3:S:1187:PEB:HBB1	1.99	0.45
2:N:135:GLN:HG2	3:N:1187:PEB:C1B	2.46	0.45
3:R:1187:PEB:HBB1	3:R:1187:PEB:HBB1	1.98	0.45
1:B:30:SER:O	1:B:34:SER:HB3	2.16	0.45
2:O:148:ARG:NH1	3:O:1187:PEB:HND	2.15	0.45
2:Q:148:ARG:NH1	3:Q:1187:PEB:HND	2.14	0.45
2:V:82:ARG:HH22	3:V:1185:PEB:C1C	2.30	0.45
3:M:1186:PEB:NA	3:M:1186:PEB:HMB2	2.30	0.45
2:Q:104:ASP:OD2	2:Q:178:ARG:NH2	2.49	0.45
1:J:139:CYS:SG	3:J:1166:PEB:HHA1	2.56	0.44
1:A:37:ARG:NH1	1:A:98:VAL:O	2.48	0.44
1:D:91:ARG:NH2	2:Q:72:TYR:OH	2.46	0.44
1:L:68:ASN:O	1:L:74:SER:HB3	2.18	0.44
3:H:1165:PEB:HMC2	2:S:77:MET:HG2	1.98	0.44
1:A:8:VAL:HB	1:A:23:ASP:OD1	2.17	0.44
3:I:1165:PEB:CMB	3:I:1165:PEB:HNA	2.30	0.44
2:W:82:ARG:NH1	3:W:1185:PEB:O1C	2.42	0.44
1:B:29:GLY:HA3	1:E:25:GLU:O	2.17	0.44
1:H:29:GLY:HA3	1:K:25:GLU:O	2.18	0.44
3:V:1187:PEB:HBB1	3:V:1187:PEB:HBB1	2.00	0.44
2:T:48:CYS:SG	2:T:152:LYS:HE2	2.58	0.44
2:W:88:LEU:O	2:W:92:THR:HG23	2.18	0.44
1:A:82:CYS:HA	3:A:1165:PEB:HAA1	1.89	0.44
1:B:37:ARG:HD2	1:B:97:LEU:O	2.18	0.43
1:D:97:LEU:HG	1:D:155:LEU:HD12	2.00	0.43
2:T:104:ASP:OD2	2:T:178:ARG:NH2	2.51	0.43
2:R:80:CYS:HA	3:R:1185:PEB:HAA1	1.86	0.43
1:A:50:ALA:O	1:A:54:GLU:HG2	2.19	0.43
2:M:148:ARG:NH1	3:M:1187:PEB:HND	2.16	0.43
2:S:48:CYS:SG	2:S:152:LYS:HE2	2.57	0.43
2:Q:70:MEN:HB2	3:Q:1185:PEB:OA	2.18	0.43
3:U:1186:PEB:HBA3	3:U:1186:PEB:HHA1	2.00	0.43
3:L:1165:PEB:HMC2	2:V:77:MET:HG2	2.00	0.43
1:G:114:ARG:NH2	5:G:2179:HOH:O	2.52	0.43
3:O:1186:PEB:HNA	3:O:1186:PEB:HMB2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:2100:HOH:O	1:K:21:SER:HB3	2.18	0.43
2:R:183:LEU:HA	2:R:183:LEU:HD23	1.78	0.43
3:T:1186:PEB:HMB2	3:T:1186:PEB:HNA	1.83	0.43
3:X:1186:PEB:HBA3	3:X:1186:PEB:HHA1	2.01	0.43
3:X:1186:PEB:HMB2	3:X:1186:PEB:NA	2.34	0.43
2:S:148:ARG:NH1	3:S:1187:PEB:HND	2.16	0.43
1:L:110:ILE:HG23	1:L:113:GLN:NE2	2.34	0.43
1:L:139:CYS:SG	3:L:1166:PEB:HHA1	2.59	0.43
2:S:34:ARG:HE	3:S:1186:PEB:CGB	2.32	0.43
3:S:1186:PEB:HMB2	3:S:1186:PEB:NA	2.32	0.43
1:A:139:CYS:SG	3:A:1166:PEB:HHA1	2.59	0.42
1:C:37:ARG:HD2	1:C:97:LEU:O	2.19	0.42
1:J:1:MET:HG3	1:J:103:GLY:HA3	2.01	0.42
2:R:148:ARG:NH1	3:R:1187:PEB:HND	2.17	0.42
1:D:37:ARG:NH1	1:D:98:VAL:O	2.52	0.42
3:F:1166:PEB:HMB2	3:F:1166:PEB:NA	2.33	0.42
1:L:62:LYS:HD3	5:L:2039:HOH:O	2.19	0.42
2:R:70:MEN:HB2	3:R:1185:PEB:OA	2.19	0.42
1:G:85:ASP:OD1	3:G:1165:PEB:H1D1	2.19	0.42
2:N:132:MET:HA	2:N:135:GLN:OE1	2.19	0.42
1:E:38:LEU:HD22	2:Q:22:MET:HE3	2.01	0.42
2:R:62:GLN:NE2	5:R:2064:HOH:O	2.52	0.42
3:F:1165:PEB:HMC2	2:P:77:MET:HG2	2.02	0.42
3:K:1166:PEB:HMB2	3:K:1166:PEB:HNA	1.85	0.42
1:L:87:LYS:NZ	5:L:2088:HOH:O	2.50	0.42
2:X:132:MET:HA	2:X:135:GLN:OE1	2.19	0.42
1:C:88:HIS:O	1:C:92:LEU:HG	2.19	0.42
1:F:155:LEU:HD23	1:F:155:LEU:HA	1.84	0.42
1:L:37:ARG:HD2	1:L:97:LEU:O	2.20	0.42
1:F:139:CYS:SG	3:F:1166:PEB:HHA1	2.60	0.42
1:G:115:GLU:HG3	1:G:118:ARG:HH12	1.85	0.41
3:S:1187:PEB:HNA	3:S:1187:PEB:HMB3	1.85	0.41
2:V:33:ASN:HB3	3:V:1186:PEB:C1C	2.50	0.41
1:A:37:ARG:NE	1:D:25:GLU:OE2	2.54	0.41
2:Q:24:ALA:O	2:Q:27:GLN:HB3	2.20	0.41
2:W:132:MET:HA	2:W:135:GLN:OE1	2.20	0.41
1:C:25:GLU:OE2	1:F:37:ARG:NE	2.53	0.41
1:B:25:GLU:OE1	1:E:30:SER:HA	2.21	0.41
1:F:87:LYS:HB3	5:F:2113:HOH:O	2.20	0.41
3:J:1166:PEB:HBA3	3:J:1166:PEB:H2A1	1.86	0.41
1:H:37:ARG:HD2	1:H:97:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:1165:PEB:HMC2	2:X:77:MET:HG2	2.01	0.41
2:O:70:MEN:HB2	3:O:1185:PEB:OA	2.21	0.41
2:S:153:LEU:HD21	2:S:155:LYS:HE2	2.03	0.41
1:C:1:MET:HG3	1:C:103:GLY:HA3	2.02	0.41
1:C:25:GLU:O	1:F:29:GLY:HA3	2.21	0.41
1:D:1:MET:HG3	1:D:103:GLY:HA3	2.03	0.41
3:I:1165:PEB:HMC2	2:T:77:MET:HG2	2.01	0.41
1:J:37:ARG:HD2	1:J:97:LEU:O	2.20	0.41
2:R:132:MET:HA	2:R:135:GLN:OE1	2.21	0.41
2:S:139:HIS:HE2	3:S:1187:PEB:HMA3	1.86	0.41
1:A:29:GLY:HA3	1:D:25:GLU:O	2.21	0.41
3:M:1187:PEB:HMB3	3:M:1187:PEB:HNA	1.86	0.41
3:C:1166:PEB:HBA3	3:C:1166:PEB:H2A1	1.90	0.41
1:L:72:ALA:O	1:L:78:PHE:HB3	2.20	0.41
1:D:45:ALA:HB2	1:D:94:GLN:NE2	2.35	0.40
3:J:1165:PEB:HNA	3:J:1165:PEB:CMB	2.35	0.40
1:G:33:ARG:HG2	1:J:25:GLU:HG2	2.04	0.40
2:M:16:THR:HG23	2:O:67:ALA:HB2	2.01	0.40
3:W:1186:PEB:NA	3:W:1186:PEB:HMB2	2.36	0.40
1:B:139:CYS:SG	3:B:1166:PEB:HHA1	2.61	0.40
3:F:1166:PEB:HBA3	3:F:1166:PEB:H2A1	1.80	0.40
1:F:37:ARG:HD2	1:F:97:LEU:O	2.21	0.40
1:G:64:PRO:HD2	5:G:2128:HOH:O	2.22	0.40
1:K:64:PRO:HD2	5:K:2136:HOH:O	2.20	0.40
3:P:1187:PEB:HBB1	3:P:1187:PEB:HHB1	2.04	0.40
3:B:1165:PEB:HBD1	2:M:72:TYR:CE1	2.56	0.40
1:G:25:GLU:OE2	1:J:37:ARG:NE	2.39	0.40
2:M:67:ALA:HB2	2:N:16:THR:HG23	2.03	0.40
2:N:108:LEU:HD21	2:N:179:VAL:HG22	2.03	0.40
2:R:102:VAL:HG23	2:R:106:ARG:HD2	2.04	0.40
2:T:155:LYS:HD2	2:T:155:LYS:HA	1.84	0.40
2:U:108:LEU:HD21	2:U:179:VAL:HG22	2.03	0.40
1:E:2:LYS:HB2	4:E:1167:GOL:H32	2.03	0.40
1:K:97:LEU:HG	1:K:155:LEU:HD12	2.03	0.40
1:D:114:ARG:NH2	5:D:2136:HOH:O	2.53	0.40
1:G:29:GLY:HA3	1:J:25:GLU:O	2.22	0.40
3:J:1165:PEB:HMB2	3:J:1165:PEB:HNA	1.85	0.40
2:N:148:ARG:HH12	3:N:1187:PEB:HND	1.70	0.40
3:O:1187:PEB:HHB1	3:O:1187:PEB:HBB1	2.04	0.40
5:I:2220:HOH:O	2:U:1:MET:N	2.52	0.40
3:V:1186:PEB:HMB2	3:V:1186:PEB:NA	2.36	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%)	3 (2%)	1 (1%)	30	16
1	C	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	D	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
1	E	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	F	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
1	G	162/164 (99%)	160 (99%)	2 (1%)	0	100	100
1	H	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	I	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
1	J	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
1	K	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	L	162/164 (99%)	160 (99%)	2 (1%)	0	100	100
2	M	181/184 (98%)	177 (98%)	4 (2%)	0	100	100
2	N	181/184 (98%)	177 (98%)	3 (2%)	1 (1%)	30	16
2	O	181/184 (98%)	178 (98%)	3 (2%)	0	100	100
2	P	181/184 (98%)	177 (98%)	4 (2%)	0	100	100
2	Q	181/184 (98%)	178 (98%)	3 (2%)	0	100	100
2	R	181/184 (98%)	174 (96%)	7 (4%)	0	100	100
2	S	181/184 (98%)	177 (98%)	4 (2%)	0	100	100
2	T	181/184 (98%)	177 (98%)	4 (2%)	0	100	100
2	U	181/184 (98%)	177 (98%)	4 (2%)	0	100	100
2	V	181/184 (98%)	177 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	W	181/184 (98%)	178 (98%)	3 (2%)	0	100	100
2	X	181/184 (98%)	176 (97%)	5 (3%)	0	100	100
All	All	4116/4176 (99%)	4026 (98%)	88 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	103	GLY
2	N	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%)	127 (100%)	0	100	100
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%)	127 (100%)	0	100	100
1	I	127/127 (100%)	127 (100%)	0	100	100
1	J	127/127 (100%)	126 (99%)	1 (1%)	86	85
1	K	127/127 (100%)	127 (100%)	0	100	100
1	L	127/127 (100%)	126 (99%)	1 (1%)	86	85
2	M	138/138 (100%)	137 (99%)	1 (1%)	88	87
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%)	138 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Q	138/138 (100%)	138 (100%)	0	100	100
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%)	138 (100%)	0	100	100
2	X	138/138 (100%)	138 (100%)	0	100	100
All	All	3180/3180 (100%)	3177 (100%)	3 (0%)	95	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	42	GLU
1	L	61	GLN
2	M	16	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	R	62	GLN

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	0.45	0	6,9,11	1.28	1 (16%)
2	MEN	N	70	2	6,8,9	0.61	0	6,9,11	1.13	1 (16%)
2	MEN	O	70	2	6,8,9	0.50	0	6,9,11	1.37	1 (16%)
2	MEN	P	70	2	6,8,9	0.44	0	6,9,11	1.34	1 (16%)
2	MEN	Q	70	2	6,8,9	0.53	0	6,9,11	1.24	1 (16%)
2	MEN	R	70	2	6,8,9	0.45	0	6,9,11	1.16	1 (16%)
2	MEN	S	70	2	6,8,9	0.45	0	6,9,11	1.41	1 (16%)
2	MEN	T	70	2	6,8,9	0.52	0	6,9,11	1.18	1 (16%)
2	MEN	U	70	2	6,8,9	0.47	0	6,9,11	1.21	1 (16%)
2	MEN	V	70	2	6,8,9	0.52	0	6,9,11	1.27	1 (16%)
2	MEN	W	70	2	6,8,9	0.45	0	6,9,11	1.24	1 (16%)
2	MEN	X	70	2	6,8,9	0.44	0	6,9,11	1.20	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	S	70	MEN	O-C-CA	-3.13	117.32	125.72
2	P	70	MEN	O-C-CA	-3.08	117.47	125.72
2	M	70	MEN	O-C-CA	-3.05	117.55	125.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	70	MEN	O-C-CA	-2.97	117.75	125.72
2	O	70	MEN	O-C-CA	-2.92	117.90	125.72
2	T	70	MEN	O-C-CA	-2.88	118.00	125.72
2	V	70	MEN	O-C-CA	-2.88	118.01	125.72
2	U	70	MEN	O-C-CA	-2.86	118.04	125.72
2	Q	70	MEN	O-C-CA	-2.86	118.05	125.72
2	X	70	MEN	O-C-CA	-2.75	118.36	125.72
2	R	70	MEN	O-C-CA	-2.67	118.56	125.72
2	N	70	MEN	O-C-CA	-2.53	118.95	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	70	MEN	1	0
2	Q	70	MEN	1	0
2	R	70	MEN	1	0
2	V	70	MEN	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

71 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	$\# Z > 2$
3	PEB	A	1165	1	37,46,46	3.41	10 (27%)	36,67,67	2.66	17 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEB	A	1166	1	37,46,46	3.27	11 (29%)	36,67,67	2.38	14 (38%)
4	GOL	A	1167	-	5,5,5	0.27	0	5,5,5	0.26	0
3	PEB	B	1165	1	37,46,46	3.35	9 (24%)	36,67,67	2.52	16 (44%)
3	PEB	B	1166	1	37,46,46	3.31	10 (27%)	36,67,67	2.31	15 (41%)
4	GOL	B	1167	-	5,5,5	0.30	0	5,5,5	0.44	0
3	PEB	C	1165	1	37,46,46	3.41	10 (27%)	36,67,67	2.45	15 (41%)
3	PEB	C	1166	1	37,46,46	3.40	10 (27%)	36,67,67	2.20	14 (38%)
3	PEB	D	1165	1	37,46,46	3.46	10 (27%)	36,67,67	2.68	17 (47%)
3	PEB	D	1166	1	37,46,46	3.38	10 (27%)	36,67,67	2.30	15 (41%)
4	GOL	D	1167	-	5,5,5	0.27	0	5,5,5	0.41	0
3	PEB	E	1165	1	37,46,46	3.52	12 (32%)	36,67,67	2.69	19 (52%)
3	PEB	E	1166	1	37,46,46	3.38	10 (27%)	36,67,67	2.31	14 (38%)
4	GOL	E	1167	-	5,5,5	0.35	0	5,5,5	0.30	0
3	PEB	F	1165	1	37,46,46	3.33	8 (21%)	36,67,67	2.53	14 (38%)
3	PEB	F	1166	1	37,46,46	3.48	10 (27%)	36,67,67	2.09	15 (41%)
3	PEB	G	1165	1	37,46,46	3.26	10 (27%)	36,67,67	2.65	18 (50%)
3	PEB	G	1166	1	37,46,46	3.48	11 (29%)	36,67,67	2.14	12 (33%)
4	GOL	G	1167	-	5,5,5	0.32	0	5,5,5	0.28	0
3	PEB	H	1165	1	37,46,46	3.43	10 (27%)	36,67,67	2.68	18 (50%)
3	PEB	H	1166	1	37,46,46	3.41	11 (29%)	36,67,67	2.30	13 (36%)
4	GOL	H	1167	-	5,5,5	0.37	0	5,5,5	0.25	0
3	PEB	I	1165	1	37,46,46	3.47	11 (29%)	36,67,67	2.60	16 (44%)
3	PEB	I	1166	1	37,46,46	3.42	12 (32%)	36,67,67	2.30	14 (38%)
4	GOL	I	1167	-	5,5,5	0.32	0	5,5,5	0.45	0
3	PEB	J	1165	1	37,46,46	3.47	10 (27%)	36,67,67	2.63	18 (50%)
3	PEB	J	1166	1	37,46,46	3.34	12 (32%)	36,67,67	2.30	13 (36%)
4	GOL	J	1167	-	5,5,5	0.29	0	5,5,5	0.14	0
3	PEB	K	1165	1	37,46,46	3.38	11 (29%)	36,67,67	2.66	19 (52%)
3	PEB	K	1166	1	37,46,46	3.34	9 (24%)	36,67,67	2.27	17 (47%)
4	GOL	K	1167	-	5,5,5	0.24	0	5,5,5	0.34	0
3	PEB	L	1165	1	37,46,46	3.34	10 (27%)	36,67,67	2.71	18 (50%)
3	PEB	L	1166	1	37,46,46	3.31	8 (21%)	36,67,67	2.27	15 (41%)
4	GOL	L	1167	-	5,5,5	0.29	0	5,5,5	0.33	0
3	PEB	M	1185	2	37,46,46	3.35	10 (27%)	36,67,67	2.62	16 (44%)
3	PEB	M	1186	2	37,46,46	3.42	11 (29%)	36,67,67	2.25	14 (38%)
3	PEB	M	1187	2	37,46,46	3.43	9 (24%)	36,67,67	2.32	15 (41%)
3	PEB	N	1185	2	37,46,46	3.37	10 (27%)	36,67,67	2.37	15 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEB	N	1186	2	37,46,46	3.54	9 (24%)	36,67,67	2.22	13 (36%)
3	PEB	N	1187	2	37,46,46	3.51	10 (27%)	36,67,67	2.28	17 (47%)
3	PEB	O	1185	2	37,46,46	3.43	9 (24%)	36,67,67	2.58	15 (41%)
3	PEB	O	1186	2	37,46,46	3.48	10 (27%)	36,67,67	2.20	14 (38%)
3	PEB	O	1187	2	37,46,46	3.40	8 (21%)	36,67,67	2.29	16 (44%)
4	GOL	O	1188	-	5,5,5	0.30	0	5,5,5	0.38	0
3	PEB	P	1185	2	37,46,46	3.31	10 (27%)	36,67,67	2.54	15 (41%)
3	PEB	P	1186	2	37,46,46	3.49	9 (24%)	36,67,67	2.10	14 (38%)
3	PEB	P	1187	2	37,46,46	3.38	9 (24%)	36,67,67	2.39	15 (41%)
3	PEB	Q	1185	2	37,46,46	3.52	11 (29%)	36,67,67	2.47	15 (41%)
3	PEB	Q	1186	2	37,46,46	3.49	9 (24%)	36,67,67	2.26	15 (41%)
3	PEB	Q	1187	2	37,46,46	3.61	10 (27%)	36,67,67	2.26	13 (36%)
3	PEB	R	1185	2	37,46,46	3.55	9 (24%)	36,67,67	2.63	15 (41%)
3	PEB	R	1186	2	37,46,46	3.42	10 (27%)	36,67,67	2.36	14 (38%)
3	PEB	R	1187	2	37,46,46	3.50	13 (35%)	36,67,67	2.33	13 (36%)
3	PEB	S	1185	2	37,46,46	3.56	10 (27%)	36,67,67	2.46	16 (44%)
3	PEB	S	1186	2	37,46,46	3.44	10 (27%)	36,67,67	2.31	16 (44%)
3	PEB	S	1187	2	37,46,46	3.43	8 (21%)	36,67,67	2.26	16 (44%)
3	PEB	T	1185	2	37,46,46	3.42	9 (24%)	36,67,67	2.38	13 (36%)
3	PEB	T	1186	2	37,46,46	3.38	9 (24%)	36,67,67	2.32	15 (41%)
3	PEB	T	1187	2	37,46,46	3.64	11 (29%)	36,67,67	2.33	15 (41%)
3	PEB	U	1185	2	37,46,46	3.34	11 (29%)	36,67,67	2.59	16 (44%)
3	PEB	U	1186	2	37,46,46	3.35	9 (24%)	36,67,67	2.29	15 (41%)
3	PEB	U	1187	2	37,46,46	3.57	10 (27%)	36,67,67	2.39	18 (50%)
3	PEB	V	1185	2	37,46,46	3.38	10 (27%)	36,67,67	2.55	16 (44%)
3	PEB	V	1186	2	37,46,46	3.46	11 (29%)	36,67,67	2.16	11 (30%)
3	PEB	V	1187	2	37,46,46	3.47	11 (29%)	36,67,67	2.25	17 (47%)
3	PEB	W	1185	2	37,46,46	3.32	11 (29%)	36,67,67	2.48	14 (38%)
3	PEB	W	1186	2	37,46,46	3.35	10 (27%)	36,67,67	2.25	16 (44%)
3	PEB	W	1187	2	37,46,46	3.53	11 (29%)	36,67,67	2.30	18 (50%)
3	PEB	X	1185	2	37,46,46	3.32	9 (24%)	36,67,67	2.75	18 (50%)
3	PEB	X	1186	2	37,46,46	3.37	10 (27%)	36,67,67	2.19	16 (44%)
3	PEB	X	1187	2	37,46,46	3.53	9 (24%)	36,67,67	2.14	13 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEB	A	1165	1	-	2/19/74/74	0/4/4/4
3	PEB	A	1166	1	-	2/19/74/74	0/4/4/4
4	GOL	A	1167	-	-	0/4/4/4	0/0/0/0
3	PEB	B	1165	1	-	2/19/74/74	0/4/4/4
3	PEB	B	1166	1	-	2/19/74/74	0/4/4/4
4	GOL	B	1167	-	-	0/4/4/4	0/0/0/0
3	PEB	C	1165	1	-	2/19/74/74	0/4/4/4
3	PEB	C	1166	1	-	2/19/74/74	0/4/4/4
3	PEB	D	1165	1	-	2/19/74/74	0/4/4/4
3	PEB	D	1166	1	-	2/19/74/74	0/4/4/4
4	GOL	D	1167	-	-	0/4/4/4	0/0/0/0
3	PEB	E	1165	1	-	2/19/74/74	0/4/4/4
3	PEB	E	1166	1	-	2/19/74/74	0/4/4/4
4	GOL	E	1167	-	-	0/4/4/4	0/0/0/0
3	PEB	F	1165	1	-	2/19/74/74	0/4/4/4
3	PEB	F	1166	1	-	2/19/74/74	0/4/4/4
3	PEB	G	1165	1	-	2/19/74/74	0/4/4/4
3	PEB	G	1166	1	-	2/19/74/74	0/4/4/4
4	GOL	G	1167	-	-	0/4/4/4	0/0/0/0
3	PEB	H	1165	1	-	2/19/74/74	0/4/4/4
3	PEB	H	1166	1	-	2/19/74/74	0/4/4/4
4	GOL	H	1167	-	-	0/4/4/4	0/0/0/0
3	PEB	I	1165	1	-	2/19/74/74	0/4/4/4
3	PEB	I	1166	1	-	2/19/74/74	0/4/4/4
4	GOL	I	1167	-	-	0/4/4/4	0/0/0/0
3	PEB	J	1165	1	-	2/19/74/74	0/4/4/4
3	PEB	J	1166	1	-	2/19/74/74	0/4/4/4
4	GOL	J	1167	-	-	0/4/4/4	0/0/0/0
3	PEB	K	1165	1	-	2/19/74/74	0/4/4/4
3	PEB	K	1166	1	-	2/19/74/74	0/4/4/4
4	GOL	K	1167	-	-	0/4/4/4	0/0/0/0
3	PEB	L	1165	1	-	2/19/74/74	0/4/4/4
3	PEB	L	1166	1	-	2/19/74/74	0/4/4/4
4	GOL	L	1167	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEB	M	1185	2	-	2/19/74/74	0/4/4/4
3	PEB	M	1186	2	-	2/19/74/74	0/4/4/4
3	PEB	M	1187	2	-	2/19/74/74	0/4/4/4
3	PEB	N	1185	2	-	2/19/74/74	0/4/4/4
3	PEB	N	1186	2	-	2/19/74/74	0/4/4/4
3	PEB	N	1187	2	-	2/19/74/74	0/4/4/4
3	PEB	O	1185	2	-	2/19/74/74	0/4/4/4
3	PEB	O	1186	2	-	2/19/74/74	0/4/4/4
3	PEB	O	1187	2	-	2/19/74/74	0/4/4/4
4	GOL	O	1188	-	-	0/4/4/4	0/0/0/0
3	PEB	P	1185	2	-	2/19/74/74	0/4/4/4
3	PEB	P	1186	2	-	2/19/74/74	0/4/4/4
3	PEB	P	1187	2	-	2/19/74/74	0/4/4/4
3	PEB	Q	1185	2	-	2/19/74/74	0/4/4/4
3	PEB	Q	1186	2	-	2/19/74/74	0/4/4/4
3	PEB	Q	1187	2	-	2/19/74/74	0/4/4/4
3	PEB	R	1185	2	-	2/19/74/74	0/4/4/4
3	PEB	R	1186	2	-	2/19/74/74	0/4/4/4
3	PEB	R	1187	2	-	2/19/74/74	0/4/4/4
3	PEB	S	1185	2	-	2/19/74/74	0/4/4/4
3	PEB	S	1186	2	-	2/19/74/74	0/4/4/4
3	PEB	S	1187	2	-	2/19/74/74	0/4/4/4
3	PEB	T	1185	2	-	2/19/74/74	0/4/4/4
3	PEB	T	1186	2	-	2/19/74/74	0/4/4/4
3	PEB	T	1187	2	-	2/19/74/74	0/4/4/4
3	PEB	U	1185	2	-	2/19/74/74	0/4/4/4
3	PEB	U	1186	2	-	2/19/74/74	0/4/4/4
3	PEB	U	1187	2	-	2/19/74/74	0/4/4/4
3	PEB	V	1185	2	-	2/19/74/74	0/4/4/4
3	PEB	V	1186	2	-	2/19/74/74	0/4/4/4
3	PEB	V	1187	2	-	2/19/74/74	0/4/4/4
3	PEB	W	1185	2	-	2/19/74/74	0/4/4/4
3	PEB	W	1186	2	-	2/19/74/74	0/4/4/4
3	PEB	W	1187	2	-	2/19/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEB	X	1185	2	-	2/19/74/74	0/4/4/4
3	PEB	X	1186	2	-	2/19/74/74	0/4/4/4
3	PEB	X	1187	2	-	2/19/74/74	0/4/4/4

All (600) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	1186	PEB	C1A-NA	-3.72	1.32	1.37
3	W	1186	PEB	C1A-NA	-3.68	1.32	1.37
3	O	1185	PEB	C1A-NA	-3.64	1.32	1.37
3	M	1186	PEB	C1A-NA	-3.55	1.33	1.37
3	B	1166	PEB	C1A-NA	-3.45	1.33	1.37
3	B	1165	PEB	C1A-NA	-3.44	1.33	1.37
3	X	1187	PEB	C1A-NA	-3.43	1.33	1.37
3	T	1186	PEB	C1A-NA	-3.39	1.33	1.37
3	U	1187	PEB	C1A-NA	-3.38	1.33	1.37
3	F	1166	PEB	C1A-NA	-3.38	1.33	1.37
3	P	1187	PEB	C1A-NA	-3.37	1.33	1.37
3	K	1166	PEB	C1A-NA	-3.36	1.33	1.37
3	E	1165	PEB	C1A-NA	-3.35	1.33	1.37
3	G	1166	PEB	C1A-NA	-3.34	1.33	1.37
3	Q	1185	PEB	C1A-NA	-3.27	1.33	1.37
3	N	1186	PEB	C1A-NA	-3.27	1.33	1.37
3	R	1186	PEB	C1A-NA	-3.26	1.33	1.37
3	I	1165	PEB	C1A-NA	-3.25	1.33	1.37
3	V	1185	PEB	C1A-NA	-3.23	1.33	1.37
3	X	1186	PEB	C1A-NA	-3.20	1.33	1.37
3	M	1187	PEB	C1A-NA	-3.20	1.33	1.37
3	O	1186	PEB	C1A-NA	-3.18	1.33	1.37
3	H	1166	PEB	C1A-NA	-3.15	1.33	1.37
3	T	1185	PEB	C1A-NA	-3.14	1.33	1.37
3	H	1165	PEB	C2A-C1A	-3.11	1.49	1.52
3	U	1186	PEB	C1A-NA	-3.10	1.33	1.37
3	N	1187	PEB	C1A-NA	-3.10	1.33	1.37
3	N	1185	PEB	C1A-NA	-3.08	1.33	1.37
3	Q	1186	PEB	C1A-NA	-3.04	1.33	1.37
3	R	1187	PEB	C1A-NA	-3.03	1.33	1.37
3	W	1187	PEB	C1A-NA	-3.02	1.33	1.37
3	C	1166	PEB	C1A-NA	-3.00	1.33	1.37
3	S	1186	PEB	C1A-NA	-2.97	1.33	1.37
3	S	1185	PEB	C1A-NA	-2.96	1.33	1.37
3	V	1187	PEB	C1A-NA	-2.95	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1166	PEB	C1A-NA	-2.93	1.33	1.37
3	E	1166	PEB	C1A-NA	-2.93	1.33	1.37
3	D	1166	PEB	C1A-NA	-2.91	1.33	1.37
3	T	1187	PEB	C1A-NA	-2.91	1.33	1.37
3	O	1187	PEB	C1A-NA	-2.90	1.33	1.37
3	K	1165	PEB	C1A-NA	-2.88	1.33	1.37
3	L	1166	PEB	C1A-NA	-2.86	1.33	1.37
3	Q	1187	PEB	C1A-NA	-2.84	1.34	1.37
3	W	1185	PEB	C1A-NA	-2.84	1.34	1.37
3	X	1185	PEB	C1A-NA	-2.84	1.34	1.37
3	S	1187	PEB	C1A-NA	-2.83	1.34	1.37
3	E	1165	PEB	C2A-C1A	-2.82	1.49	1.52
3	V	1186	PEB	C1A-NA	-2.81	1.34	1.37
3	J	1165	PEB	C1A-NA	-2.81	1.34	1.37
3	K	1165	PEB	C2A-C1A	-2.79	1.49	1.52
3	J	1166	PEB	C1A-NA	-2.77	1.34	1.37
3	U	1185	PEB	C1A-NA	-2.73	1.34	1.37
3	M	1185	PEB	C1A-NA	-2.72	1.34	1.37
3	X	1185	PEB	C2A-C1A	-2.71	1.49	1.52
3	A	1165	PEB	C2A-C1A	-2.69	1.49	1.52
3	P	1185	PEB	C1A-NA	-2.65	1.34	1.37
3	H	1165	PEB	C1A-NA	-2.64	1.34	1.37
3	L	1165	PEB	C2A-C1A	-2.62	1.49	1.52
3	A	1165	PEB	C1A-NA	-2.59	1.34	1.37
3	C	1165	PEB	C1A-NA	-2.57	1.34	1.37
3	J	1165	PEB	C2A-C1A	-2.56	1.49	1.52
3	R	1185	PEB	C1A-NA	-2.54	1.34	1.37
3	D	1165	PEB	C2A-C1A	-2.45	1.49	1.52
3	F	1165	PEB	C1A-NA	-2.43	1.34	1.37
3	A	1166	PEB	C1A-NA	-2.42	1.34	1.37
3	G	1165	PEB	C2A-C1A	-2.41	1.49	1.52
3	I	1165	PEB	C2A-C1A	-2.40	1.49	1.52
3	G	1165	PEB	C1A-NA	-2.37	1.34	1.37
3	U	1186	PEB	C2A-C1A	-2.36	1.49	1.52
3	W	1185	PEB	C2A-C1A	-2.35	1.49	1.52
3	P	1185	PEB	C2A-C1A	-2.34	1.49	1.52
3	C	1165	PEB	C2A-C1A	-2.32	1.49	1.52
3	A	1166	PEB	C2A-C1A	-2.32	1.49	1.52
3	S	1185	PEB	C2A-C1A	-2.30	1.49	1.52
3	O	1186	PEB	C2A-C1A	-2.29	1.49	1.52
3	M	1185	PEB	C2A-C1A	-2.29	1.49	1.52
3	N	1185	PEB	C2A-C1A	-2.24	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	1186	PEB	C2A-C1A	-2.22	1.50	1.52
3	U	1185	PEB	C2A-C1A	-2.21	1.50	1.52
3	B	1166	PEB	C2A-C1A	-2.21	1.50	1.52
3	S	1186	PEB	C2A-C1A	-2.19	1.50	1.52
3	Q	1185	PEB	C2A-C1A	-2.18	1.50	1.52
3	L	1165	PEB	C1A-NA	-2.18	1.34	1.37
3	T	1185	PEB	C2A-C1A	-2.18	1.50	1.52
3	M	1186	PEB	C2A-C1A	-2.13	1.50	1.52
3	D	1165	PEB	C1A-NA	-2.12	1.34	1.37
3	J	1166	PEB	C2A-C1A	-2.10	1.50	1.52
3	G	1166	PEB	C2A-C1A	-2.05	1.50	1.52
3	R	1187	PEB	C2A-C1A	-2.02	1.50	1.52
3	H	1166	PEB	C2A-C1A	-2.01	1.50	1.52
3	E	1165	PEB	C4B-C3B	2.00	1.49	1.45
3	P	1185	PEB	C1C-CHB	2.01	1.48	1.40
3	R	1186	PEB	C1D-ND	2.02	1.48	1.45
3	X	1186	PEB	C1C-CHB	2.02	1.48	1.40
3	E	1165	PEB	C1B-C2B	2.02	1.50	1.45
3	U	1185	PEB	C1B-C2B	2.02	1.50	1.45
3	W	1185	PEB	C1C-CHB	2.03	1.48	1.40
3	D	1166	PEB	C1C-CHB	2.03	1.48	1.40
3	W	1187	PEB	C4B-C3B	2.03	1.49	1.45
3	R	1187	PEB	C1D-ND	2.03	1.48	1.45
3	G	1165	PEB	C1C-CHB	2.03	1.48	1.40
3	I	1166	PEB	C4B-C3B	2.03	1.49	1.45
3	W	1186	PEB	C1D-ND	2.04	1.48	1.45
3	K	1166	PEB	C1C-CHB	2.04	1.48	1.40
3	N	1185	PEB	C1B-C2B	2.04	1.50	1.45
3	B	1166	PEB	C1C-CHB	2.04	1.48	1.40
3	C	1166	PEB	C1D-ND	2.05	1.48	1.45
3	O	1186	PEB	C1C-CHB	2.06	1.48	1.40
3	R	1186	PEB	C1C-CHB	2.07	1.48	1.40
3	P	1187	PEB	C4B-C3B	2.08	1.49	1.45
3	I	1166	PEB	C1C-CHB	2.08	1.48	1.40
3	K	1165	PEB	C1D-ND	2.08	1.48	1.45
3	W	1187	PEB	C1B-C2B	2.09	1.50	1.45
3	F	1166	PEB	C1C-CHB	2.09	1.48	1.40
3	W	1185	PEB	C1D-ND	2.09	1.48	1.45
3	Q	1185	PEB	C1B-C2B	2.09	1.50	1.45
3	Q	1187	PEB	C1D-ND	2.10	1.48	1.45
3	V	1187	PEB	C1B-C2B	2.10	1.50	1.45
3	B	1165	PEB	C1C-CHB	2.10	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1166	PEB	C1B-C2B	2.10	1.50	1.45
3	V	1185	PEB	C1C-CHB	2.11	1.48	1.40
3	M	1185	PEB	C1C-CHB	2.12	1.48	1.40
3	U	1185	PEB	C1D-ND	2.12	1.49	1.45
3	U	1187	PEB	C4B-C3B	2.12	1.49	1.45
3	I	1165	PEB	C1B-C2B	2.13	1.50	1.45
3	I	1166	PEB	C1B-C2B	2.13	1.50	1.45
3	J	1166	PEB	C1D-ND	2.14	1.49	1.45
3	M	1186	PEB	C1C-CHB	2.14	1.48	1.40
3	V	1186	PEB	C1C-CHB	2.14	1.48	1.40
3	X	1186	PEB	C1D-ND	2.15	1.49	1.45
3	V	1187	PEB	C1D-ND	2.15	1.49	1.45
3	R	1187	PEB	C1B-C2B	2.15	1.50	1.45
3	W	1186	PEB	C1C-CHB	2.16	1.48	1.40
3	G	1166	PEB	C1C-CHB	2.16	1.48	1.40
3	H	1165	PEB	C1C-CHB	2.17	1.48	1.40
3	J	1166	PEB	C1C-CHB	2.17	1.48	1.40
3	R	1187	PEB	C4B-C3B	2.17	1.49	1.45
3	I	1165	PEB	C1C-CHB	2.17	1.48	1.40
3	E	1166	PEB	C1D-ND	2.17	1.49	1.45
3	Q	1186	PEB	C1C-CHB	2.18	1.48	1.40
3	J	1165	PEB	C1C-CHB	2.18	1.48	1.40
3	N	1187	PEB	C1C-CHB	2.18	1.48	1.40
3	S	1185	PEB	C1C-CHB	2.18	1.48	1.40
3	T	1186	PEB	C1C-CHB	2.18	1.48	1.40
3	A	1166	PEB	C1C-CHB	2.18	1.48	1.40
3	E	1165	PEB	C1C-CHB	2.18	1.48	1.40
3	P	1186	PEB	C1C-CHB	2.18	1.48	1.40
3	T	1187	PEB	C1D-ND	2.19	1.49	1.45
3	E	1166	PEB	C1C-CHB	2.19	1.48	1.40
3	S	1186	PEB	C1C-CHB	2.20	1.48	1.40
3	M	1187	PEB	C1C-CHB	2.20	1.48	1.40
3	H	1166	PEB	C1C-CHB	2.21	1.48	1.40
3	L	1165	PEB	C1C-CHB	2.21	1.48	1.40
3	T	1187	PEB	C4B-C3B	2.21	1.49	1.45
3	R	1185	PEB	C1C-CHB	2.22	1.48	1.40
3	K	1165	PEB	C1C-CHB	2.22	1.48	1.40
3	Q	1185	PEB	C1C-CHB	2.22	1.48	1.40
3	H	1166	PEB	C1D-ND	2.22	1.49	1.45
3	R	1187	PEB	C1C-CHB	2.22	1.48	1.40
3	O	1185	PEB	C1B-C2B	2.26	1.50	1.45
3	C	1165	PEB	C1C-CHB	2.26	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1166	PEB	C1D-ND	2.27	1.49	1.45
3	G	1166	PEB	C1D-ND	2.27	1.49	1.45
3	V	1186	PEB	C1D-ND	2.28	1.49	1.45
3	D	1166	PEB	C1D-ND	2.28	1.49	1.45
3	W	1187	PEB	C1C-CHB	2.28	1.49	1.40
3	U	1187	PEB	C1C-CHB	2.29	1.49	1.40
3	A	1165	PEB	C1C-CHB	2.29	1.49	1.40
3	C	1166	PEB	C1C-CHB	2.29	1.49	1.40
3	A	1166	PEB	C1D-ND	2.31	1.49	1.45
3	D	1165	PEB	C1C-CHB	2.32	1.49	1.40
3	V	1185	PEB	C1B-C2B	2.32	1.51	1.45
3	S	1186	PEB	OD-C4D	2.35	1.28	1.23
3	O	1185	PEB	OD-C4D	2.37	1.28	1.23
3	N	1187	PEB	C4B-C3B	2.39	1.49	1.45
3	V	1187	PEB	C4B-C3B	2.39	1.49	1.45
3	N	1186	PEB	C1C-CHB	2.41	1.49	1.40
3	X	1187	PEB	C1C-CHB	2.42	1.49	1.40
3	M	1187	PEB	OD-C4D	2.44	1.28	1.23
3	T	1187	PEB	C1C-CHB	2.47	1.49	1.40
3	Q	1187	PEB	C1C-CHB	2.47	1.49	1.40
3	R	1186	PEB	OD-C4D	2.49	1.28	1.23
3	N	1187	PEB	OD-C4D	2.54	1.28	1.23
3	W	1185	PEB	OD-C4D	2.56	1.28	1.23
3	F	1166	PEB	C1D-ND	2.56	1.49	1.45
3	V	1185	PEB	OD-C4D	2.56	1.28	1.23
3	U	1186	PEB	OD-C4D	2.58	1.28	1.23
3	X	1185	PEB	OD-C4D	2.60	1.28	1.23
3	W	1186	PEB	OD-C4D	2.62	1.28	1.23
3	M	1185	PEB	OD-C4D	2.64	1.28	1.23
3	U	1187	PEB	OD-C4D	2.64	1.28	1.23
3	Q	1185	PEB	OD-C4D	2.64	1.28	1.23
3	E	1165	PEB	OD-C4D	2.65	1.28	1.23
3	N	1185	PEB	OD-C4D	2.70	1.28	1.23
3	O	1187	PEB	OD-C4D	2.71	1.28	1.23
3	N	1186	PEB	OD-C4D	2.73	1.28	1.23
3	B	1165	PEB	OD-C4D	2.75	1.28	1.23
3	P	1186	PEB	OD-C4D	2.77	1.28	1.23
3	X	1187	PEB	OD-C4D	2.77	1.28	1.23
3	W	1187	PEB	OD-C4D	2.77	1.28	1.23
3	Q	1186	PEB	OD-C4D	2.78	1.28	1.23
3	A	1165	PEB	OD-C4D	2.78	1.28	1.23
3	K	1166	PEB	OD-C4D	2.78	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	1185	PEB	OD-C4D	2.78	1.28	1.23
3	R	1187	PEB	OD-C4D	2.79	1.28	1.23
3	A	1166	PEB	OD-C4D	2.79	1.28	1.23
3	S	1187	PEB	OD-C4D	2.79	1.28	1.23
3	H	1165	PEB	OD-C4D	2.80	1.28	1.23
3	L	1166	PEB	OD-C4D	2.80	1.28	1.23
3	V	1186	PEB	OD-C4D	2.81	1.28	1.23
3	I	1166	PEB	OD-C4D	2.83	1.29	1.23
3	Q	1187	PEB	OD-C4D	2.83	1.29	1.23
3	K	1165	PEB	OD-C4D	2.84	1.29	1.23
3	F	1165	PEB	OD-C4D	2.85	1.29	1.23
3	T	1187	PEB	OD-C4D	2.87	1.29	1.23
3	T	1185	PEB	OD-C4D	2.88	1.29	1.23
3	X	1186	PEB	OD-C4D	2.93	1.29	1.23
3	A	1166	PEB	C2C-C3C	2.93	1.46	1.37
3	R	1185	PEB	OD-C4D	2.93	1.29	1.23
3	S	1185	PEB	OD-C4D	2.94	1.29	1.23
3	M	1186	PEB	OD-C4D	2.95	1.29	1.23
3	B	1166	PEB	OD-C4D	2.95	1.29	1.23
3	H	1166	PEB	OD-C4D	2.96	1.29	1.23
3	D	1165	PEB	OD-C4D	2.97	1.29	1.23
3	P	1187	PEB	OD-C4D	2.98	1.29	1.23
3	E	1166	PEB	OD-C4D	2.99	1.29	1.23
3	T	1186	PEB	OD-C4D	3.00	1.29	1.23
3	P	1185	PEB	OD-C4D	3.01	1.29	1.23
3	G	1166	PEB	OD-C4D	3.02	1.29	1.23
3	F	1166	PEB	OD-C4D	3.03	1.29	1.23
3	G	1165	PEB	OD-C4D	3.09	1.29	1.23
3	J	1166	PEB	OD-C4D	3.11	1.29	1.23
3	M	1186	PEB	C1D-ND	3.12	1.50	1.45
3	V	1187	PEB	OD-C4D	3.13	1.29	1.23
3	G	1165	PEB	C2C-C3C	3.13	1.47	1.37
3	C	1166	PEB	OD-C4D	3.13	1.29	1.23
3	L	1165	PEB	OD-C4D	3.15	1.29	1.23
3	O	1186	PEB	OD-C4D	3.17	1.29	1.23
3	L	1166	PEB	C2C-C3C	3.21	1.47	1.37
3	X	1187	PEB	C2C-C3C	3.21	1.47	1.37
3	M	1187	PEB	C2C-C3C	3.22	1.47	1.37
3	K	1165	PEB	C2C-C3C	3.23	1.47	1.37
3	Q	1186	PEB	C2C-C3C	3.24	1.47	1.37
3	D	1166	PEB	OD-C4D	3.24	1.29	1.23
3	I	1165	PEB	OD-C4D	3.24	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1166	PEB	C2C-C3C	3.24	1.47	1.37
3	A	1165	PEB	C2C-C3C	3.25	1.47	1.37
3	V	1187	PEB	C2C-C3C	3.26	1.47	1.37
3	L	1166	PEB	CHA-C1B	3.26	1.48	1.40
3	J	1165	PEB	OD-C4D	3.27	1.29	1.23
3	W	1187	PEB	C2C-C3C	3.27	1.47	1.37
3	T	1186	PEB	C2C-C3C	3.27	1.47	1.37
3	Q	1187	PEB	C2C-C3C	3.28	1.47	1.37
3	P	1186	PEB	C2C-C3C	3.28	1.47	1.37
3	D	1166	PEB	C2C-C3C	3.28	1.47	1.37
3	E	1166	PEB	CHA-C1B	3.29	1.48	1.40
3	S	1187	PEB	C2C-C3C	3.29	1.47	1.37
3	B	1165	PEB	C2C-C3C	3.32	1.47	1.37
3	U	1187	PEB	C2C-C3C	3.32	1.47	1.37
3	N	1185	PEB	C2C-C3C	3.32	1.47	1.37
3	I	1166	PEB	C2C-C3C	3.33	1.47	1.37
3	R	1187	PEB	C2C-C3C	3.34	1.47	1.37
3	H	1166	PEB	CHA-C1B	3.35	1.48	1.40
3	N	1186	PEB	C2C-C3C	3.36	1.47	1.37
3	O	1187	PEB	C2C-C3C	3.37	1.47	1.37
3	C	1166	PEB	CHA-C1B	3.38	1.48	1.40
3	X	1186	PEB	C2C-C3C	3.38	1.47	1.37
3	J	1166	PEB	C2C-C3C	3.38	1.47	1.37
3	C	1165	PEB	OD-C4D	3.39	1.30	1.23
3	E	1166	PEB	C2C-C3C	3.39	1.47	1.37
3	V	1185	PEB	C2C-C3C	3.40	1.47	1.37
3	T	1187	PEB	C2C-C3C	3.40	1.47	1.37
3	P	1187	PEB	C2C-C3C	3.40	1.47	1.37
3	K	1166	PEB	C2C-C3C	3.40	1.47	1.37
3	L	1165	PEB	C2C-C3C	3.41	1.47	1.37
3	O	1185	PEB	C2C-C3C	3.41	1.47	1.37
3	L	1165	PEB	CHA-C1B	3.41	1.48	1.40
3	G	1165	PEB	CHA-C1B	3.42	1.48	1.40
3	S	1185	PEB	C2C-C3C	3.42	1.47	1.37
3	J	1166	PEB	CHA-C1B	3.43	1.48	1.40
3	G	1166	PEB	C2C-C3C	3.45	1.47	1.37
3	C	1166	PEB	C2C-C3C	3.45	1.47	1.37
3	W	1186	PEB	C2C-C3C	3.45	1.47	1.37
3	R	1185	PEB	C2C-C3C	3.45	1.47	1.37
3	P	1185	PEB	C2C-C3C	3.45	1.47	1.37
3	D	1166	PEB	CHA-C1B	3.45	1.49	1.40
3	N	1187	PEB	C2C-C3C	3.46	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1165	PEB	C2C-C3C	3.46	1.47	1.37
3	D	1165	PEB	C2C-C3C	3.47	1.47	1.37
3	F	1166	PEB	CHA-C1B	3.47	1.49	1.40
3	C	1165	PEB	C2C-C3C	3.47	1.48	1.37
3	E	1165	PEB	CHA-C1B	3.48	1.49	1.40
3	F	1166	PEB	C2C-C3C	3.49	1.48	1.37
3	K	1166	PEB	CHA-C1B	3.49	1.49	1.40
3	T	1186	PEB	CHA-C1B	3.50	1.49	1.40
3	B	1166	PEB	CHA-C1B	3.51	1.49	1.40
3	T	1185	PEB	C2C-C3C	3.51	1.48	1.37
3	I	1166	PEB	CHA-C1B	3.51	1.49	1.40
3	Q	1185	PEB	C2C-C3C	3.52	1.48	1.37
3	B	1166	PEB	C2C-C3C	3.52	1.48	1.37
3	J	1165	PEB	C2C-C3C	3.52	1.48	1.37
3	F	1165	PEB	C2C-C3C	3.52	1.48	1.37
3	R	1186	PEB	C2C-C3C	3.52	1.48	1.37
3	X	1186	PEB	CHA-C1B	3.54	1.49	1.40
3	F	1165	PEB	CHA-C1B	3.55	1.49	1.40
3	H	1165	PEB	CHA-C1B	3.55	1.49	1.40
3	M	1185	PEB	C2C-C3C	3.55	1.48	1.37
3	A	1166	PEB	CHA-C1B	3.56	1.49	1.40
3	X	1185	PEB	C2C-C3C	3.56	1.48	1.37
3	W	1185	PEB	C2C-C3C	3.56	1.48	1.37
3	E	1165	PEB	C2C-C3C	3.57	1.48	1.37
3	S	1186	PEB	CHA-C1B	3.57	1.49	1.40
3	O	1187	PEB	CHA-C1B	3.57	1.49	1.40
3	V	1186	PEB	C2C-C3C	3.57	1.48	1.37
3	R	1185	PEB	CHA-C1B	3.57	1.49	1.40
3	K	1165	PEB	CHA-C1B	3.59	1.49	1.40
3	M	1186	PEB	C2C-C3C	3.59	1.48	1.37
3	U	1186	PEB	C2C-C3C	3.60	1.48	1.37
3	U	1185	PEB	C2C-C3C	3.60	1.48	1.37
3	H	1165	PEB	C2C-C3C	3.61	1.48	1.37
3	J	1165	PEB	CHA-C1B	3.62	1.49	1.40
3	A	1165	PEB	CHA-C1B	3.62	1.49	1.40
3	O	1186	PEB	C2C-C3C	3.62	1.48	1.37
3	S	1186	PEB	C2C-C3C	3.63	1.48	1.37
3	M	1186	PEB	CHA-C1B	3.66	1.49	1.40
3	T	1187	PEB	CHA-C1B	3.68	1.49	1.40
3	X	1187	PEB	CHA-C1B	3.71	1.49	1.40
3	D	1165	PEB	CHA-C1B	3.71	1.49	1.40
3	B	1165	PEB	CHA-C1B	3.72	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	1186	PEB	CHA-C1B	3.72	1.49	1.40
3	N	1187	PEB	CHA-C1B	3.73	1.49	1.40
3	P	1185	PEB	CHA-C1B	3.73	1.49	1.40
3	V	1185	PEB	CHA-C1B	3.74	1.49	1.40
3	W	1187	PEB	CHA-C1B	3.74	1.49	1.40
3	T	1185	PEB	CHA-C1B	3.76	1.49	1.40
3	O	1186	PEB	CHA-C1B	3.77	1.49	1.40
3	V	1187	PEB	CHA-C1B	3.79	1.49	1.40
3	G	1166	PEB	CHA-C1B	3.80	1.49	1.40
3	U	1186	PEB	CHA-C1B	3.80	1.49	1.40
3	W	1186	PEB	CHA-C1B	3.82	1.49	1.40
3	R	1187	PEB	CHA-C1B	3.83	1.49	1.40
3	X	1185	PEB	CHA-C1B	3.83	1.49	1.40
3	Q	1186	PEB	CHA-C1B	3.83	1.49	1.40
3	P	1187	PEB	CHA-C1B	3.86	1.49	1.40
3	W	1185	PEB	CHA-C1B	3.88	1.50	1.40
3	Q	1187	PEB	CHA-C1B	3.89	1.50	1.40
3	S	1185	PEB	CHA-C1B	3.91	1.50	1.40
3	S	1187	PEB	CHA-C1B	3.92	1.50	1.40
3	I	1165	PEB	CHA-C1B	3.94	1.50	1.40
3	C	1165	PEB	CHA-C1B	3.96	1.50	1.40
3	U	1185	PEB	CHA-C1B	3.96	1.50	1.40
3	U	1187	PEB	CHA-C1B	3.98	1.50	1.40
3	O	1185	PEB	CHA-C1B	3.99	1.50	1.40
3	P	1186	PEB	CHA-C1B	4.00	1.50	1.40
3	Q	1185	PEB	CHA-C1B	4.05	1.50	1.40
3	N	1185	PEB	CHA-C1B	4.05	1.50	1.40
3	M	1187	PEB	CHA-C1B	4.08	1.50	1.40
3	M	1185	PEB	CHA-C1B	4.14	1.50	1.40
3	V	1186	PEB	CHA-C1B	4.23	1.50	1.40
3	N	1186	PEB	CHA-C1B	4.24	1.50	1.40
3	X	1185	PEB	C3B-C2B	4.54	1.46	1.36
3	W	1185	PEB	C3B-C2B	4.65	1.46	1.36
3	O	1185	PEB	C3B-C2B	4.73	1.47	1.36
3	J	1165	PEB	C3B-C2B	4.79	1.47	1.36
3	S	1186	PEB	C3B-C2B	4.89	1.47	1.36
3	Q	1185	PEB	C3C-C4C	4.90	1.49	1.42
3	G	1165	PEB	C3B-C2B	4.91	1.47	1.36
3	O	1187	PEB	C3B-C2B	4.92	1.47	1.36
3	B	1165	PEB	C3B-C2B	4.92	1.47	1.36
3	V	1185	PEB	C3B-C2B	4.93	1.47	1.36
3	M	1185	PEB	C3B-C2B	4.95	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	1185	PEB	C3B-C2B	4.95	1.47	1.36
3	A	1165	PEB	C3B-C2B	4.96	1.47	1.36
3	L	1166	PEB	C3B-C2B	4.97	1.47	1.36
3	P	1187	PEB	C3B-C2B	4.98	1.47	1.36
3	M	1187	PEB	C3B-C2B	4.99	1.47	1.36
3	P	1185	PEB	C3B-C2B	4.99	1.47	1.36
3	X	1187	PEB	C3B-C2B	4.99	1.47	1.36
3	F	1165	PEB	C3B-C2B	4.99	1.47	1.36
3	K	1165	PEB	C3B-C2B	5.03	1.47	1.36
3	N	1185	PEB	C3B-C2B	5.04	1.47	1.36
3	T	1186	PEB	C3B-C2B	5.04	1.47	1.36
3	V	1187	PEB	C3C-C4C	5.04	1.49	1.42
3	T	1185	PEB	C3B-C2B	5.05	1.47	1.36
3	P	1186	PEB	C3B-C2B	5.05	1.47	1.36
3	V	1187	PEB	C3B-C2B	5.06	1.47	1.36
3	H	1166	PEB	C3C-C4C	5.08	1.49	1.42
3	A	1165	PEB	C3C-C4C	5.09	1.49	1.42
3	D	1165	PEB	C3B-C2B	5.10	1.47	1.36
3	C	1165	PEB	C3B-C2B	5.10	1.47	1.36
3	U	1185	PEB	C3B-C2B	5.12	1.47	1.36
3	L	1165	PEB	C3B-C2B	5.12	1.47	1.36
3	U	1186	PEB	C3B-C2B	5.13	1.47	1.36
3	X	1186	PEB	C3B-C2B	5.14	1.47	1.36
3	M	1186	PEB	C3B-C2B	5.14	1.47	1.36
3	N	1186	PEB	C3B-C2B	5.15	1.47	1.36
3	A	1166	PEB	C3C-C4C	5.16	1.49	1.42
3	O	1186	PEB	C3B-C2B	5.16	1.47	1.36
3	X	1187	PEB	C3C-C4C	5.16	1.49	1.42
3	A	1166	PEB	C3B-C2B	5.17	1.48	1.36
3	B	1166	PEB	C3B-C2B	5.18	1.48	1.36
3	H	1165	PEB	C3B-C2B	5.21	1.48	1.36
3	U	1187	PEB	C3B-C2B	5.22	1.48	1.36
3	R	1186	PEB	C3B-C2B	5.22	1.48	1.36
3	H	1166	PEB	C3B-C2B	5.22	1.48	1.36
3	D	1165	PEB	C3C-C4C	5.23	1.49	1.42
3	Q	1187	PEB	C3B-C2B	5.26	1.48	1.36
3	I	1166	PEB	C3B-C2B	5.27	1.48	1.36
3	E	1166	PEB	C3B-C2B	5.27	1.48	1.36
3	S	1187	PEB	C3B-C2B	5.27	1.48	1.36
3	R	1186	PEB	C3C-C4C	5.27	1.49	1.42
3	H	1165	PEB	C3C-C4C	5.28	1.49	1.42
3	D	1166	PEB	C3C-C4C	5.28	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	1185	PEB	C3B-C2B	5.29	1.48	1.36
3	J	1166	PEB	C3B-C2B	5.29	1.48	1.36
3	O	1187	PEB	C3C-C4C	5.29	1.49	1.42
3	F	1166	PEB	C3B-C2B	5.31	1.48	1.36
3	C	1166	PEB	C3B-C2B	5.33	1.48	1.36
3	T	1187	PEB	C3B-C2B	5.34	1.48	1.36
3	K	1166	PEB	C3C-C4C	5.34	1.49	1.42
3	T	1185	PEB	C3C-C4C	5.34	1.49	1.42
3	D	1166	PEB	C3B-C2B	5.35	1.48	1.36
3	W	1186	PEB	C3B-C2B	5.36	1.48	1.36
3	C	1165	PEB	C3C-C4C	5.36	1.49	1.42
3	Q	1186	PEB	C3B-C2B	5.39	1.48	1.36
3	R	1187	PEB	C3B-C2B	5.39	1.48	1.36
3	Q	1185	PEB	C3B-C2B	5.40	1.48	1.36
3	V	1186	PEB	C3B-C2B	5.40	1.48	1.36
3	I	1165	PEB	C3B-C2B	5.42	1.48	1.36
3	T	1187	PEB	C3C-C4C	5.43	1.50	1.42
3	I	1165	PEB	C3C-C4C	5.47	1.50	1.42
3	K	1166	PEB	C3B-C2B	5.47	1.48	1.36
3	M	1187	PEB	C3C-C4C	5.48	1.50	1.42
3	R	1185	PEB	C3C-C4C	5.48	1.50	1.42
3	E	1165	PEB	C3B-C2B	5.49	1.48	1.36
3	P	1187	PEB	C3C-C4C	5.51	1.50	1.42
3	G	1166	PEB	C3B-C2B	5.52	1.48	1.36
3	N	1187	PEB	C3B-C2B	5.54	1.48	1.36
3	S	1186	PEB	C3C-C4C	5.54	1.50	1.42
3	P	1185	PEB	C3C-C4C	5.55	1.50	1.42
3	J	1166	PEB	C3C-C4C	5.62	1.50	1.42
3	B	1165	PEB	C3C-C4C	5.62	1.50	1.42
3	C	1166	PEB	C3C-C4C	5.63	1.50	1.42
3	W	1187	PEB	C3B-C2B	5.64	1.49	1.36
3	P	1186	PEB	C3C-C4C	5.65	1.50	1.42
3	G	1166	PEB	C3C-C4C	5.66	1.50	1.42
3	J	1165	PEB	C3C-C4C	5.68	1.50	1.42
3	B	1166	PEB	C3C-C4C	5.69	1.50	1.42
3	W	1186	PEB	C3C-C4C	5.69	1.50	1.42
3	I	1166	PEB	C3C-C4C	5.71	1.50	1.42
3	O	1185	PEB	C3C-C4C	5.72	1.50	1.42
3	E	1166	PEB	C3C-C4C	5.73	1.50	1.42
3	V	1186	PEB	C3C-C4C	5.73	1.50	1.42
3	U	1186	PEB	C3C-C4C	5.73	1.50	1.42
3	S	1185	PEB	C3C-C4C	5.74	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	1165	PEB	C3C-C4C	5.75	1.50	1.42
3	W	1185	PEB	C3C-C4C	5.75	1.50	1.42
3	K	1165	PEB	C3C-C4C	5.76	1.50	1.42
3	O	1186	PEB	C3C-C4C	5.77	1.50	1.42
3	U	1185	PEB	C3C-C4C	5.81	1.50	1.42
3	R	1187	PEB	C3C-C4C	5.81	1.50	1.42
3	Q	1187	PEB	C3C-C4C	5.83	1.50	1.42
3	W	1187	PEB	C3C-C4C	5.84	1.50	1.42
3	N	1187	PEB	C3C-C4C	5.84	1.50	1.42
3	X	1185	PEB	C3C-C4C	5.88	1.50	1.42
3	E	1165	PEB	C3C-C4C	5.90	1.50	1.42
3	M	1186	PEB	C3C-C4C	5.91	1.50	1.42
3	Q	1186	PEB	C3C-C4C	5.94	1.50	1.42
3	M	1185	PEB	C3C-C4C	5.95	1.50	1.42
3	L	1166	PEB	C3C-C4C	5.96	1.50	1.42
3	N	1185	PEB	C3C-C4C	5.98	1.50	1.42
3	V	1185	PEB	C3C-C4C	6.02	1.50	1.42
3	F	1166	PEB	C3C-C4C	6.02	1.50	1.42
3	U	1187	PEB	C3C-C4C	6.03	1.50	1.42
3	N	1186	PEB	C3C-C4C	6.06	1.51	1.42
3	T	1186	PEB	C3C-C4C	6.08	1.51	1.42
3	S	1187	PEB	C3C-C4C	6.17	1.51	1.42
3	X	1186	PEB	C3C-C4C	6.18	1.51	1.42
3	F	1165	PEB	C3C-C4C	6.22	1.51	1.42
3	G	1165	PEB	C3C-C4C	6.27	1.51	1.42
3	J	1166	PEB	C2D-C3D	8.34	1.45	1.34
3	B	1166	PEB	C2D-C3D	8.50	1.45	1.34
3	A	1166	PEB	C2D-C3D	8.55	1.45	1.34
3	M	1185	PEB	C2D-C3D	8.64	1.45	1.34
3	W	1186	PEB	C2D-C3D	8.68	1.45	1.34
3	X	1186	PEB	C2D-C3D	8.71	1.46	1.34
3	P	1187	PEB	C2D-C3D	8.73	1.46	1.34
3	U	1186	PEB	C2D-C3D	8.74	1.46	1.34
3	C	1165	PEB	C2D-C3D	8.76	1.46	1.34
3	K	1166	PEB	C2D-C3D	8.78	1.46	1.34
3	A	1165	PEB	C2D-C3D	8.82	1.46	1.34
3	L	1166	PEB	C2D-C3D	8.83	1.46	1.34
3	K	1165	PEB	C2D-C3D	8.90	1.46	1.34
3	G	1166	PEB	C2D-C3D	8.99	1.46	1.34
3	M	1186	PEB	C2D-C3D	8.99	1.46	1.34
3	T	1185	PEB	C2D-C3D	9.00	1.46	1.34
3	B	1165	PEB	C2D-C3D	9.00	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	1187	PEB	C2D-C3D	9.01	1.46	1.34
3	V	1185	PEB	C2D-C3D	9.01	1.46	1.34
3	N	1186	PEB	C2D-C3D	9.03	1.46	1.34
3	X	1185	PEB	C2D-C3D	9.03	1.46	1.34
3	D	1165	PEB	C2D-C3D	9.04	1.46	1.34
3	P	1186	PEB	C2D-C3D	9.04	1.46	1.34
3	O	1185	PEB	C2D-C3D	9.09	1.46	1.34
3	F	1165	PEB	C2D-C3D	9.12	1.46	1.34
3	N	1185	PEB	C2D-C3D	9.13	1.46	1.34
3	C	1166	PEB	C2D-C3D	9.15	1.46	1.34
3	J	1165	PEB	C2D-C3D	9.17	1.46	1.34
3	F	1166	PEB	C2D-C3D	9.17	1.46	1.34
3	U	1185	PEB	C2D-C3D	9.17	1.46	1.34
3	I	1166	PEB	C2D-C3D	9.20	1.46	1.34
3	X	1187	PEB	C2D-C3D	9.23	1.46	1.34
3	U	1187	PEB	C2D-C3D	9.23	1.46	1.34
3	M	1187	PEB	C2D-C3D	9.24	1.46	1.34
3	W	1187	PEB	C2D-C3D	9.28	1.46	1.34
3	O	1187	PEB	C2D-C3D	9.28	1.46	1.34
3	N	1187	PEB	C2D-C3D	9.30	1.46	1.34
3	V	1186	PEB	C2D-C3D	9.30	1.46	1.34
3	S	1185	PEB	C2D-C3D	9.30	1.46	1.34
3	P	1185	PEB	C2D-C3D	9.31	1.46	1.34
3	E	1165	PEB	C2D-C3D	9.35	1.46	1.34
3	G	1165	PEB	C2D-C3D	9.35	1.46	1.34
3	L	1165	PEB	C2D-C3D	9.37	1.46	1.34
3	H	1165	PEB	C2D-C3D	9.38	1.46	1.34
3	D	1166	PEB	C2D-C3D	9.39	1.46	1.34
3	E	1166	PEB	C2D-C3D	9.39	1.46	1.34
3	T	1186	PEB	C2D-C3D	9.39	1.46	1.34
3	S	1186	PEB	C2D-C3D	9.39	1.46	1.34
3	R	1187	PEB	C2D-C3D	9.40	1.46	1.34
3	Q	1186	PEB	C2D-C3D	9.46	1.46	1.34
3	O	1186	PEB	C2D-C3D	9.48	1.47	1.34
3	I	1165	PEB	C2D-C3D	9.49	1.47	1.34
3	H	1166	PEB	C2D-C3D	9.53	1.47	1.34
3	W	1185	PEB	C2D-C3D	9.53	1.47	1.34
3	Q	1187	PEB	C2D-C3D	9.57	1.47	1.34
3	Q	1185	PEB	C2D-C3D	9.60	1.47	1.34
3	S	1187	PEB	C2D-C3D	9.68	1.47	1.34
3	R	1185	PEB	C2D-C3D	9.77	1.47	1.34
3	R	1186	PEB	C2D-C3D	9.79	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	1187	PEB	C2D-C3D	9.89	1.47	1.34
3	G	1165	PEB	CHB-C4B	13.30	1.47	1.35
3	W	1185	PEB	CHB-C4B	13.89	1.47	1.35
3	P	1185	PEB	CHB-C4B	13.97	1.47	1.35
3	U	1185	PEB	CHB-C4B	14.07	1.48	1.35
3	X	1185	PEB	CHB-C4B	14.17	1.48	1.35
3	F	1165	PEB	CHB-C4B	14.19	1.48	1.35
3	L	1165	PEB	CHB-C4B	14.20	1.48	1.35
3	B	1166	PEB	CHB-C4B	14.26	1.48	1.35
3	A	1166	PEB	CHB-C4B	14.27	1.48	1.35
3	T	1186	PEB	CHB-C4B	14.27	1.48	1.35
3	N	1185	PEB	CHB-C4B	14.35	1.48	1.35
3	D	1166	PEB	CHB-C4B	14.37	1.48	1.35
3	W	1186	PEB	CHB-C4B	14.38	1.48	1.35
3	L	1166	PEB	CHB-C4B	14.40	1.48	1.35
3	E	1166	PEB	CHB-C4B	14.41	1.48	1.35
3	K	1165	PEB	CHB-C4B	14.48	1.48	1.35
3	B	1165	PEB	CHB-C4B	14.50	1.48	1.35
3	M	1185	PEB	CHB-C4B	14.50	1.48	1.35
3	K	1166	PEB	CHB-C4B	14.51	1.48	1.35
3	M	1186	PEB	CHB-C4B	14.51	1.48	1.35
3	R	1186	PEB	CHB-C4B	14.53	1.48	1.35
3	X	1186	PEB	CHB-C4B	14.56	1.48	1.35
3	J	1166	PEB	CHB-C4B	14.57	1.48	1.35
3	U	1186	PEB	CHB-C4B	14.62	1.48	1.35
3	V	1185	PEB	CHB-C4B	14.62	1.48	1.35
3	S	1187	PEB	CHB-C4B	14.62	1.48	1.35
3	H	1166	PEB	CHB-C4B	14.65	1.48	1.35
3	I	1165	PEB	CHB-C4B	14.66	1.48	1.35
3	C	1166	PEB	CHB-C4B	14.70	1.48	1.35
3	I	1166	PEB	CHB-C4B	14.77	1.48	1.35
3	P	1187	PEB	CHB-C4B	14.80	1.48	1.35
3	V	1186	PEB	CHB-C4B	14.86	1.48	1.35
3	H	1165	PEB	CHB-C4B	14.87	1.48	1.35
3	C	1165	PEB	CHB-C4B	14.95	1.48	1.35
3	O	1187	PEB	CHB-C4B	14.96	1.48	1.35
3	O	1185	PEB	CHB-C4B	15.02	1.48	1.35
3	O	1186	PEB	CHB-C4B	15.05	1.48	1.35
3	F	1166	PEB	CHB-C4B	15.08	1.48	1.35
3	M	1187	PEB	CHB-C4B	15.08	1.48	1.35
3	G	1166	PEB	CHB-C4B	15.10	1.48	1.35
3	S	1186	PEB	CHB-C4B	15.11	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	1185	PEB	CHB-C4B	15.15	1.48	1.35
3	Q	1186	PEB	CHB-C4B	15.16	1.49	1.35
3	E	1165	PEB	CHB-C4B	15.20	1.49	1.35
3	R	1187	PEB	CHB-C4B	15.21	1.49	1.35
3	A	1165	PEB	CHB-C4B	15.22	1.49	1.35
3	N	1187	PEB	CHB-C4B	15.26	1.49	1.35
3	J	1165	PEB	CHB-C4B	15.32	1.49	1.35
3	V	1187	PEB	CHB-C4B	15.35	1.49	1.35
3	P	1186	PEB	CHB-C4B	15.37	1.49	1.35
3	D	1165	PEB	CHB-C4B	15.45	1.49	1.35
3	Q	1185	PEB	CHB-C4B	15.48	1.49	1.35
3	W	1187	PEB	CHB-C4B	15.50	1.49	1.35
3	N	1186	PEB	CHB-C4B	15.70	1.49	1.35
3	U	1187	PEB	CHB-C4B	15.71	1.49	1.35
3	R	1185	PEB	CHB-C4B	15.75	1.49	1.35
3	S	1185	PEB	CHB-C4B	15.75	1.49	1.35
3	X	1187	PEB	CHB-C4B	15.90	1.49	1.35
3	Q	1187	PEB	CHB-C4B	16.18	1.49	1.35
3	T	1187	PEB	CHB-C4B	16.24	1.49	1.35

All (919) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	1185	PEB	OA-C1A-C2A	-7.05	120.63	126.30
3	O	1185	PEB	C2D-C3D-C4D	-6.62	99.21	108.25
3	M	1185	PEB	OA-C1A-C2A	-6.60	120.99	126.30
3	K	1165	PEB	CHA-C1B-NB	-6.44	112.86	124.89
3	A	1165	PEB	OA-C1A-C2A	-6.37	121.17	126.30
3	Q	1185	PEB	C2D-C3D-C4D	-6.37	99.56	108.25
3	L	1165	PEB	OA-C1A-C2A	-6.36	121.18	126.30
3	F	1165	PEB	CHA-C1B-NB	-6.34	113.04	124.89
3	R	1185	PEB	OA-C1A-C2A	-6.33	121.21	126.30
3	S	1186	PEB	C2D-C3D-C4D	-6.32	99.62	108.25
3	W	1185	PEB	OA-C1A-C2A	-6.32	121.22	126.30
3	V	1185	PEB	C2D-C3D-C4D	-6.30	99.65	108.25
3	X	1185	PEB	C2D-C3D-C4D	-6.29	99.66	108.25
3	D	1165	PEB	OA-C1A-C2A	-6.29	121.24	126.30
3	N	1186	PEB	C2D-C3D-C4D	-6.23	99.74	108.25
3	W	1186	PEB	C2D-C3D-C4D	-6.21	99.77	108.25
3	Q	1186	PEB	C2D-C3D-C4D	-6.21	99.77	108.25
3	S	1187	PEB	C2D-C3D-C4D	-6.19	99.80	108.25
3	T	1187	PEB	C2D-C3D-C4D	-6.16	99.83	108.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	W	1185	PEB	C2D-C3D-C4D	-6.16	99.84	108.25
3	R	1186	PEB	C2D-C3D-C4D	-6.15	99.85	108.25
3	U	1186	PEB	C2D-C3D-C4D	-6.15	99.85	108.25
3	L	1166	PEB	C2D-C3D-C4D	-6.10	99.93	108.25
3	I	1165	PEB	CHA-C1B-NB	-6.09	113.51	124.89
3	K	1166	PEB	C2D-C3D-C4D	-6.09	99.94	108.25
3	M	1185	PEB	C2D-C3D-C4D	-6.06	99.97	108.25
3	P	1185	PEB	C2D-C3D-C4D	-6.06	99.98	108.25
3	M	1187	PEB	C2D-C3D-C4D	-6.05	99.99	108.25
3	L	1165	PEB	C2D-C3D-C4D	-6.05	99.99	108.25
3	N	1185	PEB	C2D-C3D-C4D	-6.05	99.99	108.25
3	B	1165	PEB	CHA-C1B-NB	-6.05	113.60	124.89
3	S	1185	PEB	C2D-C3D-C4D	-6.02	100.04	108.25
3	T	1185	PEB	C2D-C3D-C4D	-6.01	100.04	108.25
3	H	1165	PEB	C2D-C3D-C4D	-6.01	100.05	108.25
3	D	1165	PEB	CHC-C4C-C3C	-5.99	122.88	130.95
3	B	1165	PEB	C2D-C3D-C4D	-5.99	100.07	108.25
3	T	1187	PEB	CHC-C4C-C3C	-5.99	122.89	130.95
3	G	1165	PEB	CHA-C1B-NB	-5.97	113.74	124.89
3	O	1187	PEB	C2D-C3D-C4D	-5.97	100.10	108.25
3	Q	1187	PEB	C2D-C3D-C4D	-5.97	100.10	108.25
3	E	1165	PEB	OA-C1A-C2A	-5.96	121.50	126.30
3	O	1186	PEB	C2D-C3D-C4D	-5.96	100.11	108.25
3	J	1165	PEB	CHA-C1B-NB	-5.95	113.78	124.89
3	T	1186	PEB	C2D-C3D-C4D	-5.94	100.14	108.25
3	E	1165	PEB	C2D-C3D-C4D	-5.93	100.15	108.25
3	P	1187	PEB	C2D-C3D-C4D	-5.93	100.15	108.25
3	J	1165	PEB	C2D-C3D-C4D	-5.93	100.16	108.25
3	X	1187	PEB	C2D-C3D-C4D	-5.93	100.16	108.25
3	H	1166	PEB	CHC-C4C-C3C	-5.92	122.98	130.95
3	U	1187	PEB	C2D-C3D-C4D	-5.90	100.19	108.25
3	N	1187	PEB	C2D-C3D-C4D	-5.90	100.20	108.25
3	V	1186	PEB	C2D-C3D-C4D	-5.89	100.20	108.25
3	R	1185	PEB	C2D-C3D-C4D	-5.87	100.23	108.25
3	U	1185	PEB	C2D-C3D-C4D	-5.87	100.24	108.25
3	E	1165	PEB	CHA-C1B-NB	-5.86	113.95	124.89
3	B	1166	PEB	C2D-C3D-C4D	-5.85	100.26	108.25
3	F	1165	PEB	C2D-C3D-C4D	-5.85	100.27	108.25
3	A	1165	PEB	CHA-C1B-NB	-5.84	113.97	124.89
3	X	1186	PEB	C2D-C3D-C4D	-5.84	100.27	108.25
3	L	1165	PEB	CHA-C1B-NB	-5.84	113.99	124.89
3	G	1165	PEB	C2D-C3D-C4D	-5.79	100.35	108.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1165	PEB	OA-C1A-C2A	-5.77	121.66	126.30
3	E	1166	PEB	C2D-C3D-C4D	-5.74	100.41	108.25
3	A	1165	PEB	C2D-C3D-C4D	-5.74	100.42	108.25
3	A	1166	PEB	C2D-C3D-C4D	-5.73	100.42	108.25
3	P	1186	PEB	C2D-C3D-C4D	-5.72	100.44	108.25
3	H	1166	PEB	C2D-C3D-C4D	-5.71	100.45	108.25
3	D	1165	PEB	C2D-C3D-C4D	-5.69	100.48	108.25
3	G	1166	PEB	C2D-C3D-C4D	-5.69	100.48	108.25
3	R	1187	PEB	C2D-C3D-C4D	-5.68	100.50	108.25
3	C	1166	PEB	C2D-C3D-C4D	-5.64	100.55	108.25
3	J	1165	PEB	OA-C1A-C2A	-5.61	121.79	126.30
3	I	1165	PEB	C2D-C3D-C4D	-5.60	100.60	108.25
3	W	1187	PEB	C2D-C3D-C4D	-5.57	100.65	108.25
3	P	1185	PEB	OA-C1A-C2A	-5.55	121.83	126.30
3	Q	1187	PEB	CHC-C4C-C3C	-5.54	123.49	130.95
3	I	1166	PEB	C2D-C3D-C4D	-5.53	100.69	108.25
3	C	1165	PEB	CHA-C1B-NB	-5.52	114.58	124.89
3	M	1186	PEB	C2D-C3D-C4D	-5.51	100.73	108.25
3	J	1166	PEB	OA-C1A-C2A	-5.50	121.88	126.30
3	K	1165	PEB	C2D-C3D-C4D	-5.50	100.75	108.25
3	D	1166	PEB	C2D-C3D-C4D	-5.49	100.76	108.25
3	H	1165	PEB	CHC-C4C-C3C	-5.47	123.59	130.95
3	F	1166	PEB	C2D-C3D-C4D	-5.45	100.81	108.25
3	H	1165	PEB	CHA-C1B-NB	-5.43	114.75	124.89
3	V	1187	PEB	C2D-C3D-C4D	-5.41	100.86	108.25
3	P	1187	PEB	CHC-C4C-C3C	-5.41	123.66	130.95
3	Q	1185	PEB	CHC-C4C-C3C	-5.38	123.70	130.95
3	U	1185	PEB	CHC-C4C-C3C	-5.35	123.75	130.95
3	E	1166	PEB	CHC-C4C-C3C	-5.33	123.77	130.95
3	A	1166	PEB	OA-C1A-C2A	-5.33	122.01	126.30
3	C	1165	PEB	C2D-C3D-C4D	-5.33	100.98	108.25
3	G	1165	PEB	OA-C1A-C2A	-5.32	122.02	126.30
3	A	1165	PEB	CHC-C4C-C3C	-5.31	123.80	130.95
3	J	1166	PEB	C2D-C3D-C4D	-5.31	101.00	108.25
3	D	1165	PEB	CHA-C1B-NB	-5.29	115.01	124.89
3	O	1185	PEB	OA-C1A-C2A	-5.29	122.05	126.30
3	S	1185	PEB	OA-C1A-C2A	-5.28	122.05	126.30
3	U	1185	PEB	OA-C1A-C2A	-5.23	122.09	126.30
3	J	1165	PEB	CHC-C4C-C3C	-5.22	123.92	130.95
3	M	1186	PEB	CHC-C4C-C3C	-5.21	123.94	130.95
3	V	1185	PEB	CHA-C1B-NB	-5.19	115.19	124.89
3	U	1186	PEB	OA-C1A-C2A	-5.18	122.14	126.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1165	PEB	CHC-C4C-C3C	-5.16	124.00	130.95
3	R	1187	PEB	CHC-C4C-C3C	-5.14	124.02	130.95
3	V	1185	PEB	OA-C1A-C2A	-5.14	122.16	126.30
3	V	1186	PEB	CHC-C4C-C3C	-5.14	124.03	130.95
3	I	1165	PEB	CHC-C4C-C3C	-5.13	124.04	130.95
3	M	1185	PEB	CHC-C4C-C3C	-5.12	124.05	130.95
3	M	1187	PEB	CHC-C4C-C3C	-5.12	124.06	130.95
3	A	1166	PEB	CHC-C4C-C3C	-5.06	124.14	130.95
3	X	1185	PEB	CHA-C1B-NB	-4.99	115.56	124.89
3	N	1187	PEB	CHC-C4C-C3C	-4.96	124.27	130.95
3	R	1185	PEB	CHA-C1B-NB	-4.94	115.66	124.89
3	R	1185	PEB	CHC-C4C-C3C	-4.94	124.30	130.95
3	K	1165	PEB	OA-C1A-C2A	-4.93	122.33	126.30
3	P	1185	PEB	CHC-C4C-C3C	-4.93	124.31	130.95
3	R	1187	PEB	OA-C1A-C2A	-4.89	122.37	126.30
3	R	1186	PEB	CHC-C4C-C3C	-4.89	124.37	130.95
3	X	1185	PEB	CHC-C4C-C3C	-4.87	124.39	130.95
3	T	1185	PEB	CHC-C4C-C3C	-4.87	124.40	130.95
3	C	1165	PEB	OA-C1A-C2A	-4.81	122.43	126.30
3	T	1185	PEB	OA-C1A-C2A	-4.81	122.43	126.30
3	S	1185	PEB	CHA-C1B-NB	-4.80	115.93	124.89
3	O	1186	PEB	CHC-C4C-C3C	-4.79	124.50	130.95
3	I	1166	PEB	CHC-C4C-C3C	-4.78	124.51	130.95
3	N	1185	PEB	OA-C1A-C2A	-4.76	122.47	126.30
3	U	1185	PEB	CHA-C1B-NB	-4.75	116.01	124.89
3	K	1166	PEB	CHC-C4C-C3C	-4.75	124.55	130.95
3	I	1165	PEB	OA-C1A-C2A	-4.73	122.49	126.30
3	D	1166	PEB	CHC-C4C-C3C	-4.73	124.59	130.95
3	S	1186	PEB	CHC-C4C-C3C	-4.72	124.60	130.95
3	V	1187	PEB	CHC-C4C-C3C	-4.70	124.63	130.95
3	M	1185	PEB	CHA-C1B-NB	-4.68	116.15	124.89
3	K	1165	PEB	CHC-C4C-C3C	-4.68	124.65	130.95
3	U	1187	PEB	OA-C1A-C2A	-4.66	122.55	126.30
3	O	1186	PEB	OA-C1A-C2A	-4.63	122.58	126.30
3	X	1187	PEB	CHC-C4C-C3C	-4.61	124.74	130.95
3	N	1186	PEB	CHC-C4C-C3C	-4.61	124.75	130.95
3	S	1186	PEB	OA-C1A-C2A	-4.60	122.59	126.30
3	C	1165	PEB	CHC-C4C-C3C	-4.59	124.76	130.95
3	B	1165	PEB	CHC-C4C-C3C	-4.59	124.77	130.95
3	U	1187	PEB	CHC-C4C-C3C	-4.58	124.78	130.95
3	I	1166	PEB	OA-C1A-C2A	-4.56	122.63	126.30
3	Q	1186	PEB	CHC-C4C-C3C	-4.56	124.81	130.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	1185	PEB	CHA-C1B-NB	-4.55	116.40	124.89
3	F	1166	PEB	CHC-C4C-C3C	-4.53	124.85	130.95
3	T	1186	PEB	CHC-C4C-C3C	-4.49	124.90	130.95
3	E	1165	PEB	CHC-C4C-C3C	-4.49	124.91	130.95
3	H	1166	PEB	OA-C1A-C2A	-4.48	122.70	126.30
3	L	1166	PEB	CHC-C4C-C3C	-4.47	124.94	130.95
3	Q	1185	PEB	OA-C1A-C2A	-4.46	122.71	126.30
3	B	1166	PEB	CHC-C4C-C3C	-4.45	124.96	130.95
3	D	1166	PEB	OA-C1A-C2A	-4.42	122.75	126.30
3	G	1165	PEB	CHC-C4C-C3C	-4.41	125.02	130.95
3	Q	1185	PEB	CHA-C1B-NB	-4.40	116.68	124.89
3	P	1185	PEB	CHA-C1B-NB	-4.39	116.69	124.89
3	G	1166	PEB	CHC-C4C-C3C	-4.37	125.06	130.95
3	S	1187	PEB	OA-C1A-C2A	-4.36	122.79	126.30
3	S	1185	PEB	CHC-C4C-C3C	-4.34	125.11	130.95
3	W	1186	PEB	CHC-C4C-C3C	-4.34	125.11	130.95
3	B	1166	PEB	OA-C1A-C2A	-4.32	122.82	126.30
3	W	1187	PEB	CHC-C4C-C3C	-4.29	125.17	130.95
3	X	1186	PEB	CHC-C4C-C3C	-4.27	125.20	130.95
3	J	1166	PEB	CHC-C4C-C3C	-4.26	125.21	130.95
3	F	1165	PEB	OA-C1A-C2A	-4.26	122.87	126.30
3	R	1186	PEB	OA-C1A-C2A	-4.24	122.89	126.30
3	M	1186	PEB	OA-C1A-C2A	-4.22	122.90	126.30
3	N	1185	PEB	CHC-C4C-C3C	-4.22	125.27	130.95
3	O	1185	PEB	CHC-C4C-C3C	-4.15	125.36	130.95
3	N	1185	PEB	CHA-C1B-NB	-4.15	117.14	124.89
3	W	1185	PEB	CHC-C4C-C3C	-4.12	125.40	130.95
3	O	1187	PEB	OA-C1A-C2A	-4.12	122.98	126.30
3	G	1166	PEB	OA-C1A-C2A	-4.07	123.02	126.30
3	C	1166	PEB	OA-C1A-C2A	-4.05	123.04	126.30
3	V	1185	PEB	CHC-C4C-C3C	-4.03	125.52	130.95
3	K	1165	PEB	CHB-C4B-NB	-4.03	121.58	128.71
3	L	1166	PEB	OA-C1A-C2A	-3.98	123.10	126.30
3	B	1165	PEB	CHB-C4B-NB	-3.97	121.67	128.71
3	W	1187	PEB	OA-C1A-C2A	-3.97	123.10	126.30
3	C	1166	PEB	CHC-C4C-C3C	-3.96	125.62	130.95
3	W	1185	PEB	CHA-C1B-NB	-3.95	117.51	124.89
3	B	1165	PEB	OA-C1A-C2A	-3.95	123.12	126.30
3	E	1165	PEB	CHB-C4B-NB	-3.95	121.72	128.71
3	V	1186	PEB	OA-C1A-C2A	-3.93	123.14	126.30
3	F	1165	PEB	CHC-C4C-C3C	-3.90	125.70	130.95
3	T	1185	PEB	CHA-C1B-NB	-3.89	117.62	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	1187	PEB	CHC-C4C-C3C	-3.85	125.77	130.95
3	P	1186	PEB	CHC-C4C-C3C	-3.84	125.78	130.95
3	A	1166	PEB	OD-C4D-C3D	-3.83	120.51	130.06
3	U	1186	PEB	CHC-C4C-C3C	-3.82	125.81	130.95
3	I	1165	PEB	CHB-C4B-NB	-3.82	121.95	128.71
3	T	1187	PEB	OA-C1A-C2A	-3.81	123.23	126.30
3	K	1166	PEB	C4B-C3B-C2B	-3.78	102.69	106.80
3	H	1165	PEB	CMA-C2A-C1A	-3.74	104.38	112.39
3	C	1165	PEB	CHB-C4B-NB	-3.70	122.16	128.71
3	R	1186	PEB	CHA-C1B-NB	-3.69	117.99	124.89
3	M	1186	PEB	OD-C4D-C3D	-3.69	120.86	130.06
3	S	1187	PEB	CHC-C4C-C3C	-3.69	125.98	130.95
3	T	1186	PEB	CHA-C1B-NB	-3.65	118.07	124.89
3	Q	1187	PEB	OD-C4D-C3D	-3.65	120.98	130.06
3	S	1187	PEB	C4B-C3B-C2B	-3.63	102.85	106.80
3	V	1187	PEB	OA-C1A-C2A	-3.62	123.38	126.30
3	M	1187	PEB	OD-C4D-C3D	-3.62	121.03	130.06
3	Q	1187	PEB	OA-C1A-C2A	-3.60	123.40	126.30
3	T	1186	PEB	OA-C1A-C2A	-3.55	123.44	126.30
3	E	1166	PEB	CHA-C1B-NB	-3.53	118.30	124.89
3	V	1187	PEB	CBC-CAC-C2C	-3.52	106.30	112.49
3	P	1185	PEB	C4B-C3B-C2B	-3.51	102.98	106.80
3	E	1166	PEB	CHB-C4B-NB	-3.51	122.49	128.71
3	X	1186	PEB	OA-C1A-C2A	-3.49	123.49	126.30
3	M	1187	PEB	CAC-CBC-CGC	-3.46	106.04	112.78
3	U	1185	PEB	C4B-C3B-C2B	-3.45	103.04	106.80
3	P	1187	PEB	CAC-CBC-CGC	-3.44	106.08	112.78
3	E	1166	PEB	OA-C1A-C2A	-3.44	123.53	126.30
3	J	1165	PEB	CHB-C4B-NB	-3.43	122.64	128.71
3	T	1186	PEB	CAB-CBB-CGB	-3.38	106.20	112.78
3	V	1187	PEB	C4B-C3B-C2B	-3.38	103.12	106.80
3	M	1186	PEB	C4B-C3B-C2B	-3.37	103.13	106.80
3	N	1187	PEB	C4B-C3B-C2B	-3.37	103.13	106.80
3	H	1165	PEB	CHB-C4B-NB	-3.37	122.75	128.71
3	D	1165	PEB	CHB-C4B-NB	-3.35	122.78	128.71
3	B	1166	PEB	C4B-C3B-C2B	-3.34	103.17	106.80
3	P	1186	PEB	OA-C1A-C2A	-3.33	123.62	126.30
3	H	1166	PEB	C4B-C3B-C2B	-3.33	103.18	106.80
3	W	1186	PEB	C4B-C3B-C2B	-3.30	103.21	106.80
3	T	1186	PEB	OD-C4D-C3D	-3.30	121.84	130.06
3	X	1185	PEB	OD-C4D-C3D	-3.29	121.87	130.06
3	T	1187	PEB	OD-C4D-C3D	-3.28	121.88	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	1187	PEB	CHB-C4B-NB	-3.28	122.90	128.71
3	V	1186	PEB	C4B-C3B-C2B	-3.28	103.23	106.80
3	X	1186	PEB	OD-C4D-C3D	-3.28	121.90	130.06
3	N	1187	PEB	OA-C1A-C2A	-3.25	123.68	126.30
3	J	1166	PEB	C1B-C2B-C3B	-3.24	102.69	106.43
3	V	1186	PEB	OD-C4D-C3D	-3.24	121.98	130.06
3	D	1166	PEB	C4B-C3B-C2B	-3.24	103.27	106.80
3	V	1187	PEB	OD-C4D-C3D	-3.24	121.99	130.06
3	R	1187	PEB	OD-C4D-C3D	-3.23	122.02	130.06
3	Q	1186	PEB	CHA-C1B-NB	-3.22	118.87	124.89
3	A	1165	PEB	CHB-C4B-NB	-3.21	123.03	128.71
3	N	1186	PEB	OA-C1A-C2A	-3.21	123.72	126.30
3	Q	1186	PEB	OD-C4D-C3D	-3.20	122.08	130.06
3	O	1186	PEB	OD-C4D-C3D	-3.20	122.09	130.06
3	Q	1186	PEB	OA-C1A-C2A	-3.19	123.73	126.30
3	L	1166	PEB	C4B-C3B-C2B	-3.19	103.33	106.80
3	W	1187	PEB	C4B-C3B-C2B	-3.19	103.33	106.80
3	U	1186	PEB	C4B-C3B-C2B	-3.19	103.33	106.80
3	P	1187	PEB	CHB-C4B-NB	-3.17	123.09	128.71
3	E	1166	PEB	C4B-C3B-C2B	-3.17	103.35	106.80
3	G	1165	PEB	CHB-C4B-NB	-3.17	123.10	128.71
3	I	1166	PEB	C4B-C3B-C2B	-3.17	103.35	106.80
3	W	1185	PEB	OD-C4D-C3D	-3.16	122.18	130.06
3	M	1185	PEB	OD-C4D-C3D	-3.16	122.18	130.06
3	F	1165	PEB	C4B-C3B-C2B	-3.16	103.36	106.80
3	D	1165	PEB	OD-C4D-C3D	-3.15	122.20	130.06
3	N	1186	PEB	C4B-C3B-C2B	-3.15	103.37	106.80
3	P	1187	PEB	OA-C1A-C2A	-3.15	123.76	126.30
3	Q	1186	PEB	C4B-C3B-C2B	-3.15	103.37	106.80
3	E	1165	PEB	C4B-C3B-C2B	-3.12	103.40	106.80
3	Q	1185	PEB	OD-C4D-C3D	-3.12	122.28	130.06
3	H	1165	PEB	C4B-C3B-C2B	-3.11	103.41	106.80
3	U	1187	PEB	OD-C4D-C3D	-3.10	122.32	130.06
3	W	1186	PEB	CHA-C1B-NB	-3.10	119.09	124.89
3	T	1185	PEB	OD-C4D-C3D	-3.10	122.33	130.06
3	N	1187	PEB	OD-C4D-C3D	-3.10	122.33	130.06
3	T	1186	PEB	C4B-C3B-C2B	-3.10	103.43	106.80
3	D	1166	PEB	CHB-C4B-NB	-3.09	123.24	128.71
3	Q	1185	PEB	CHB-C4B-NB	-3.09	123.24	128.71
3	F	1165	PEB	OD-C4D-C3D	-3.08	122.37	130.06
3	L	1165	PEB	CHB-C4B-NB	-3.08	123.25	128.71
3	C	1166	PEB	C1B-C2B-C3B	-3.08	102.88	106.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	1166	PEB	CHB-C4B-NB	-3.07	123.27	128.71
3	F	1165	PEB	CHB-C4B-NB	-3.07	123.27	128.71
3	X	1187	PEB	OD-C4D-C3D	-3.06	122.42	130.06
3	L	1166	PEB	OD-C4D-C3D	-3.06	122.43	130.06
3	F	1166	PEB	OA-C1A-C2A	-3.06	123.83	126.30
3	E	1166	PEB	C1B-C2B-C3B	-3.06	102.90	106.43
3	Q	1187	PEB	C4B-C3B-C2B	-3.05	103.48	106.80
3	N	1186	PEB	CHA-C1B-NB	-3.04	119.22	124.89
3	E	1166	PEB	OD-C4D-C3D	-3.03	122.50	130.06
3	O	1187	PEB	C4B-C3B-C2B	-3.02	103.51	106.80
3	R	1186	PEB	OD-C4D-C3D	-3.02	122.53	130.06
3	J	1165	PEB	C4B-C3B-C2B	-3.02	103.51	106.80
3	X	1186	PEB	C4B-C3B-C2B	-3.02	103.52	106.80
3	D	1166	PEB	C1B-C2B-C3B	-3.01	102.95	106.43
3	M	1187	PEB	OA-C1A-C2A	-3.01	123.88	126.30
3	O	1186	PEB	C4B-C3B-C2B	-3.01	103.53	106.80
3	S	1186	PEB	OD-C4D-C3D	-3.00	122.57	130.06
3	L	1165	PEB	C4B-C3B-C2B	-3.00	103.53	106.80
3	P	1186	PEB	OD-C4D-C3D	-2.99	122.61	130.06
3	P	1187	PEB	C1B-C2B-C3B	-2.98	102.99	106.43
3	A	1166	PEB	CBC-CAC-C2C	-2.97	107.27	112.49
3	E	1165	PEB	OD-C4D-ND	-2.97	120.88	126.06
3	U	1185	PEB	CHB-C4B-NB	-2.97	123.46	128.71
3	T	1187	PEB	CHB-C4B-NB	-2.97	123.46	128.71
3	T	1185	PEB	C4B-C3B-C2B	-2.96	103.58	106.80
3	P	1186	PEB	C4B-C3B-C2B	-2.96	103.58	106.80
3	D	1166	PEB	OD-C4D-C3D	-2.95	122.70	130.06
3	M	1185	PEB	C4B-C3B-C2B	-2.95	103.59	106.80
3	C	1165	PEB	C4B-C3B-C2B	-2.95	103.59	106.80
3	K	1166	PEB	OD-C4D-C3D	-2.95	122.72	130.06
3	B	1166	PEB	OD-C4D-C3D	-2.94	122.72	130.06
3	S	1185	PEB	OD-C4D-C3D	-2.94	122.73	130.06
3	U	1185	PEB	OD-C4D-C3D	-2.94	122.73	130.06
3	R	1186	PEB	C4B-C3B-C2B	-2.93	103.61	106.80
3	A	1166	PEB	C4B-C3B-C2B	-2.93	103.61	106.80
3	H	1166	PEB	OD-C4D-C3D	-2.92	122.77	130.06
3	F	1166	PEB	C1B-C2B-C3B	-2.92	103.06	106.43
3	G	1165	PEB	OD-C4D-C3D	-2.91	122.80	130.06
3	K	1165	PEB	C4B-C3B-C2B	-2.91	103.63	106.80
3	R	1185	PEB	OD-C4D-C3D	-2.91	122.81	130.06
3	U	1187	PEB	C4B-C3B-C2B	-2.90	103.64	106.80
3	N	1185	PEB	C4B-C3B-C2B	-2.89	103.65	106.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	1187	PEB	OD-C4D-C3D	-2.89	122.86	130.06
3	I	1166	PEB	OD-C4D-C3D	-2.88	122.87	130.06
3	J	1166	PEB	OD-C4D-C3D	-2.88	122.88	130.06
3	T	1186	PEB	C1B-C2B-C3B	-2.88	103.11	106.43
3	W	1187	PEB	CBC-CAC-C2C	-2.88	107.43	112.49
3	W	1187	PEB	OD-C4D-C3D	-2.87	122.90	130.06
3	N	1185	PEB	OD-C4D-C3D	-2.87	122.90	130.06
3	P	1185	PEB	CHB-C4B-NB	-2.87	123.62	128.71
3	O	1185	PEB	OD-C4D-C3D	-2.87	122.91	130.06
3	L	1166	PEB	CBC-CAC-C2C	-2.87	107.44	112.49
3	G	1166	PEB	OD-C4D-C3D	-2.87	122.92	130.06
3	R	1185	PEB	C1B-C2B-C3B	-2.87	103.12	106.43
3	Q	1185	PEB	C4B-C3B-C2B	-2.86	103.69	106.80
3	O	1187	PEB	OD-C4D-C3D	-2.85	122.95	130.06
3	G	1165	PEB	C4B-C3B-C2B	-2.85	103.70	106.80
3	R	1187	PEB	C4B-C3B-C2B	-2.85	103.70	106.80
3	I	1166	PEB	CHA-C1B-NB	-2.85	119.57	124.89
3	L	1166	PEB	CHA-C1B-NB	-2.84	119.59	124.89
3	P	1185	PEB	OD-C4D-C3D	-2.83	123.00	130.06
3	H	1165	PEB	OD-C4D-C3D	-2.83	123.00	130.06
3	K	1166	PEB	OA-C1A-C2A	-2.83	124.02	126.30
3	P	1187	PEB	OD-C4D-C3D	-2.83	123.00	130.06
3	W	1186	PEB	OA-C1A-C2A	-2.83	124.02	126.30
3	V	1186	PEB	CAA-C3A-C2A	-2.83	107.12	114.17
3	U	1186	PEB	CHB-C4B-C3B	-2.83	119.04	125.48
3	I	1166	PEB	CHB-C4B-NB	-2.82	123.71	128.71
3	O	1185	PEB	CAB-CBB-CGB	-2.82	107.30	112.78
3	C	1166	PEB	C4B-C3B-C2B	-2.82	103.73	106.80
3	V	1185	PEB	OD-C4D-C3D	-2.81	123.05	130.06
3	H	1166	PEB	C1B-C2B-C3B	-2.80	103.20	106.43
3	M	1187	PEB	C4B-C3B-C2B	-2.80	103.75	106.80
3	A	1165	PEB	OD-C4D-C3D	-2.80	123.09	130.06
3	R	1187	PEB	CHA-C1B-NB	-2.80	119.67	124.89
3	H	1166	PEB	CHB-C4B-NB	-2.79	123.77	128.71
3	W	1187	PEB	CHB-C4B-NB	-2.79	123.77	128.71
3	A	1165	PEB	C4B-C3B-C2B	-2.79	103.77	106.80
3	C	1166	PEB	OD-C4D-C3D	-2.78	123.12	130.06
3	U	1187	PEB	C1B-C2B-C3B	-2.78	103.22	106.43
3	G	1166	PEB	C1B-C2B-C3B	-2.78	103.22	106.43
3	T	1187	PEB	CHA-C1B-NB	-2.77	119.71	124.89
3	K	1165	PEB	OD-C4D-C3D	-2.77	123.15	130.06
3	A	1166	PEB	C1B-C2B-C3B	-2.77	103.23	106.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	1166	PEB	CHA-C1B-NB	-2.77	119.71	124.89
3	R	1186	PEB	C1B-C2B-C3B	-2.77	103.24	106.43
3	G	1165	PEB	C1B-C2B-C3B	-2.76	103.25	106.43
3	I	1165	PEB	C4B-C3B-C2B	-2.76	103.80	106.80
3	F	1166	PEB	C4B-C3B-C2B	-2.76	103.80	106.80
3	W	1186	PEB	OD-C4D-ND	-2.75	121.26	126.06
3	I	1166	PEB	C1B-C2B-C3B	-2.75	103.26	106.43
3	S	1187	PEB	CAC-CBC-CGC	-2.74	107.44	112.78
3	R	1187	PEB	C1B-C2B-C3B	-2.74	103.27	106.43
3	V	1185	PEB	C1B-C2B-C3B	-2.74	103.27	106.43
3	U	1186	PEB	OD-C4D-ND	-2.73	121.29	126.06
3	Q	1187	PEB	CBC-CAC-C2C	-2.73	107.69	112.49
3	X	1187	PEB	C4B-C3B-C2B	-2.73	103.83	106.80
3	V	1187	PEB	CHB-C4B-NB	-2.73	123.88	128.71
3	B	1165	PEB	OD-C4D-C3D	-2.73	123.27	130.06
3	W	1185	PEB	C1B-C2B-C3B	-2.72	103.29	106.43
3	X	1186	PEB	C1B-C2B-C3B	-2.72	103.30	106.43
3	S	1186	PEB	C4B-C3B-C2B	-2.71	103.85	106.80
3	F	1166	PEB	OD-C4D-C3D	-2.71	123.30	130.06
3	N	1187	PEB	CHA-C1B-NB	-2.71	119.82	124.89
3	W	1185	PEB	CBA-CAA-C3A	-2.71	106.72	113.43
3	R	1187	PEB	CHB-C4B-NB	-2.71	123.91	128.71
3	M	1186	PEB	CAA-C3A-C2A	-2.70	107.42	114.17
3	I	1165	PEB	OD-C4D-C3D	-2.70	123.33	130.06
3	T	1187	PEB	C1B-C2B-C3B	-2.70	103.32	106.43
3	K	1165	PEB	C1B-C2B-C3B	-2.70	103.32	106.43
3	B	1166	PEB	CHA-C1B-NB	-2.69	119.86	124.89
3	I	1165	PEB	C1B-C2B-C3B	-2.69	103.33	106.43
3	X	1187	PEB	CAC-CBC-CGC	-2.69	107.55	112.78
3	T	1187	PEB	C4B-C3B-C2B	-2.69	103.88	106.80
3	W	1186	PEB	OD-C4D-C3D	-2.69	123.37	130.06
3	B	1165	PEB	C1B-C2B-C3B	-2.68	103.34	106.43
3	P	1187	PEB	C4B-C3B-C2B	-2.68	103.88	106.80
3	J	1166	PEB	CHA-C1B-NB	-2.68	119.89	124.89
3	G	1166	PEB	CHA-C1B-NB	-2.67	119.89	124.89
3	X	1186	PEB	CHA-C1B-NB	-2.67	119.90	124.89
3	U	1187	PEB	CMA-C2A-C1A	-2.67	106.68	112.39
3	P	1186	PEB	CHA-C1B-NB	-2.66	119.92	124.89
3	A	1166	PEB	CHA-C1B-NB	-2.66	119.92	124.89
3	B	1166	PEB	C1B-C2B-C3B	-2.66	103.36	106.43
3	F	1165	PEB	C1B-C2B-C3B	-2.65	103.37	106.43
3	L	1165	PEB	CBA-CAA-C3A	-2.65	106.86	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1166	PEB	C4B-C3B-C2B	-2.65	103.91	106.80
3	L	1166	PEB	C1B-C2B-C3B	-2.65	103.37	106.43
3	U	1186	PEB	OD-C4D-C3D	-2.65	123.45	130.06
3	N	1186	PEB	OD-C4D-ND	-2.65	121.44	126.06
3	S	1185	PEB	C1B-C2B-C3B	-2.65	103.38	106.43
3	J	1166	PEB	C4B-C3B-C2B	-2.64	103.93	106.80
3	C	1166	PEB	CHB-C4B-NB	-2.63	124.06	128.71
3	B	1165	PEB	OD-C4D-ND	-2.63	121.48	126.06
3	N	1187	PEB	CHB-C4B-NB	-2.62	124.07	128.71
3	P	1186	PEB	CHB-C4B-C3B	-2.62	119.52	125.48
3	O	1185	PEB	OD-C4D-ND	-2.61	121.50	126.06
3	Q	1185	PEB	CAC-CBC-CGC	-2.61	107.71	112.78
3	S	1186	PEB	C1B-C2B-C3B	-2.60	103.43	106.43
3	D	1165	PEB	C1B-C2B-C3B	-2.59	103.44	106.43
3	U	1187	PEB	CHA-C1B-NB	-2.59	120.05	124.89
3	O	1185	PEB	C1B-C2B-C3B	-2.59	103.45	106.43
3	J	1165	PEB	OD-C4D-ND	-2.58	121.56	126.06
3	O	1187	PEB	CHA-C1B-NB	-2.58	120.07	124.89
3	B	1165	PEB	C4B-C3B-C2B	-2.58	103.99	106.80
3	I	1166	PEB	CBC-CAC-C2C	-2.58	107.96	112.49
3	E	1165	PEB	CAC-CBC-CGC	-2.56	107.79	112.78
3	O	1186	PEB	CHA-C1B-NB	-2.56	120.10	124.89
3	N	1186	PEB	OD-C4D-C3D	-2.56	123.68	130.06
3	B	1166	PEB	CHB-C4B-NB	-2.55	124.19	128.71
3	X	1186	PEB	CAB-CBB-CGB	-2.55	107.82	112.78
3	I	1165	PEB	CMA-C2A-C1A	-2.55	106.94	112.39
3	D	1166	PEB	CAB-CBB-CGB	-2.54	107.83	112.78
3	O	1187	PEB	C1B-C2B-C3B	-2.54	103.50	106.43
3	C	1165	PEB	OD-C4D-C3D	-2.54	123.73	130.06
3	L	1165	PEB	OD-C4D-C3D	-2.54	123.73	130.06
3	L	1165	PEB	CAC-CBC-CGC	-2.54	107.84	112.78
3	L	1165	PEB	C1B-C2B-C3B	-2.54	103.50	106.43
3	X	1185	PEB	C1B-C2B-C3B	-2.54	103.50	106.43
3	B	1166	PEB	CAB-CBB-CGB	-2.53	107.86	112.78
3	O	1187	PEB	CHB-C4B-NB	-2.53	124.23	128.71
3	W	1186	PEB	C1B-C2B-C3B	-2.50	103.54	106.43
3	W	1186	PEB	CHB-C4B-NB	-2.50	124.28	128.71
3	Q	1186	PEB	CHB-C4B-NB	-2.49	124.30	128.71
3	T	1185	PEB	CHB-C4B-NB	-2.49	124.30	128.71
3	D	1166	PEB	CHA-C1B-NB	-2.49	120.24	124.89
3	V	1185	PEB	C4B-C3B-C2B	-2.49	104.09	106.80
3	R	1185	PEB	CHB-C4B-NB	-2.48	124.32	128.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	1186	PEB	CHA-C1B-NB	-2.48	120.26	124.89
3	F	1166	PEB	CHA-C1B-NB	-2.47	120.27	124.89
3	K	1166	PEB	C1B-C2B-C3B	-2.46	103.59	106.43
3	X	1187	PEB	C1B-C2B-C3B	-2.45	103.60	106.43
3	D	1165	PEB	C4B-C3B-C2B	-2.45	104.13	106.80
3	E	1165	PEB	OD-C4D-C3D	-2.45	123.96	130.06
3	E	1165	PEB	C1B-C2B-C3B	-2.45	103.61	106.43
3	K	1166	PEB	CBC-CAC-C2C	-2.44	108.20	112.49
3	V	1186	PEB	CHA-C1B-NB	-2.44	120.34	124.89
3	J	1165	PEB	OD-C4D-C3D	-2.43	124.00	130.06
3	T	1185	PEB	C1B-C2B-C3B	-2.43	103.63	106.43
3	V	1185	PEB	OD-C4D-ND	-2.43	121.83	126.06
3	H	1165	PEB	CAC-CBC-CGC	-2.43	108.06	112.78
3	W	1187	PEB	CHA-C1B-NB	-2.42	120.36	124.89
3	V	1186	PEB	CHB-C4B-NB	-2.42	124.42	128.71
3	W	1185	PEB	C4B-C3B-C2B	-2.41	104.17	106.80
3	Q	1186	PEB	C1B-C2B-C3B	-2.41	103.65	106.43
3	J	1166	PEB	CHB-C4B-NB	-2.40	124.45	128.71
3	N	1187	PEB	C1B-C2B-C3B	-2.40	103.66	106.43
3	J	1165	PEB	C1B-C2B-C3B	-2.40	103.66	106.43
3	U	1186	PEB	CHA-C1B-NB	-2.40	120.40	124.89
3	E	1165	PEB	CMA-C2A-C1A	-2.40	107.26	112.39
3	X	1187	PEB	CHB-C4B-NB	-2.40	124.47	128.71
3	S	1185	PEB	C4B-C3B-C2B	-2.40	104.19	106.80
3	T	1186	PEB	CHB-C4B-NB	-2.39	124.47	128.71
3	A	1166	PEB	CHB-C4B-NB	-2.39	124.48	128.71
3	L	1165	PEB	OD-C4D-ND	-2.39	121.89	126.06
3	W	1186	PEB	CAA-C3A-C2A	-2.39	108.21	114.17
3	X	1185	PEB	C4B-C3B-C2B	-2.39	104.20	106.80
3	W	1187	PEB	C1B-C2B-C3B	-2.38	103.69	106.43
3	N	1185	PEB	CHB-C4B-NB	-2.37	124.51	128.71
3	T	1187	PEB	CAC-CBC-CGC	-2.37	108.17	112.78
3	Q	1187	PEB	CHB-C4B-NB	-2.37	124.52	128.71
3	R	1186	PEB	CHB-C4B-NB	-2.37	124.52	128.71
3	Q	1186	PEB	CAC-CBC-CGC	-2.37	108.18	112.78
3	V	1187	PEB	C1B-C2B-C3B	-2.36	103.70	106.43
3	H	1166	PEB	CHA-C1B-NB	-2.35	120.50	124.89
3	S	1186	PEB	CHA-C1B-NB	-2.35	120.51	124.89
3	R	1185	PEB	C4B-C3B-C2B	-2.34	104.25	106.80
3	A	1165	PEB	C1B-C2B-C3B	-2.33	103.74	106.43
3	N	1186	PEB	CAA-C3A-C2A	-2.33	108.36	114.17
3	M	1186	PEB	CHB-C4B-NB	-2.32	124.60	128.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	1186	PEB	OD-C4D-ND	-2.32	122.01	126.06
3	L	1166	PEB	CHB-C4B-NB	-2.32	124.60	128.71
3	Q	1185	PEB	C1B-C2B-C3B	-2.32	103.76	106.43
3	D	1165	PEB	CBA-CAA-C3A	-2.31	107.70	113.43
3	S	1185	PEB	CHB-C4B-NB	-2.31	124.62	128.71
3	H	1165	PEB	OD-C4D-ND	-2.31	122.03	126.06
3	S	1187	PEB	CHB-C4B-C3B	-2.31	120.22	125.48
3	N	1185	PEB	OD-C4D-ND	-2.30	122.04	126.06
3	H	1165	PEB	C1B-C2B-C3B	-2.30	103.78	106.43
3	U	1187	PEB	CBD-CAD-C3D	-2.30	115.42	127.70
3	W	1186	PEB	CAC-CBC-CGC	-2.29	108.32	112.78
3	J	1165	PEB	CMA-C2A-C1A	-2.29	107.49	112.39
3	C	1165	PEB	OD-C4D-ND	-2.28	122.08	126.06
3	E	1166	PEB	CBC-CAC-C2C	-2.28	108.49	112.49
3	M	1187	PEB	C1B-C2B-C3B	-2.27	103.81	106.43
3	V	1185	PEB	CAB-CBB-CGB	-2.25	108.40	112.78
3	O	1186	PEB	C1B-C2B-C3B	-2.25	103.84	106.43
3	W	1187	PEB	CBD-CAD-C3D	-2.24	115.75	127.70
3	V	1185	PEB	CHB-C4B-C3B	-2.23	120.39	125.48
3	K	1165	PEB	OD-C4D-ND	-2.23	122.17	126.06
3	K	1165	PEB	CBA-CAA-C3A	-2.23	107.91	113.43
3	M	1187	PEB	CHB-C4B-NB	-2.22	124.77	128.71
3	W	1185	PEB	CHB-C4B-NB	-2.22	124.79	128.71
3	S	1187	PEB	CHB-C4B-NB	-2.21	124.79	128.71
3	X	1186	PEB	CHB-C4B-C3B	-2.21	120.45	125.48
3	X	1186	PEB	CHB-C4B-NB	-2.21	124.80	128.71
3	C	1166	PEB	CHA-C1B-NB	-2.21	120.77	124.89
3	U	1186	PEB	CAB-CBB-CGB	-2.20	108.49	112.78
3	I	1165	PEB	OD-C4D-ND	-2.19	122.25	126.06
3	X	1185	PEB	CMA-C2A-C1A	-2.19	107.71	112.39
3	G	1166	PEB	CHB-C4B-NB	-2.19	124.84	128.71
3	P	1185	PEB	OD-C4D-ND	-2.18	122.25	126.06
3	X	1185	PEB	CHB-C4B-NB	-2.18	124.85	128.71
3	M	1185	PEB	CHB-C4B-NB	-2.18	124.85	128.71
3	U	1185	PEB	C1B-C2B-C3B	-2.17	103.92	106.43
3	O	1187	PEB	CBC-CAC-C2C	-2.17	108.68	112.49
3	N	1186	PEB	CAC-CBC-CGC	-2.16	108.57	112.78
3	N	1185	PEB	C1B-C2B-C3B	-2.16	103.94	106.43
3	F	1166	PEB	OD-C4D-ND	-2.16	122.29	126.06
3	P	1187	PEB	CHA-C1B-NB	-2.16	120.85	124.89
3	X	1186	PEB	CAA-C3A-C2A	-2.16	108.78	114.17
3	Q	1186	PEB	CAA-C3A-C2A	-2.16	108.79	114.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	1186	PEB	CAA-C3A-C2A	-2.16	108.79	114.17
3	O	1186	PEB	CAA-C3A-C2A	-2.15	108.80	114.17
3	N	1185	PEB	CAC-CBC-CGC	-2.15	108.61	112.78
3	C	1165	PEB	C1B-C2B-C3B	-2.14	103.96	106.43
3	U	1187	PEB	CBC-CAC-C2C	-2.14	108.72	112.49
3	W	1187	PEB	OD-C4D-ND	-2.13	122.34	126.06
3	D	1166	PEB	CBC-CAC-C2C	-2.13	108.74	112.49
3	W	1187	PEB	CAC-CBC-CGC	-2.13	108.64	112.78
3	F	1166	PEB	CHB-C4B-NB	-2.12	124.96	128.71
3	Q	1185	PEB	OD-C4D-ND	-2.11	122.37	126.06
3	U	1185	PEB	CAC-CBC-CGC	-2.11	108.67	112.78
3	M	1185	PEB	CBA-CAA-C3A	-2.11	108.21	113.43
3	M	1185	PEB	OD-C4D-ND	-2.11	122.39	126.06
3	G	1165	PEB	CAC-CBC-CGC	-2.10	108.69	112.78
3	B	1166	PEB	OD-C4D-ND	-2.09	122.41	126.06
3	S	1187	PEB	OD-C4D-ND	-2.09	122.42	126.06
3	V	1187	PEB	CHA-C1B-NB	-2.09	120.99	124.89
3	T	1185	PEB	CMA-C2A-C1A	-2.08	107.93	112.39
3	S	1185	PEB	CBA-CAA-C3A	-2.08	108.27	113.43
3	S	1186	PEB	CHB-C4B-C3B	-2.08	120.75	125.48
3	P	1185	PEB	CAC-CBC-CGC	-2.08	108.74	112.78
3	R	1185	PEB	OD-C4D-ND	-2.08	122.44	126.06
3	K	1166	PEB	OD-C4D-ND	-2.07	122.45	126.06
3	X	1185	PEB	CAB-CBB-CGB	-2.07	108.75	112.78
3	L	1166	PEB	CHB-C4B-C3B	-2.07	120.77	125.48
3	O	1186	PEB	CHB-C4B-NB	-2.07	125.05	128.71
3	M	1186	PEB	C1B-C2B-C3B	-2.07	104.05	106.43
3	G	1165	PEB	CBA-CAA-C3A	-2.06	108.32	113.43
3	S	1185	PEB	OD-C4D-ND	-2.06	122.46	126.06
3	T	1186	PEB	CHB-C4B-C3B	-2.06	120.79	125.48
3	V	1187	PEB	CBD-CAD-C3D	-2.06	116.71	127.70
3	K	1166	PEB	CAA-C3A-C2A	-2.06	109.04	114.17
3	A	1165	PEB	OD-C4D-ND	-2.05	122.49	126.06
3	M	1187	PEB	CHA-C1B-NB	-2.05	121.06	124.89
3	M	1185	PEB	C1B-C2B-C3B	-2.05	104.07	106.43
3	G	1165	PEB	OD-C4D-ND	-2.04	122.50	126.06
3	N	1187	PEB	CBD-CAD-C3D	-2.04	116.80	127.70
3	N	1187	PEB	OD-C4D-ND	-2.04	122.50	126.06
3	K	1165	PEB	CAC-CBC-CGC	-2.04	108.82	112.78
3	W	1186	PEB	CAB-CBB-CGB	-2.03	108.82	112.78
3	R	1186	PEB	OD-C4D-ND	-2.03	122.51	126.06
3	S	1187	PEB	C1B-C2B-C3B	-2.03	104.09	106.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	1186	PEB	CMA-C2A-C1A	-2.03	108.04	112.39
3	F	1166	PEB	CHB-C4B-C3B	-2.03	120.86	125.48
3	Q	1187	PEB	CHA-C1B-NB	-2.03	121.10	124.89
3	S	1186	PEB	CAC-CBC-CGC	-2.02	108.85	112.78
3	O	1185	PEB	CHB-C4B-C3B	-2.02	120.88	125.48
3	N	1187	PEB	CBC-CAC-C2C	-2.02	108.94	112.49
3	U	1185	PEB	OD-C4D-ND	-2.02	122.54	126.06
3	X	1187	PEB	CHA-C1B-NB	-2.01	121.13	124.89
3	X	1185	PEB	CHB-C4B-C3B	-2.00	120.92	125.48
3	U	1186	PEB	C3A-C4A-NA	2.03	109.89	107.94
3	A	1165	PEB	CAB-C3B-C4B	2.03	128.57	125.00
3	Q	1186	PEB	C3A-C4A-NA	2.06	109.92	107.94
3	U	1187	PEB	CAD-C3D-C4D	2.08	129.57	123.58
3	X	1187	PEB	C2A-C1A-NA	2.09	110.37	108.31
3	P	1186	PEB	C3A-C4A-NA	2.09	109.95	107.94
3	R	1187	PEB	CAB-C3B-C4B	2.09	128.67	125.00
3	M	1186	PEB	C3A-C4A-NA	2.10	109.96	107.94
3	W	1185	PEB	C3A-C4A-NA	2.10	109.96	107.94
3	X	1186	PEB	C3A-C4A-NA	2.11	109.97	107.94
3	E	1165	PEB	CAB-C3B-C4B	2.11	128.70	125.00
3	T	1186	PEB	CAD-C3D-C4D	2.12	129.69	123.58
3	D	1165	PEB	C3B-C4B-NB	2.13	113.23	109.98
3	S	1187	PEB	CAB-C3B-C4B	2.14	128.75	125.00
3	B	1165	PEB	CAD-C3D-C4D	2.15	129.77	123.58
3	C	1165	PEB	C2A-C1A-NA	2.15	110.43	108.31
3	L	1165	PEB	CAD-C3D-C4D	2.15	129.77	123.58
3	O	1187	PEB	CAD-C3D-C4D	2.15	129.77	123.58
3	U	1185	PEB	C3A-C4A-NA	2.16	110.02	107.94
3	M	1187	PEB	CMC-C3C-C4C	2.16	129.34	127.13
3	S	1185	PEB	C3B-C4B-NB	2.17	113.28	109.98
3	N	1187	PEB	CAB-C3B-C4B	2.17	128.81	125.00
3	I	1165	PEB	C2A-C1A-NA	2.18	110.46	108.31
3	J	1165	PEB	C3A-C4A-NA	2.18	110.04	107.94
3	V	1187	PEB	CMC-C3C-C4C	2.19	129.36	127.13
3	C	1165	PEB	C3A-C4A-NA	2.19	110.04	107.94
3	C	1165	PEB	C3B-C4B-NB	2.19	113.32	109.98
3	D	1165	PEB	C3A-C4A-NA	2.19	110.05	107.94
3	L	1165	PEB	C2A-C1A-NA	2.21	110.49	108.31
3	J	1165	PEB	CAB-C3B-C4B	2.21	128.87	125.00
3	J	1165	PEB	OA-C1A-NA	2.21	127.55	124.84
3	F	1165	PEB	CMC-C3C-C4C	2.21	129.39	127.13
3	U	1186	PEB	CMC-C3C-C4C	2.22	129.40	127.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	1187	PEB	C3B-C4B-NB	2.22	113.36	109.98
3	B	1165	PEB	CAB-C3B-C4B	2.23	128.91	125.00
3	H	1165	PEB	C3A-C4A-NA	2.23	110.09	107.94
3	P	1185	PEB	C3A-C4A-NA	2.24	110.09	107.94
3	F	1165	PEB	CAD-C3D-C4D	2.24	130.04	123.58
3	P	1186	PEB	CMC-C3C-C4C	2.24	129.42	127.13
3	E	1165	PEB	CAD-C3D-C4D	2.25	130.06	123.58
3	D	1165	PEB	C2A-C1A-NA	2.26	110.54	108.31
3	T	1187	PEB	CAB-C3B-C4B	2.26	128.96	125.00
3	K	1166	PEB	CMC-C3C-C4C	2.26	129.44	127.13
3	V	1187	PEB	CAB-C3B-C4B	2.26	128.97	125.00
3	H	1165	PEB	CAD-C3D-C4D	2.27	130.12	123.58
3	Q	1187	PEB	C3B-C4B-NB	2.27	113.44	109.98
3	H	1165	PEB	CAB-C3B-C4B	2.27	128.99	125.00
3	G	1165	PEB	CAD-C3D-C4D	2.27	130.12	123.58
3	V	1187	PEB	CAD-C3D-C4D	2.28	130.15	123.58
3	X	1187	PEB	C3B-C4B-NB	2.28	113.46	109.98
3	A	1165	PEB	C3B-C4B-NB	2.29	113.48	109.98
3	R	1185	PEB	C3B-C4B-NB	2.30	113.48	109.98
3	K	1166	PEB	C3A-C4A-NA	2.31	110.16	107.94
3	S	1186	PEB	CAD-C3D-C4D	2.32	130.25	123.58
3	J	1165	PEB	C3B-C4B-NB	2.32	113.52	109.98
3	I	1165	PEB	C3B-C4B-NB	2.33	113.53	109.98
3	U	1187	PEB	CAB-C3B-C4B	2.33	129.08	125.00
3	S	1186	PEB	C3A-C4A-NA	2.33	110.18	107.94
3	K	1166	PEB	CMB-C2B-C1B	2.33	128.79	125.06
3	W	1185	PEB	CAD-C3D-C4D	2.34	130.32	123.58
3	H	1166	PEB	CAD-C3D-C4D	2.34	130.32	123.58
3	G	1165	PEB	OA-C1A-NA	2.34	127.71	124.84
3	N	1186	PEB	C2A-C1A-NA	2.35	110.63	108.31
3	Q	1185	PEB	CAD-C3D-C4D	2.35	130.34	123.58
3	O	1186	PEB	C3A-C4A-NA	2.35	110.20	107.94
3	L	1166	PEB	C2A-C1A-NA	2.35	110.64	108.31
3	T	1186	PEB	CMC-C3C-C4C	2.36	129.54	127.13
3	D	1166	PEB	CAD-C3D-C4D	2.36	130.37	123.58
3	W	1187	PEB	CAB-C3B-C4B	2.37	129.15	125.00
3	A	1166	PEB	C3A-C4A-NA	2.37	110.22	107.94
3	S	1185	PEB	C3A-C4A-NA	2.37	110.22	107.94
3	D	1166	PEB	CMB-C2B-C1B	2.37	128.86	125.06
3	M	1186	PEB	C2A-C1A-NA	2.37	110.66	108.31
3	N	1187	PEB	CMC-C3C-C4C	2.37	129.56	127.13
3	I	1165	PEB	C3A-C4A-NA	2.38	110.22	107.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1165	PEB	C2A-C1A-NA	2.38	110.66	108.31
3	B	1166	PEB	C3A-C4A-NA	2.38	110.23	107.94
3	Q	1186	PEB	CAD-C3D-C4D	2.38	130.44	123.58
3	T	1186	PEB	C3A-C4A-NA	2.39	110.23	107.94
3	J	1165	PEB	CAD-C3D-C4D	2.39	130.45	123.58
3	O	1185	PEB	C3B-C4B-NB	2.39	113.62	109.98
3	N	1185	PEB	CHA-C1B-C2B	2.39	130.41	124.71
3	I	1166	PEB	CAD-C3D-C4D	2.39	130.45	123.58
3	E	1165	PEB	OA-C1A-NA	2.39	127.77	124.84
3	D	1165	PEB	CAB-C3B-C4B	2.39	129.19	125.00
3	U	1187	PEB	C3B-C4B-NB	2.39	113.63	109.98
3	I	1165	PEB	CAD-C3D-C4D	2.40	130.48	123.58
3	X	1185	PEB	OA-C1A-NA	2.40	127.78	124.84
3	B	1165	PEB	C2A-C1A-NA	2.41	110.70	108.31
3	N	1185	PEB	CAD-C3D-C4D	2.42	130.54	123.58
3	K	1165	PEB	C2A-C1A-NA	2.42	110.70	108.31
3	X	1186	PEB	C2A-C1A-NA	2.42	110.70	108.31
3	N	1186	PEB	C3B-C4B-NB	2.42	113.67	109.98
3	F	1166	PEB	C2A-C1A-NA	2.43	110.71	108.31
3	M	1187	PEB	C3B-C4B-NB	2.43	113.68	109.98
3	T	1187	PEB	CAD-C3D-C4D	2.43	130.57	123.58
3	A	1165	PEB	OA-C1A-NA	2.43	127.81	124.84
3	K	1165	PEB	C3B-C4B-NB	2.43	113.69	109.98
3	X	1186	PEB	CAD-C3D-C4D	2.43	130.58	123.58
3	Q	1186	PEB	CMC-C3C-C4C	2.43	129.62	127.13
3	R	1186	PEB	CAD-C3D-C4D	2.44	130.60	123.58
3	O	1186	PEB	C2A-C1A-NA	2.44	110.72	108.31
3	O	1186	PEB	CAD-C3D-C4D	2.44	130.62	123.58
3	E	1165	PEB	C2A-C1A-NA	2.45	110.73	108.31
3	S	1185	PEB	CAD-C3D-C4D	2.45	130.64	123.58
3	K	1166	PEB	C2A-C1A-NA	2.46	110.74	108.31
3	F	1166	PEB	C3A-C4A-NA	2.46	110.30	107.94
3	O	1187	PEB	CMC-C3C-C4C	2.46	129.64	127.13
3	V	1186	PEB	C3B-C4B-NB	2.46	113.73	109.98
3	Q	1185	PEB	C3B-C4B-NB	2.47	113.74	109.98
3	G	1165	PEB	CMC-C3C-C4C	2.47	129.65	127.13
3	U	1187	PEB	CMC-C3C-C4C	2.47	129.66	127.13
3	D	1165	PEB	CAD-C3D-C4D	2.48	130.71	123.58
3	A	1165	PEB	CAD-C3D-C4D	2.48	130.72	123.58
3	W	1186	PEB	C3A-C4A-NA	2.48	110.33	107.94
3	O	1187	PEB	CAB-C3B-C4B	2.48	129.36	125.00
3	E	1165	PEB	C3B-C4B-NB	2.48	113.77	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1166	PEB	CAD-C3D-C4D	2.48	130.74	123.58
3	R	1185	PEB	CAD-C3D-C4D	2.48	130.74	123.58
3	F	1166	PEB	CAD-C3D-C4D	2.49	130.75	123.58
3	P	1187	PEB	C2A-C1A-NA	2.50	110.78	108.31
3	B	1165	PEB	C3B-C4B-NB	2.50	113.80	109.98
3	L	1165	PEB	C3B-C4B-NB	2.51	113.80	109.98
3	K	1165	PEB	CAB-C3B-C4B	2.51	129.40	125.00
3	K	1165	PEB	CAD-C3D-C4D	2.51	130.81	123.58
3	O	1186	PEB	C3B-C4B-NB	2.52	113.82	109.98
3	H	1165	PEB	C3B-C4B-NB	2.52	113.82	109.98
3	P	1185	PEB	CHA-C1B-C2B	2.52	130.73	124.71
3	K	1165	PEB	CMC-C3C-C4C	2.53	129.71	127.13
3	R	1187	PEB	C3B-C4B-NB	2.54	113.85	109.98
3	M	1185	PEB	C3B-C4B-NB	2.54	113.85	109.98
3	G	1166	PEB	C3B-C4B-NB	2.55	113.86	109.98
3	W	1187	PEB	C3B-C4B-NB	2.55	113.87	109.98
3	U	1187	PEB	C3A-C4A-NA	2.56	110.40	107.94
3	E	1166	PEB	C2A-C1A-NA	2.56	110.84	108.31
3	P	1186	PEB	C3B-C4B-NB	2.56	113.89	109.98
3	U	1186	PEB	CMB-C2B-C1B	2.56	129.16	125.06
3	J	1166	PEB	CAD-C3D-C4D	2.58	131.02	123.58
3	O	1185	PEB	CAD-C3D-C4D	2.59	131.03	123.58
3	G	1166	PEB	CAD-C3D-C4D	2.59	131.04	123.58
3	P	1186	PEB	CAD-C3D-C4D	2.60	131.06	123.58
3	N	1187	PEB	C3B-C4B-NB	2.60	113.94	109.98
3	O	1185	PEB	C3A-C4A-NA	2.60	110.44	107.94
3	C	1166	PEB	CMC-C3C-C4C	2.60	129.79	127.13
3	L	1166	PEB	CMB-C2B-C1B	2.60	129.23	125.06
3	P	1186	PEB	C2A-C1A-NA	2.61	110.89	108.31
3	V	1187	PEB	C3B-C4B-NB	2.61	113.96	109.98
3	S	1186	PEB	C3B-C4B-NB	2.61	113.97	109.98
3	A	1166	PEB	CMB-C2B-C1B	2.62	129.24	125.06
3	S	1187	PEB	CMC-C3C-C4C	2.62	129.81	127.13
3	Q	1187	PEB	CAB-C3B-C4B	2.62	129.60	125.00
3	H	1166	PEB	CMB-C2B-C1B	2.63	129.26	125.06
3	G	1165	PEB	C3A-C4A-NA	2.63	110.47	107.94
3	L	1166	PEB	CAD-C3D-C4D	2.63	131.17	123.58
3	M	1185	PEB	C3A-C4A-NA	2.64	110.47	107.94
3	F	1165	PEB	C3A-C4A-NA	2.64	110.48	107.94
3	U	1186	PEB	C2A-C1A-NA	2.64	110.92	108.31
3	L	1165	PEB	C3A-C4A-NA	2.65	110.49	107.94
3	M	1186	PEB	CAD-C3D-C4D	2.65	131.23	123.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1166	PEB	C2A-C1A-NA	2.66	110.94	108.31
3	I	1166	PEB	C2A-C1A-NA	2.66	110.94	108.31
3	V	1185	PEB	CAD-C3D-C4D	2.66	131.25	123.58
3	P	1187	PEB	CAD-C3D-C4D	2.66	131.25	123.58
3	Q	1186	PEB	C3B-C4B-NB	2.67	114.05	109.98
3	P	1187	PEB	C3B-C4B-NB	2.67	114.05	109.98
3	X	1185	PEB	CAD-C3D-C4D	2.68	131.31	123.58
3	Q	1185	PEB	CHA-C1B-C2B	2.69	131.14	124.71
3	S	1186	PEB	C2A-C1A-NA	2.69	110.97	108.31
3	X	1187	PEB	CAB-C3B-C4B	2.69	129.72	125.00
3	R	1185	PEB	CHA-C1B-C2B	2.69	131.15	124.71
3	C	1166	PEB	C3B-C4B-NB	2.71	114.11	109.98
3	T	1185	PEB	C3B-C4B-NB	2.71	114.12	109.98
3	S	1187	PEB	C3A-C4A-NA	2.72	110.56	107.94
3	U	1186	PEB	C3B-C4B-NB	2.72	114.13	109.98
3	T	1185	PEB	CAD-C3D-C4D	2.72	131.43	123.58
3	A	1165	PEB	C2A-C1A-NA	2.73	111.01	108.31
3	U	1185	PEB	CAD-C3D-C4D	2.74	131.46	123.58
3	O	1187	PEB	C3B-C4B-NB	2.74	114.16	109.98
3	U	1185	PEB	CHA-C1B-C2B	2.75	131.27	124.71
3	H	1165	PEB	OA-C1A-NA	2.75	128.21	124.84
3	X	1185	PEB	C3B-C4B-NB	2.75	114.17	109.98
3	A	1166	PEB	CAD-C3D-C4D	2.75	131.50	123.58
3	G	1165	PEB	C3B-C4B-NB	2.75	114.18	109.98
3	F	1166	PEB	C3B-C4B-NB	2.75	114.18	109.98
3	M	1185	PEB	CHA-C1B-C2B	2.75	131.29	124.71
3	C	1166	PEB	C2A-C1A-NA	2.75	111.03	108.31
3	C	1165	PEB	CAD-C3D-C4D	2.76	131.51	123.58
3	V	1185	PEB	C3B-C4B-NB	2.76	114.18	109.98
3	D	1165	PEB	OA-C1A-NA	2.76	128.22	124.84
3	J	1166	PEB	C3B-C4B-NB	2.76	114.19	109.98
3	C	1166	PEB	CAD-C3D-C4D	2.76	131.53	123.58
3	M	1187	PEB	CAB-C3B-C4B	2.77	129.86	125.00
3	V	1187	PEB	CMB-C2B-C1B	2.80	129.53	125.06
3	V	1186	PEB	CMB-C2B-C1B	2.80	129.53	125.06
3	E	1166	PEB	CMB-C2B-C1B	2.80	129.54	125.06
3	Q	1185	PEB	C2A-C1A-NA	2.81	111.08	108.31
3	W	1185	PEB	C3B-C4B-NB	2.81	114.26	109.98
3	O	1185	PEB	CHA-C1B-C2B	2.81	131.42	124.71
3	H	1166	PEB	C3A-C4A-NA	2.81	110.64	107.94
3	J	1166	PEB	C3A-C4A-NA	2.81	110.64	107.94
3	Q	1187	PEB	C3A-C4A-NA	2.82	110.65	107.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	1186	PEB	CAD-C3D-C4D	2.82	131.71	123.58
3	T	1185	PEB	C2A-C1A-NA	2.83	111.11	108.31
3	A	1165	PEB	C3A-C4A-NA	2.83	110.66	107.94
3	O	1186	PEB	CMB-C2B-C1B	2.83	129.59	125.06
3	S	1185	PEB	CHA-C1B-C2B	2.83	131.48	124.71
3	P	1187	PEB	CAB-C3B-C4B	2.84	129.97	125.00
3	M	1185	PEB	CAD-C3D-C4D	2.84	131.75	123.58
3	L	1165	PEB	OA-C1A-NA	2.84	128.32	124.84
3	S	1187	PEB	C2A-C1A-NA	2.85	111.13	108.31
3	M	1186	PEB	C3B-C4B-NB	2.86	114.34	109.98
3	W	1186	PEB	CMB-C2B-C1B	2.86	129.64	125.06
3	S	1187	PEB	CMB-C2B-C1B	2.86	129.64	125.06
3	E	1165	PEB	C3A-C4A-NA	2.87	110.70	107.94
3	K	1165	PEB	C3A-C4A-NA	2.87	110.70	107.94
3	T	1187	PEB	CMB-C2B-C1B	2.88	129.67	125.06
3	X	1185	PEB	CHA-C1B-C2B	2.89	131.61	124.71
3	R	1186	PEB	C3B-C4B-NB	2.89	114.38	109.98
3	H	1166	PEB	C2A-C1A-NA	2.90	111.17	108.31
3	K	1166	PEB	CAD-C3D-C4D	2.91	131.96	123.58
3	F	1165	PEB	C3B-C4B-NB	2.91	114.42	109.98
3	V	1185	PEB	C3A-C4A-NA	2.91	110.74	107.94
3	R	1187	PEB	C2A-C1A-NA	2.92	111.20	108.31
3	N	1185	PEB	C3B-C4B-NB	2.93	114.44	109.98
3	W	1187	PEB	CMC-C3C-C4C	2.93	130.13	127.13
3	A	1166	PEB	C3B-C4B-NB	2.95	114.47	109.98
3	B	1165	PEB	C3A-C4A-NA	2.95	110.78	107.94
3	W	1186	PEB	CAD-C3D-C4D	2.96	132.10	123.58
3	G	1166	PEB	C2A-C1A-NA	2.96	111.24	108.31
3	W	1186	PEB	C3B-C4B-NB	2.97	114.50	109.98
3	N	1186	PEB	CAD-C3D-C4D	2.98	132.16	123.58
3	B	1166	PEB	CAD-C3D-C4D	2.98	132.16	123.58
3	E	1166	PEB	C3B-C4B-NB	2.98	114.53	109.98
3	B	1166	PEB	CMB-C2B-C1B	2.99	129.84	125.06
3	I	1166	PEB	C3B-C4B-NB	2.99	114.54	109.98
3	X	1185	PEB	C3A-C4A-NA	3.00	110.82	107.94
3	Q	1187	PEB	C2A-C1A-NA	3.00	111.28	108.31
3	N	1187	PEB	C3A-C4A-NA	3.01	110.83	107.94
3	H	1166	PEB	C3B-C4B-NB	3.02	114.58	109.98
3	I	1166	PEB	C3A-C4A-NA	3.02	110.84	107.94
3	P	1185	PEB	C3B-C4B-NB	3.03	114.60	109.98
3	D	1165	PEB	CHA-C1B-C2B	3.03	131.96	124.71
3	R	1186	PEB	C3A-C4A-NA	3.04	110.86	107.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	1186	PEB	C2A-C1A-NA	3.04	111.31	108.31
3	W	1187	PEB	C3A-C4A-NA	3.05	110.87	107.94
3	W	1187	PEB	CMB-C2B-C1B	3.05	129.93	125.06
3	L	1166	PEB	C3B-C4B-NB	3.05	114.63	109.98
3	P	1185	PEB	CAD-C3D-C4D	3.05	132.36	123.58
3	L	1166	PEB	C3A-C4A-NA	3.07	110.89	107.94
3	B	1166	PEB	C3B-C4B-NB	3.07	114.66	109.98
3	D	1166	PEB	C3B-C4B-NB	3.08	114.67	109.98
3	T	1187	PEB	C2A-C1A-NA	3.08	111.35	108.31
3	V	1185	PEB	CHA-C1B-C2B	3.09	132.11	124.71
3	R	1187	PEB	C3A-C4A-NA	3.10	110.92	107.94
3	U	1186	PEB	CAD-C3D-C4D	3.10	132.50	123.58
3	Q	1186	PEB	CMB-C2B-C1B	3.10	130.02	125.06
3	L	1165	PEB	CHA-C1B-C2B	3.11	132.13	124.71
3	N	1187	PEB	C2A-C1A-NA	3.11	111.38	108.31
3	T	1186	PEB	C3B-C4B-NB	3.12	114.74	109.98
3	M	1187	PEB	C3A-C4A-NA	3.12	110.94	107.94
3	X	1186	PEB	C3B-C4B-NB	3.13	114.75	109.98
3	I	1166	PEB	CMB-C2B-C1B	3.13	130.07	125.06
3	G	1166	PEB	CMB-C2B-C1B	3.13	130.07	125.06
3	U	1185	PEB	C2A-C1A-NA	3.14	111.41	108.31
3	H	1165	PEB	CHA-C1B-C2B	3.14	132.22	124.71
3	F	1166	PEB	CMB-C2B-C1B	3.14	130.09	125.06
3	B	1166	PEB	C2A-C1A-NA	3.15	111.42	108.31
3	C	1166	PEB	C3A-C4A-NA	3.16	110.97	107.94
3	M	1186	PEB	CMB-C2B-C1B	3.17	130.13	125.06
3	J	1166	PEB	C2A-C1A-NA	3.19	111.46	108.31
3	E	1166	PEB	C3A-C4A-NA	3.19	111.01	107.94
3	U	1187	PEB	CMB-C2B-C1B	3.19	130.17	125.06
3	O	1187	PEB	C3A-C4A-NA	3.20	111.02	107.94
3	X	1186	PEB	CMB-C2B-C1B	3.20	130.18	125.06
3	N	1187	PEB	CMB-C2B-C1B	3.21	130.19	125.06
3	V	1187	PEB	C2A-C1A-NA	3.21	111.48	108.31
3	P	1186	PEB	CMB-C2B-C1B	3.22	130.21	125.06
3	T	1187	PEB	C3A-C4A-NA	3.22	111.04	107.94
3	T	1186	PEB	CMB-C2B-C1B	3.23	130.23	125.06
3	R	1187	PEB	CMB-C2B-C1B	3.24	130.25	125.06
3	N	1186	PEB	CMB-C2B-C1B	3.24	130.25	125.06
3	S	1187	PEB	C3B-C4B-NB	3.25	114.94	109.98
3	S	1185	PEB	C2A-C1A-NA	3.26	111.53	108.31
3	N	1185	PEB	C2A-C1A-NA	3.27	111.54	108.31
3	U	1185	PEB	C3B-C4B-NB	3.27	114.96	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	1166	PEB	C3B-C4B-NB	3.27	114.96	109.98
3	X	1187	PEB	C3A-C4A-NA	3.28	111.09	107.94
3	O	1185	PEB	C2A-C1A-NA	3.30	111.57	108.31
3	A	1165	PEB	CHA-C1B-C2B	3.32	132.65	124.71
3	X	1185	PEB	C2A-C1A-NA	3.32	111.59	108.31
3	P	1187	PEB	C3A-C4A-NA	3.33	111.14	107.94
3	Q	1187	PEB	CMB-C2B-C1B	3.33	130.39	125.06
3	C	1166	PEB	CMB-C2B-C1B	3.38	130.46	125.06
3	O	1187	PEB	CMB-C2B-C1B	3.41	130.51	125.06
3	R	1185	PEB	C3A-C4A-NA	3.41	111.22	107.94
3	V	1187	PEB	C3A-C4A-NA	3.42	111.22	107.94
3	A	1166	PEB	C2A-C1A-NA	3.42	111.69	108.31
3	E	1165	PEB	CHA-C1B-C2B	3.45	132.95	124.71
3	D	1166	PEB	C3A-C4A-NA	3.45	111.25	107.94
3	B	1165	PEB	CHA-C1B-C2B	3.46	132.98	124.71
3	J	1165	PEB	CHA-C1B-C2B	3.47	133.01	124.71
3	M	1187	PEB	C2A-C1A-NA	3.48	111.75	108.31
3	W	1187	PEB	C2A-C1A-NA	3.54	111.80	108.31
3	R	1185	PEB	C2A-C1A-NA	3.56	111.82	108.31
3	G	1165	PEB	CHA-C1B-C2B	3.57	133.25	124.71
3	S	1186	PEB	CMB-C2B-C1B	3.58	130.78	125.06
3	C	1165	PEB	CHA-C1B-C2B	3.58	133.28	124.71
3	M	1185	PEB	C2A-C1A-NA	3.62	111.89	108.31
3	N	1185	PEB	CMB-C2B-C1B	3.63	130.87	125.06
3	W	1185	PEB	CMB-C2B-C1B	3.65	130.90	125.06
3	K	1165	PEB	CHA-C1B-C2B	3.65	133.44	124.71
3	M	1187	PEB	CMB-C2B-C1B	3.66	130.91	125.06
3	X	1187	PEB	CMB-C2B-C1B	3.66	130.91	125.06
3	R	1186	PEB	CMB-C2B-C1B	3.68	130.95	125.06
3	P	1185	PEB	CMB-C2B-C1B	3.68	130.95	125.06
3	A	1165	PEB	CMB-C2B-C1B	3.71	130.99	125.06
3	O	1187	PEB	C2A-C1A-NA	3.79	112.05	108.31
3	I	1165	PEB	CHA-C1B-C2B	3.81	133.81	124.71
3	V	1185	PEB	C2A-C1A-NA	3.82	112.08	108.31
3	F	1165	PEB	CHA-C1B-C2B	3.82	133.84	124.71
3	P	1185	PEB	C2A-C1A-NA	3.83	112.09	108.31
3	T	1185	PEB	CMB-C2B-C1B	3.89	131.28	125.06
3	U	1187	PEB	C2A-C1A-NA	3.91	112.17	108.31
3	W	1185	PEB	C2A-C1A-NA	3.91	112.18	108.31
3	B	1165	PEB	CMB-C2B-C1B	4.01	131.47	125.06
3	Q	1185	PEB	CMB-C2B-C1B	4.04	131.52	125.06
3	D	1165	PEB	CMB-C2B-C1B	4.04	131.53	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1165	PEB	CMB-C2B-C1B	4.09	131.60	125.06
3	L	1165	PEB	CMB-C2B-C1B	4.11	131.63	125.06
3	J	1166	PEB	CMB-C2B-C1B	4.11	131.63	125.06
3	C	1165	PEB	CMB-C2B-C1B	4.11	131.64	125.06
3	K	1165	PEB	CMB-C2B-C1B	4.12	131.65	125.06
3	M	1185	PEB	CMB-C2B-C1B	4.17	131.72	125.06
3	E	1165	PEB	CMB-C2B-C1B	4.17	131.73	125.06
3	J	1165	PEB	CMB-C2B-C1B	4.23	131.83	125.06
3	P	1187	PEB	CMB-C2B-C1B	4.27	131.89	125.06
3	F	1165	PEB	CMB-C2B-C1B	4.32	131.97	125.06
3	I	1165	PEB	CMB-C2B-C1B	4.34	132.00	125.06
3	U	1185	PEB	CMB-C2B-C1B	4.40	132.09	125.06
3	S	1185	PEB	CMB-C2B-C1B	4.53	132.30	125.06
3	V	1185	PEB	CMB-C2B-C1B	4.69	132.56	125.06
3	R	1185	PEB	CMB-C2B-C1B	4.90	132.90	125.06
3	G	1165	PEB	CMB-C2B-C1B	4.93	132.94	125.06
3	X	1185	PEB	CMB-C2B-C1B	5.07	133.17	125.06
3	O	1185	PEB	CMB-C2B-C1B	5.64	134.08	125.06

There are no chirality outliers.

All (120) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	1166	PEB	C4A-CHA-C1B-C2B
3	D	1166	PEB	C4A-CHA-C1B-C2B
3	E	1166	PEB	C4A-CHA-C1B-C2B
3	C	1166	PEB	C4A-CHA-C1B-C2B
3	I	1166	PEB	C4A-CHA-C1B-C2B
3	A	1166	PEB	C4A-CHA-C1B-C2B
3	J	1166	PEB	C4A-CHA-C1B-C2B
3	F	1166	PEB	C4A-CHA-C1B-C2B
3	X	1187	PEB	C4A-CHA-C1B-C2B
3	L	1166	PEB	C4A-CHA-C1B-C2B
3	T	1187	PEB	C4A-CHA-C1B-C2B
3	V	1187	PEB	C4A-CHA-C1B-C2B
3	K	1166	PEB	C4A-CHA-C1B-C2B
3	O	1187	PEB	C4A-CHA-C1B-C2B
3	W	1186	PEB	C4A-CHA-C1B-C2B
3	B	1166	PEB	C4A-CHA-C1B-C2B
3	S	1187	PEB	C4A-CHA-C1B-C2B
3	O	1186	PEB	C4A-CHA-C1B-C2B
3	T	1186	PEB	C4A-CHA-C1B-C2B

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Mol	Chain	Res	Type	Atoms
3	R	1187	PEB	C4A-CHA-C1B-C2B
3	G	1166	PEB	C4A-CHA-C1B-C2B
3	N	1187	PEB	C4A-CHA-C1B-C2B
3	M	1187	PEB	C4A-CHA-C1B-C2B
3	W	1187	PEB	C4A-CHA-C1B-C2B
3	X	1186	PEB	C4A-CHA-C1B-C2B
3	S	1186	PEB	C4A-CHA-C1B-C2B
3	Q	1187	PEB	C4A-CHA-C1B-C2B
3	U	1187	PEB	C4A-CHA-C1B-C2B
3	P	1187	PEB	C4A-CHA-C1B-C2B
3	M	1186	PEB	C4A-CHA-C1B-C2B
3	P	1186	PEB	C4A-CHA-C1B-C2B
3	R	1186	PEB	C4A-CHA-C1B-C2B
3	Q	1186	PEB	C4A-CHA-C1B-C2B
3	V	1186	PEB	C4A-CHA-C1B-C2B
3	H	1166	PEB	C4A-CHA-C1B-NB
3	U	1186	PEB	C4A-CHA-C1B-C2B
3	N	1186	PEB	C4A-CHA-C1B-C2B
3	E	1166	PEB	C4A-CHA-C1B-NB
3	D	1166	PEB	C4A-CHA-C1B-NB
3	F	1166	PEB	C4A-CHA-C1B-NB
3	C	1166	PEB	C4A-CHA-C1B-NB
3	I	1166	PEB	C4A-CHA-C1B-NB
3	T	1185	PEB	C4A-CHA-C1B-C2B
3	A	1166	PEB	C4A-CHA-C1B-NB
3	J	1166	PEB	C4A-CHA-C1B-NB
3	T	1186	PEB	C4A-CHA-C1B-NB
3	L	1166	PEB	C4A-CHA-C1B-NB
3	W	1186	PEB	C4A-CHA-C1B-NB
3	O	1186	PEB	C4A-CHA-C1B-NB
3	G	1166	PEB	C4A-CHA-C1B-NB
3	K	1166	PEB	C4A-CHA-C1B-NB
3	O	1187	PEB	C4A-CHA-C1B-NB
3	T	1187	PEB	C4A-CHA-C1B-NB
3	W	1185	PEB	C4A-CHA-C1B-C2B
3	X	1186	PEB	C4A-CHA-C1B-NB
3	B	1166	PEB	C4A-CHA-C1B-NB
3	R	1185	PEB	C4A-CHA-C1B-C2B
3	M	1186	PEB	C4A-CHA-C1B-NB
3	X	1187	PEB	C4A-CHA-C1B-NB
3	P	1186	PEB	C4A-CHA-C1B-NB
3	S	1186	PEB	C4A-CHA-C1B-NB

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Mol	Chain	Res	Type	Atoms
3	V	1187	PEB	C4A-CHA-C1B-NB
3	Q	1185	PEB	C4A-CHA-C1B-C2B
3	R	1186	PEB	C4A-CHA-C1B-NB
3	N	1187	PEB	C4A-CHA-C1B-NB
3	S	1187	PEB	C4A-CHA-C1B-NB
3	N	1185	PEB	C4A-CHA-C1B-C2B
3	X	1185	PEB	C4A-CHA-C1B-C2B
3	Q	1186	PEB	C4A-CHA-C1B-NB
3	U	1186	PEB	C4A-CHA-C1B-NB
3	R	1187	PEB	C4A-CHA-C1B-NB
3	M	1185	PEB	C4A-CHA-C1B-C2B
3	P	1185	PEB	C4A-CHA-C1B-C2B
3	S	1185	PEB	C4A-CHA-C1B-C2B
3	V	1186	PEB	C4A-CHA-C1B-NB
3	V	1185	PEB	C4A-CHA-C1B-C2B
3	W	1187	PEB	C4A-CHA-C1B-NB
3	N	1186	PEB	C4A-CHA-C1B-NB
3	U	1187	PEB	C4A-CHA-C1B-NB
3	Q	1187	PEB	C4A-CHA-C1B-NB
3	O	1185	PEB	C4A-CHA-C1B-C2B
3	M	1187	PEB	C4A-CHA-C1B-NB
3	U	1185	PEB	C4A-CHA-C1B-C2B
3	P	1187	PEB	C4A-CHA-C1B-NB
3	T	1185	PEB	C4A-CHA-C1B-NB
3	R	1185	PEB	C4A-CHA-C1B-NB
3	W	1185	PEB	C4A-CHA-C1B-NB
3	M	1185	PEB	C4A-CHA-C1B-NB
3	V	1185	PEB	C4A-CHA-C1B-NB
3	X	1185	PEB	C4A-CHA-C1B-NB
3	N	1185	PEB	C4A-CHA-C1B-NB
3	Q	1185	PEB	C4A-CHA-C1B-NB
3	I	1165	PEB	C4A-CHA-C1B-C2B
3	S	1185	PEB	C4A-CHA-C1B-NB
3	P	1185	PEB	C4A-CHA-C1B-NB
3	D	1165	PEB	C4A-CHA-C1B-C2B
3	U	1185	PEB	C4A-CHA-C1B-NB
3	O	1185	PEB	C4A-CHA-C1B-NB
3	H	1165	PEB	C4A-CHA-C1B-C2B
3	I	1165	PEB	C4A-CHA-C1B-NB
3	E	1165	PEB	C4A-CHA-C1B-C2B
3	D	1165	PEB	C4A-CHA-C1B-NB
3	J	1165	PEB	C4A-CHA-C1B-C2B

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Mol	Chain	Res	Type	Atoms
3	G	1165	PEB	C4A-CHA-C1B-C2B
3	H	1165	PEB	C4A-CHA-C1B-NB
3	A	1165	PEB	C4A-CHA-C1B-C2B
3	E	1165	PEB	C4A-CHA-C1B-NB
3	F	1165	PEB	C4A-CHA-C1B-C2B
3	K	1165	PEB	C4A-CHA-C1B-C2B
3	J	1165	PEB	C4A-CHA-C1B-NB
3	A	1165	PEB	C4A-CHA-C1B-NB
3	K	1165	PEB	C4A-CHA-C1B-NB
3	L	1165	PEB	C4A-CHA-C1B-C2B
3	L	1165	PEB	C4A-CHA-C1B-NB
3	C	1165	PEB	C4A-CHA-C1B-C2B
3	B	1165	PEB	C4A-CHA-C1B-C2B
3	G	1165	PEB	C4A-CHA-C1B-NB
3	B	1165	PEB	C4A-CHA-C1B-NB
3	F	1165	PEB	C4A-CHA-C1B-NB
3	C	1165	PEB	C4A-CHA-C1B-NB

There are no ring outliers.

57 monomers are involved in 121 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1165	PEB	2	0
3	A	1166	PEB	1	0
3	B	1165	PEB	1	0
3	B	1166	PEB	2	0
3	C	1166	PEB	1	0
3	D	1165	PEB	1	0
3	E	1165	PEB	3	0
4	E	1167	GOL	1	0
3	F	1165	PEB	1	0
3	F	1166	PEB	3	0
3	G	1165	PEB	1	0
3	G	1166	PEB	2	0
3	H	1165	PEB	3	0
3	I	1165	PEB	3	0
3	J	1165	PEB	3	0
3	J	1166	PEB	2	0
3	K	1165	PEB	1	0
3	K	1166	PEB	2	0
3	L	1165	PEB	1	0
3	L	1166	PEB	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	1185	PEB	1	0
3	M	1186	PEB	2	0
3	M	1187	PEB	3	0
3	N	1185	PEB	2	0
3	N	1186	PEB	1	0
3	N	1187	PEB	4	0
3	O	1185	PEB	3	0
3	O	1186	PEB	1	0
3	O	1187	PEB	2	0
4	O	1188	GOL	1	0
3	P	1185	PEB	1	0
3	P	1186	PEB	1	0
3	P	1187	PEB	3	0
3	Q	1185	PEB	2	0
3	Q	1186	PEB	2	0
3	Q	1187	PEB	3	0
3	R	1185	PEB	4	0
3	R	1186	PEB	2	0
3	R	1187	PEB	3	0
3	S	1185	PEB	1	0
3	S	1186	PEB	4	0
3	S	1187	PEB	5	0
3	T	1185	PEB	2	0
3	T	1186	PEB	2	0
3	T	1187	PEB	1	0
3	U	1185	PEB	2	0
3	U	1186	PEB	3	0
3	U	1187	PEB	3	0
3	V	1185	PEB	4	0
3	V	1186	PEB	3	0
3	V	1187	PEB	2	0
3	W	1185	PEB	2	0
3	W	1186	PEB	2	0
3	W	1187	PEB	3	0
3	X	1185	PEB	1	0
3	X	1186	PEB	3	0
3	X	1187	PEB	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th 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 ²)	Q<0.9
1	A	164/164 (100%)	-0.15	0 100 100	7, 12, 23, 32	0
1	B	164/164 (100%)	-0.10	0 100 100	10, 15, 24, 29	0
1	C	164/164 (100%)	-0.09	0 100 100	11, 18, 29, 37	0
1	D	164/164 (100%)	0.12	0 100 100	9, 18, 30, 35	0
1	E	164/164 (100%)	0.13	3 (1%) 71 78	10, 19, 33, 39	0
1	F	164/164 (100%)	0.16	0 100 100	15, 21, 27, 34	0
1	G	164/164 (100%)	-0.08	0 100 100	10, 17, 26, 32	0
1	H	164/164 (100%)	0.06	1 (0%) 90 93	11, 18, 28, 34	0
1	I	164/164 (100%)	0.20	1 (0%) 90 93	11, 20, 34, 44	0
1	J	164/164 (100%)	-0.20	0 100 100	8, 14, 26, 33	0
1	K	164/164 (100%)	0.01	0 100 100	10, 16, 26, 32	0
1	L	164/164 (100%)	-0.17	0 100 100	8, 13, 22, 29	0
2	M	183/184 (99%)	-0.12	1 (0%) 91 94	8, 14, 25, 41	0
2	N	183/184 (99%)	0.04	5 (2%) 58 67	12, 19, 33, 45	0
2	O	183/184 (99%)	-0.16	1 (0%) 91 94	10, 17, 27, 37	0
2	P	183/184 (99%)	0.13	7 (3%) 44 54	9, 18, 32, 50	0
2	Q	183/184 (99%)	0.05	5 (2%) 58 67	10, 18, 30, 44	0
2	R	183/184 (99%)	0.54	17 (9%) 11 16	16, 25, 38, 54	0
2	S	183/184 (99%)	0.05	5 (2%) 58 67	10, 18, 29, 45	0
2	T	183/184 (99%)	0.16	8 (4%) 38 47	12, 21, 33, 44	0
2	U	183/184 (99%)	0.20	10 (5%) 29 37	9, 18, 35, 52	0
2	V	183/184 (99%)	-0.14	1 (0%) 91 94	9, 15, 25, 37	0
2	W	183/184 (99%)	0.02	2 (1%) 82 87	11, 18, 30, 44	0
2	X	183/184 (99%)	-0.11	1 (0%) 91 94	9, 15, 26, 39	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4164/4176 (99%)	0.02	68 (1%) 74 81	7, 17, 31, 54	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	150	GLY	4.0
2	R	183	LEU	3.7
2	R	110	GLY	3.7
2	U	24	ALA	3.6
2	U	21	ASP	3.6
2	R	109	ASN	3.5
2	U	20	ALA	3.4
2	W	162	GLU	3.3
2	Q	21	ASP	3.3
2	R	111	LEU	3.2
2	R	21	ASP	3.2
2	R	20	ALA	3.2
2	Q	150	GLY	3.1
2	Q	22	MET	3.1
1	E	75	THR	3.0
2	R	22	MET	3.0
2	U	22	MET	3.0
2	T	114	THR	3.0
2	P	22	MET	3.0
2	M	24	ALA	2.9
2	R	113	GLU	2.9
2	S	24	ALA	2.8
2	V	150	GLY	2.7
2	P	24	ALA	2.7
2	U	150	GLY	2.7
1	H	80	ALA	2.7
2	R	120	VAL	2.7
2	Q	151	GLY	2.6
2	R	19	VAL	2.6
2	P	109	ASN	2.6
2	P	20	ALA	2.6
2	T	16	THR	2.6
2	N	162	GLU	2.5
2	T	109	ASN	2.5
2	S	16	THR	2.5
2	P	21	ASP	2.5
2	R	117	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	T	113	GLU	2.4
2	R	160	VAL	2.4
2	U	184	SER	2.4
1	E	76	ASP	2.4
1	E	46	GLY	2.4
2	R	116	ALA	2.3
2	R	114	THR	2.3
2	T	22	MET	2.3
2	X	22	MET	2.3
2	N	184	SER	2.2
2	U	113	GLU	2.2
2	U	109	ASN	2.2
2	Q	23	GLY	2.2
2	W	110	GLY	2.2
2	R	64	LEU	2.2
2	R	115	TYR	2.2
2	U	17	SER	2.2
2	T	118	LEU	2.2
1	I	74	SER	2.1
2	N	96	LEU	2.1
2	N	109	ASN	2.1
2	S	21	ASP	2.1
2	T	163	ASP	2.1
2	P	16	THR	2.1
2	U	16	THR	2.1
2	S	118	LEU	2.1
2	R	118	LEU	2.1
2	N	110	GLY	2.1
2	S	22	MET	2.0
2	P	67	ALA	2.0
2	T	21	ASP	2.0

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

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, 95th 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(\AA^2)	Q<0.9
2	MEN	M	70	9/10	0.97	0.08	-	12,13,15,17	0
2	MEN	U	70	9/10	0.95	0.09	-	14,17,19,20	0
2	MEN	O	70	9/10	0.95	0.08	-	12,14,17,19	0
2	MEN	N	70	9/10	0.95	0.10	-	15,17,19,19	0
2	MEN	P	70	9/10	0.93	0.13	-	15,17,21,21	0
2	MEN	S	70	9/10	0.94	0.10	-	17,18,21,21	0
2	MEN	R	70	9/10	0.95	0.10	-	23,24,28,29	0
2	MEN	T	70	9/10	0.95	0.11	-	18,21,24,25	0
2	MEN	W	70	9/10	0.97	0.09	-	10,13,15,17	0
2	MEN	V	70	9/10	0.97	0.10	-	10,14,18,20	0
2	MEN	Q	70	9/10	0.96	0.08	-	13,15,17,19	0
2	MEN	X	70	9/10	0.95	0.08	-	13,14,17,18	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, 95th 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(\AA^2)	Q<0.9
4	GOL	E	1167	6/6	0.85	0.20	7.03	20,23,26,40	0
4	GOL	K	1167	6/6	0.81	0.22	5.63	26,31,32,35	0
4	GOL	A	1167	6/6	0.71	0.19	4.34	21,24,29,32	0
4	GOL	H	1167	6/6	0.81	0.16	4.11	25,34,42,42	0
4	GOL	J	1167	6/6	0.80	0.15	4.01	25,28,29,40	0
4	GOL	O	1188	6/6	0.80	0.13	3.20	30,32,34,38	0
3	PEB	J	1166	43/43	0.95	0.12	2.23	8,14,19,24	0
3	PEB	D	1166	43/43	0.90	0.16	1.97	18,30,36,39	0
3	PEB	O	1187	43/43	0.94	0.14	1.81	12,16,22,27	0
3	PEB	C	1166	43/43	0.94	0.12	1.79	10,16,23,27	0
3	PEB	X	1187	43/43	0.94	0.12	1.78	10,14,22,28	0
3	PEB	F	1166	43/43	0.88	0.19	1.76	20,28,31,36	0
4	GOL	B	1167	6/6	0.87	0.14	1.71	27,28,30,33	0
3	PEB	Q	1186	43/43	0.85	0.15	1.54	11,19,31,39	0
3	PEB	M	1187	43/43	0.94	0.11	1.37	9,14,22,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	PEB	R	1186	43/43	0.88	0.17	1.32	16,24,30,39	0
3	PEB	Q	1187	43/43	0.92	0.12	1.23	12,17,23,26	0
3	PEB	T	1186	43/43	0.88	0.15	1.17	11,21,32,34	0
3	PEB	W	1187	43/43	0.93	0.12	1.15	12,17,21,25	0
4	GOL	D	1167	6/6	0.86	0.16	1.14	21,23,26,38	0
3	PEB	I	1166	43/43	0.89	0.16	1.13	20,30,36,40	0
3	PEB	H	1166	43/43	0.90	0.15	1.09	19,28,36,42	0
3	PEB	E	1166	43/43	0.91	0.14	1.08	18,28,32,36	0
3	PEB	N	1187	43/43	0.93	0.13	0.96	14,20,26,30	0
3	PEB	I	1165	43/43	0.88	0.13	0.90	17,25,30,36	0
3	PEB	T	1187	43/43	0.92	0.12	0.89	15,21,30,33	0
3	PEB	V	1187	43/43	0.94	0.12	0.86	10,15,18,27	0
3	PEB	R	1187	43/43	0.91	0.13	0.84	15,23,31,38	0
3	PEB	M	1185	43/43	0.93	0.12	0.78	9,14,23,29	0
3	PEB	G	1166	43/43	0.94	0.12	0.76	11,21,25,29	0
4	GOL	I	1167	6/6	0.92	0.12	0.74	24,28,30,31	0
3	PEB	E	1165	43/43	0.91	0.13	0.74	19,23,30,43	0
3	PEB	R	1185	43/43	0.89	0.17	0.68	19,26,34,42	0
3	PEB	X	1185	43/43	0.94	0.11	0.67	8,13,24,31	0
3	PEB	B	1166	43/43	0.95	0.09	0.67	9,16,24,28	0
3	PEB	S	1186	43/43	0.94	0.12	0.65	11,17,25,37	0
3	PEB	A	1166	43/43	0.95	0.09	0.55	10,15,18,19	0
3	PEB	V	1185	43/43	0.93	0.11	0.54	10,15,24,37	0
3	PEB	J	1165	43/43	0.93	0.11	0.46	12,16,21,26	0
3	PEB	K	1166	43/43	0.94	0.10	0.46	10,16,22,28	0
3	PEB	S	1185	43/43	0.93	0.12	0.41	13,18,26,36	0
3	PEB	H	1165	43/43	0.93	0.11	0.40	13,19,25,34	0
3	PEB	W	1186	43/43	0.87	0.14	0.36	15,22,31,34	0
3	PEB	V	1186	43/43	0.91	0.11	0.35	9,17,25,34	0
3	PEB	M	1186	43/43	0.92	0.12	0.34	11,17,25,34	0
4	GOL	L	1167	6/6	0.91	0.10	0.33	21,22,29,31	0
3	PEB	O	1185	43/43	0.94	0.10	0.32	10,16,26,32	0
3	PEB	C	1165	43/43	0.93	0.11	0.32	11,19,25,32	0
3	PEB	A	1165	43/43	0.94	0.10	0.27	8,13,17,25	0
3	PEB	F	1165	43/43	0.92	0.12	0.20	14,19,22,25	0
3	PEB	D	1165	43/43	0.90	0.11	0.15	15,20,26,36	0
3	PEB	X	1186	43/43	0.92	0.12	0.13	12,17,24,31	0
3	PEB	T	1185	43/43	0.93	0.12	0.12	18,22,30,35	0
3	PEB	K	1165	43/43	0.94	0.10	0.04	10,16,21,27	0
3	PEB	U	1186	43/43	0.93	0.11	0.03	8,15,23,27	0
3	PEB	G	1165	43/43	0.94	0.10	0.03	12,17,22,29	0
3	PEB	P	1186	43/43	0.94	0.11	0.02	10,16,22,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	PEB	O	1186	43/43	0.91	0.12	-0.06	14,21,33,41	0
3	PEB	L	1166	43/43	0.96	0.09	-0.09	6,12,16,19	0
3	PEB	P	1185	43/43	0.93	0.12	-0.09	11,17,30,37	0
3	PEB	W	1185	43/43	0.94	0.10	-0.14	11,15,23,28	0
3	PEB	N	1185	43/43	0.94	0.10	-0.15	12,17,23,31	0
3	PEB	N	1186	43/43	0.91	0.12	-0.16	14,22,26,29	0
3	PEB	U	1185	43/43	0.93	0.11	-0.16	10,16,26,31	0
3	PEB	Q	1185	43/43	0.93	0.10	-0.18	12,17,27,30	0
3	PEB	P	1187	43/43	0.94	0.10	-0.23	8,13,21,29	0
3	PEB	U	1187	43/43	0.95	0.09	-0.25	8,14,21,30	0
4	GOL	G	1167	6/6	0.88	0.11	-0.28	21,25,28,32	0
3	PEB	B	1165	43/43	0.94	0.10	-0.33	10,14,22,29	0
3	PEB	S	1187	43/43	0.94	0.10	-0.42	10,16,21,26	0
3	PEB	L	1165	43/43	0.95	0.09	-0.46	9,13,16,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.