



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:20 AM UTC

PDB ID : 9BKX / pdb_00009bkx
Title : Mycobacterium tuberculosis encapsulin in complex with DyP
Authors : Cuthbert, B.J.; Batot, G.O.; Contreras, H.; Chen, X.; Burley, K.H.; Goulding, C.W.
Deposited on : 2024-04-29
Resolution : 3.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

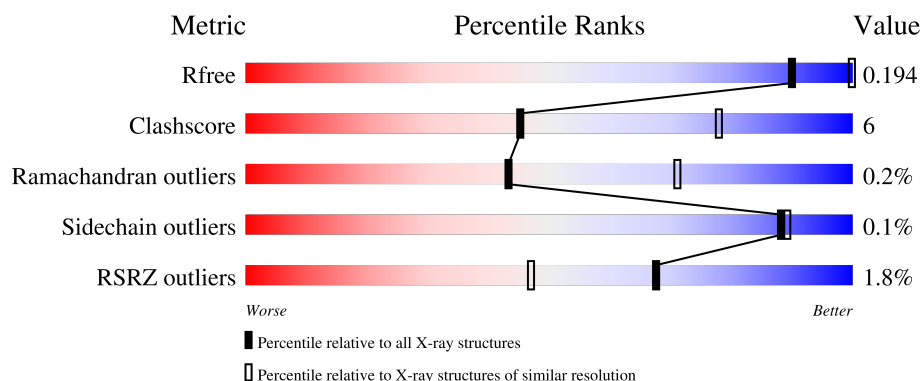
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

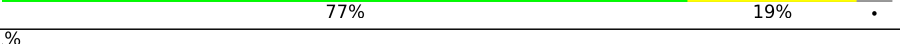
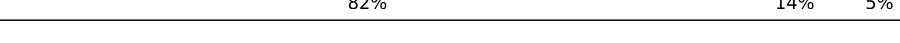
The reported resolution of this entry is 3.15 Å.

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.



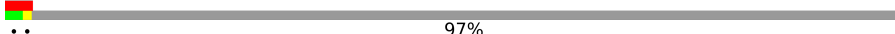
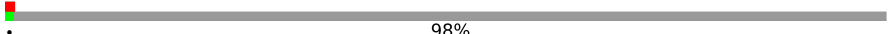
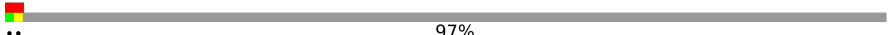
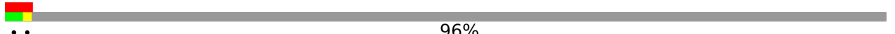
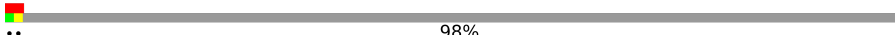
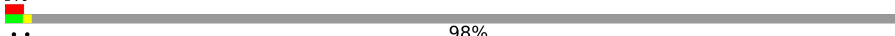
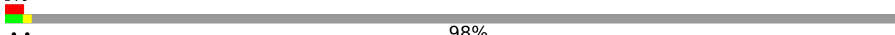
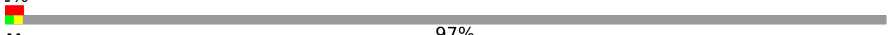
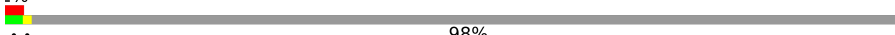
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	279	 84% 12% .
1	B	279	 80% 15% 5%
1	C	279	 77% 19% .
1	D	279	 82% 14% 5%
1	E	279	 85% 12% .

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Mol	Chain	Length	Quality of chain
1	F	279	 78%17%5%
1	G	279	 84%12%5%
1	H	279	 81%15%5%
1	I	279	 85%11%5%
1	J	279	 85%11%5%
1	K	279	 80%15%5%
1	L	279	 82%12%5%
1	M	279	 83%12%5%
1	N	279	 80%15%5%
1	O	279	 79%16%5%
1	P	279	 82%13%5%
1	Q	279	 84%11%5%
1	R	279	 83%13%5%
1	S	279	 84%12%5%
1	T	279	 85%10%5%
2	d	335	 97%
2	g	335	 98%
2	h	335	 97%
2	i	335	 96%
2	p	335	 98%
2	q	335	 98%
2	r	335	 98%
2	s	335	 97%
2	t	335	 98%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 42837 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 Type 1 encapsulin shell protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	1	0
			2040	1282	358	398	2			
1	B	265	Total	C	N	O	S	0	0	0
			2030	1276	354	398	2			
1	C	268	Total	C	N	O	S	0	1	0
			2055	1293	359	401	2			
1	D	266	Total	C	N	O	S	0	1	0
			2042	1284	355	401	2			
1	E	272	Total	C	N	O	S	0	0	0
			2075	1305	361	407	2			
1	F	266	Total	C	N	O	S	0	0	0
			2035	1279	355	399	2			
1	G	266	Total	C	N	O	S	0	0	0
			2035	1279	354	400	2			
1	H	267	Total	C	N	O	S	0	0	0
			2044	1284	356	402	2			
1	I	267	Total	C	N	O	S	0	0	0
			2044	1284	356	402	2			
1	J	267	Total	C	N	O	S	0	0	0
			2040	1282	356	400	2			
1	K	266	Total	C	N	O	S	0	0	0
			2039	1281	355	401	2			
1	L	265	Total	C	N	O	S	0	2	0
			2039	1281	356	400	2			
1	M	266	Total	C	N	O	S	0	0	0
			2031	1277	355	397	2			
1	N	266	Total	C	N	O	S	0	0	0
			2035	1278	354	401	2			
1	O	266	Total	C	N	O	S	0	0	0
			2035	1279	355	399	2			
1	P	266	Total	C	N	O	S	0	0	0
			2027	1274	354	397	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	265	Total	C	N	O	S	0	0	0
			2023	1272	353	396	2			
1	R	266	Total	C	N	O	S	0	0	0
			2035	1278	354	401	2			
1	S	267	Total	C	N	O	S	0	3	0
			2065	1299	362	402	2			
1	T	266	Total	C	N	O	S	0	0	0
			2039	1281	355	401	2			

There are 280 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	266	LYS	-	expression tag	UNP I6WZG6
A	267	LEU	-	expression tag	UNP I6WZG6
A	268	ALA	-	expression tag	UNP I6WZG6
A	269	ALA	-	expression tag	UNP I6WZG6
A	270	ALA	-	expression tag	UNP I6WZG6
A	271	ALA	-	expression tag	UNP I6WZG6
A	272	LEU	-	expression tag	UNP I6WZG6
A	273	GLU	-	expression tag	UNP I6WZG6
A	274	HIS	-	expression tag	UNP I6WZG6
A	275	HIS	-	expression tag	UNP I6WZG6
A	276	HIS	-	expression tag	UNP I6WZG6
A	277	HIS	-	expression tag	UNP I6WZG6
A	278	HIS	-	expression tag	UNP I6WZG6
A	279	HIS	-	expression tag	UNP I6WZG6
B	266	LYS	-	expression tag	UNP I6WZG6
B	267	LEU	-	expression tag	UNP I6WZG6
B	268	ALA	-	expression tag	UNP I6WZG6
B	269	ALA	-	expression tag	UNP I6WZG6
B	270	ALA	-	expression tag	UNP I6WZG6
B	271	ALA	-	expression tag	UNP I6WZG6
B	272	LEU	-	expression tag	UNP I6WZG6
B	273	GLU	-	expression tag	UNP I6WZG6
B	274	HIS	-	expression tag	UNP I6WZG6
B	275	HIS	-	expression tag	UNP I6WZG6
B	276	HIS	-	expression tag	UNP I6WZG6
B	277	HIS	-	expression tag	UNP I6WZG6
B	278	HIS	-	expression tag	UNP I6WZG6
B	279	HIS	-	expression tag	UNP I6WZG6
C	266	LYS	-	expression tag	UNP I6WZG6
C	267	LEU	-	expression tag	UNP I6WZG6
C	268	ALA	-	expression tag	UNP I6WZG6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	269	ALA	-	expression tag	UNP I6WZG6
C	270	ALA	-	expression tag	UNP I6WZG6
C	271	ALA	-	expression tag	UNP I6WZG6
C	272	LEU	-	expression tag	UNP I6WZG6
C	273	GLU	-	expression tag	UNP I6WZG6
C	274	HIS	-	expression tag	UNP I6WZG6
C	275	HIS	-	expression tag	UNP I6WZG6
C	276	HIS	-	expression tag	UNP I6WZG6
C	277	HIS	-	expression tag	UNP I6WZG6
C	278	HIS	-	expression tag	UNP I6WZG6
C	279	HIS	-	expression tag	UNP I6WZG6
D	266	LYS	-	expression tag	UNP I6WZG6
D	267	LEU	-	expression tag	UNP I6WZG6
D	268	ALA	-	expression tag	UNP I6WZG6
D	269	ALA	-	expression tag	UNP I6WZG6
D	270	ALA	-	expression tag	UNP I6WZG6
D	271	ALA	-	expression tag	UNP I6WZG6
D	272	LEU	-	expression tag	UNP I6WZG6
D	273	GLU	-	expression tag	UNP I6WZG6
D	274	HIS	-	expression tag	UNP I6WZG6
D	275	HIS	-	expression tag	UNP I6WZG6
D	276	HIS	-	expression tag	UNP I6WZG6
D	277	HIS	-	expression tag	UNP I6WZG6
D	278	HIS	-	expression tag	UNP I6WZG6
D	279	HIS	-	expression tag	UNP I6WZG6
E	266	LYS	-	expression tag	UNP I6WZG6
E	267	LEU	-	expression tag	UNP I6WZG6
E	268	ALA	-	expression tag	UNP I6WZG6
E	269	ALA	-	expression tag	UNP I6WZG6
E	270	ALA	-	expression tag	UNP I6WZG6
E	271	ALA	-	expression tag	UNP I6WZG6
E	272	LEU	-	expression tag	UNP I6WZG6
E	273	GLU	-	expression tag	UNP I6WZG6
E	274	HIS	-	expression tag	UNP I6WZG6
E	275	HIS	-	expression tag	UNP I6WZG6
E	276	HIS	-	expression tag	UNP I6WZG6
E	277	HIS	-	expression tag	UNP I6WZG6
E	278	HIS	-	expression tag	UNP I6WZG6
E	279	HIS	-	expression tag	UNP I6WZG6
F	266	LYS	-	expression tag	UNP I6WZG6
F	267	LEU	-	expression tag	UNP I6WZG6
F	268	ALA	-	expression tag	UNP I6WZG6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	269	ALA	-	expression tag	UNP I6WZG6
F	270	ALA	-	expression tag	UNP I6WZG6
F	271	ALA	-	expression tag	UNP I6WZG6
F	272	LEU	-	expression tag	UNP I6WZG6
F	273	GLU	-	expression tag	UNP I6WZG6
F	274	HIS	-	expression tag	UNP I6WZG6
F	275	HIS	-	expression tag	UNP I6WZG6
F	276	HIS	-	expression tag	UNP I6WZG6
F	277	HIS	-	expression tag	UNP I6WZG6
F	278	HIS	-	expression tag	UNP I6WZG6
F	279	HIS	-	expression tag	UNP I6WZG6
G	266	LYS	-	expression tag	UNP I6WZG6
G	267	LEU	-	expression tag	UNP I6WZG6
G	268	ALA	-	expression tag	UNP I6WZG6
G	269	ALA	-	expression tag	UNP I6WZG6
G	270	ALA	-	expression tag	UNP I6WZG6
G	271	ALA	-	expression tag	UNP I6WZG6
G	272	LEU	-	expression tag	UNP I6WZG6
G	273	GLU	-	expression tag	UNP I6WZG6
G	274	HIS	-	expression tag	UNP I6WZG6
G	275	HIS	-	expression tag	UNP I6WZG6
G	276	HIS	-	expression tag	UNP I6WZG6
G	277	HIS	-	expression tag	UNP I6WZG6
G	278	HIS	-	expression tag	UNP I6WZG6
G	279	HIS	-	expression tag	UNP I6WZG6
H	266	LYS	-	expression tag	UNP I6WZG6
H	267	LEU	-	expression tag	UNP I6WZG6
H	268	ALA	-	expression tag	UNP I6WZG6
H	269	ALA	-	expression tag	UNP I6WZG6
H	270	ALA	-	expression tag	UNP I6WZG6
H	271	ALA	-	expression tag	UNP I6WZG6
H	272	LEU	-	expression tag	UNP I6WZG6
H	273	GLU	-	expression tag	UNP I6WZG6
H	274	HIS	-	expression tag	UNP I6WZG6
H	275	HIS	-	expression tag	UNP I6WZG6
H	276	HIS	-	expression tag	UNP I6WZG6
H	277	HIS	-	expression tag	UNP I6WZG6
H	278	HIS	-	expression tag	UNP I6WZG6
H	279	HIS	-	expression tag	UNP I6WZG6
I	266	LYS	-	expression tag	UNP I6WZG6
I	267	LEU	-	expression tag	UNP I6WZG6
I	268	ALA	-	expression tag	UNP I6WZG6

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Chain	Residue	Modelled	Actual	Comment	Reference
I	269	ALA	-	expression tag	UNP I6WZG6
I	270	ALA	-	expression tag	UNP I6WZG6
I	271	ALA	-	expression tag	UNP I6WZG6
I	272	LEU	-	expression tag	UNP I6WZG6
I	273	GLU	-	expression tag	UNP I6WZG6
I	274	HIS	-	expression tag	UNP I6WZG6
I	275	HIS	-	expression tag	UNP I6WZG6
I	276	HIS	-	expression tag	UNP I6WZG6
I	277	HIS	-	expression tag	UNP I6WZG6
I	278	HIS	-	expression tag	UNP I6WZG6
I	279	HIS	-	expression tag	UNP I6WZG6
J	266	LYS	-	expression tag	UNP I6WZG6
J	267	LEU	-	expression tag	UNP I6WZG6
J	268	ALA	-	expression tag	UNP I6WZG6
J	269	ALA	-	expression tag	UNP I6WZG6
J	270	ALA	-	expression tag	UNP I6WZG6
J	271	ALA	-	expression tag	UNP I6WZG6
J	272	LEU	-	expression tag	UNP I6WZG6
J	273	GLU	-	expression tag	UNP I6WZG6
J	274	HIS	-	expression tag	UNP I6WZG6
J	275	HIS	-	expression tag	UNP I6WZG6
J	276	HIS	-	expression tag	UNP I6WZG6
J	277	HIS	-	expression tag	UNP I6WZG6
J	278	HIS	-	expression tag	UNP I6WZG6
J	279	HIS	-	expression tag	UNP I6WZG6
K	266	LYS	-	expression tag	UNP I6WZG6
K	267	LEU	-	expression tag	UNP I6WZG6
K	268	ALA	-	expression tag	UNP I6WZG6
K	269	ALA	-	expression tag	UNP I6WZG6
K	270	ALA	-	expression tag	UNP I6WZG6
K	271	ALA	-	expression tag	UNP I6WZG6
K	272	LEU	-	expression tag	UNP I6WZG6
K	273	GLU	-	expression tag	UNP I6WZG6
K	274	HIS	-	expression tag	UNP I6WZG6
K	275	HIS	-	expression tag	UNP I6WZG6
K	276	HIS	-	expression tag	UNP I6WZG6
K	277	HIS	-	expression tag	UNP I6WZG6
K	278	HIS	-	expression tag	UNP I6WZG6
K	279	HIS	-	expression tag	UNP I6WZG6
L	266	LYS	-	expression tag	UNP I6WZG6
L	267	LEU	-	expression tag	UNP I6WZG6
L	268	ALA	-	expression tag	UNP I6WZG6

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Chain	Residue	Modelled	Actual	Comment	Reference
L	269	ALA	-	expression tag	UNP I6WZG6
L	270	ALA	-	expression tag	UNP I6WZG6
L	271	ALA	-	expression tag	UNP I6WZG6
L	272	LEU	-	expression tag	UNP I6WZG6
L	273	GLU	-	expression tag	UNP I6WZG6
L	274	HIS	-	expression tag	UNP I6WZG6
L	275	HIS	-	expression tag	UNP I6WZG6
L	276	HIS	-	expression tag	UNP I6WZG6
L	277	HIS	-	expression tag	UNP I6WZG6
L	278	HIS	-	expression tag	UNP I6WZG6
L	279	HIS	-	expression tag	UNP I6WZG6
M	266	LYS	-	expression tag	UNP I6WZG6
M	267	LEU	-	expression tag	UNP I6WZG6
M	268	ALA	-	expression tag	UNP I6WZG6
M	269	ALA	-	expression tag	UNP I6WZG6
M	270	ALA	-	expression tag	UNP I6WZG6
M	271	ALA	-	expression tag	UNP I6WZG6
M	272	LEU	-	expression tag	UNP I6WZG6
M	273	GLU	-	expression tag	UNP I6WZG6
M	274	HIS	-	expression tag	UNP I6WZG6
M	275	HIS	-	expression tag	UNP I6WZG6
M	276	HIS	-	expression tag	UNP I6WZG6
M	277	HIS	-	expression tag	UNP I6WZG6
M	278	HIS	-	expression tag	UNP I6WZG6
M	279	HIS	-	expression tag	UNP I6WZG6
N	266	LYS	-	expression tag	UNP I6WZG6
N	267	LEU	-	expression tag	UNP I6WZG6
N	268	ALA	-	expression tag	UNP I6WZG6
N	269	ALA	-	expression tag	UNP I6WZG6
N	270	ALA	-	expression tag	UNP I6WZG6
N	271	ALA	-	expression tag	UNP I6WZG6
N	272	LEU	-	expression tag	UNP I6WZG6
N	273	GLU	-	expression tag	UNP I6WZG6
N	274	HIS	-	expression tag	UNP I6WZG6
N	275	HIS	-	expression tag	UNP I6WZG6
N	276	HIS	-	expression tag	UNP I6WZG6
N	277	HIS	-	expression tag	UNP I6WZG6
N	278	HIS	-	expression tag	UNP I6WZG6
N	279	HIS	-	expression tag	UNP I6WZG6
O	266	LYS	-	expression tag	UNP I6WZG6
O	267	LEU	-	expression tag	UNP I6WZG6
O	268	ALA	-	expression tag	UNP I6WZG6

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Chain	Residue	Modelled	Actual	Comment	Reference
O	269	ALA	-	expression tag	UNP I6WZG6
O	270	ALA	-	expression tag	UNP I6WZG6
O	271	ALA	-	expression tag	UNP I6WZG6
O	272	LEU	-	expression tag	UNP I6WZG6
O	273	GLU	-	expression tag	UNP I6WZG6
O	274	HIS	-	expression tag	UNP I6WZG6
O	275	HIS	-	expression tag	UNP I6WZG6
O	276	HIS	-	expression tag	UNP I6WZG6
O	277	HIS	-	expression tag	UNP I6WZG6
O	278	HIS	-	expression tag	UNP I6WZG6
O	279	HIS	-	expression tag	UNP I6WZG6
P	266	LYS	-	expression tag	UNP I6WZG6
P	267	LEU	-	expression tag	UNP I6WZG6
P	268	ALA	-	expression tag	UNP I6WZG6
P	269	ALA	-	expression tag	UNP I6WZG6
P	270	ALA	-	expression tag	UNP I6WZG6
P	271	ALA	-	expression tag	UNP I6WZG6
P	272	LEU	-	expression tag	UNP I6WZG6
P	273	GLU	-	expression tag	UNP I6WZG6
P	274	HIS	-	expression tag	UNP I6WZG6
P	275	HIS	-	expression tag	UNP I6WZG6
P	276	HIS	-	expression tag	UNP I6WZG6
P	277	HIS	-	expression tag	UNP I6WZG6
P	278	HIS	-	expression tag	UNP I6WZG6
P	279	HIS	-	expression tag	UNP I6WZG6
Q	266	LYS	-	expression tag	UNP I6WZG6
Q	267	LEU	-	expression tag	UNP I6WZG6
Q	268	ALA	-	expression tag	UNP I6WZG6
Q	269	ALA	-	expression tag	UNP I6WZG6
Q	270	ALA	-	expression tag	UNP I6WZG6
Q	271	ALA	-	expression tag	UNP I6WZG6
Q	272	LEU	-	expression tag	UNP I6WZG6
Q	273	GLU	-	expression tag	UNP I6WZG6
Q	274	HIS	-	expression tag	UNP I6WZG6
Q	275	HIS	-	expression tag	UNP I6WZG6
Q	276	HIS	-	expression tag	UNP I6WZG6
Q	277	HIS	-	expression tag	UNP I6WZG6
Q	278	HIS	-	expression tag	UNP I6WZG6
Q	279	HIS	-	expression tag	UNP I6WZG6
R	266	LYS	-	expression tag	UNP I6WZG6
R	267	LEU	-	expression tag	UNP I6WZG6
R	268	ALA	-	expression tag	UNP I6WZG6

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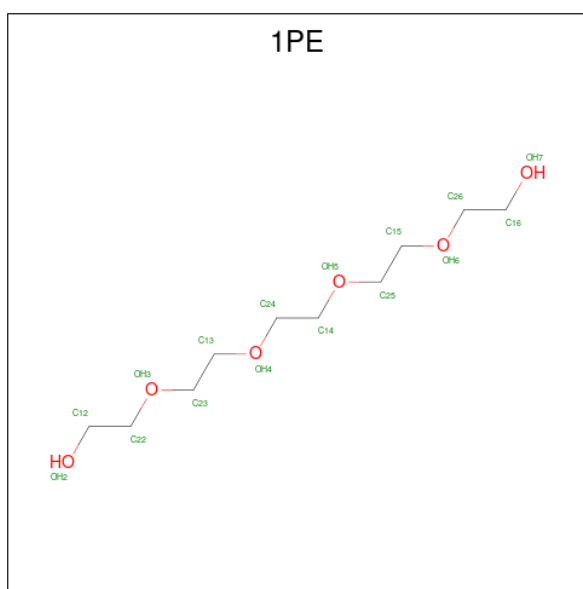
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Chain	Residue	Modelled	Actual	Comment	Reference
R	269	ALA	-	expression tag	UNP I6WZG6
R	270	ALA	-	expression tag	UNP I6WZG6
R	271	ALA	-	expression tag	UNP I6WZG6
R	272	LEU	-	expression tag	UNP I6WZG6
R	273	GLU	-	expression tag	UNP I6WZG6
R	274	HIS	-	expression tag	UNP I6WZG6
R	275	HIS	-	expression tag	UNP I6WZG6
R	276	HIS	-	expression tag	UNP I6WZG6
R	277	HIS	-	expression tag	UNP I6WZG6
R	278	HIS	-	expression tag	UNP I6WZG6
R	279	HIS	-	expression tag	UNP I6WZG6
S	266	LYS	-	expression tag	UNP I6WZG6
S	267	LEU	-	expression tag	UNP I6WZG6
S	268	ALA	-	expression tag	UNP I6WZG6
S	269	ALA	-	expression tag	UNP I6WZG6
S	270	ALA	-	expression tag	UNP I6WZG6
S	271	ALA	-	expression tag	UNP I6WZG6
S	272	LEU	-	expression tag	UNP I6WZG6
S	273	GLU	-	expression tag	UNP I6WZG6
S	274	HIS	-	expression tag	UNP I6WZG6
S	275	HIS	-	expression tag	UNP I6WZG6
S	276	HIS	-	expression tag	UNP I6WZG6
S	277	HIS	-	expression tag	UNP I6WZG6
S	278	HIS	-	expression tag	UNP I6WZG6
S	279	HIS	-	expression tag	UNP I6WZG6
T	266	LYS	-	expression tag	UNP I6WZG6
T	267	LEU	-	expression tag	UNP I6WZG6
T	268	ALA	-	expression tag	UNP I6WZG6
T	269	ALA	-	expression tag	UNP I6WZG6
T	270	ALA	-	expression tag	UNP I6WZG6
T	271	ALA	-	expression tag	UNP I6WZG6
T	272	LEU	-	expression tag	UNP I6WZG6
T	273	GLU	-	expression tag	UNP I6WZG6
T	274	HIS	-	expression tag	UNP I6WZG6
T	275	HIS	-	expression tag	UNP I6WZG6
T	276	HIS	-	expression tag	UNP I6WZG6
T	277	HIS	-	expression tag	UNP I6WZG6
T	278	HIS	-	expression tag	UNP I6WZG6
T	279	HIS	-	expression tag	UNP I6WZG6

- Molecule 2 is a protein called Dye-decolorizing peroxidase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	d	10	Total	C	N	O	0	0	0
			54	33	10	11			
2	g	6	Total	C	N	O	0	0	0
			35	23	6	6			
2	h	9	Total	C	N	O	0	0	0
			50	31	9	10			
2	i	12	Total	C	N	O	0	0	0
			74	47	12	15			
2	p	8	Total	C	N	O	0	0	0
			44	28	8	8			
2	q	8	Total	C	N	O	0	0	0
			43	25	8	10			
2	r	8	Total	C	N	O	0	0	0
			48	31	8	9			
2	s	10	Total	C	N	O	0	0	0
			60	39	11	10			
2	t	8	Total	C	N	O	0	0	0
			50	32	8	10			

- Molecule 3 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			10	6	4		

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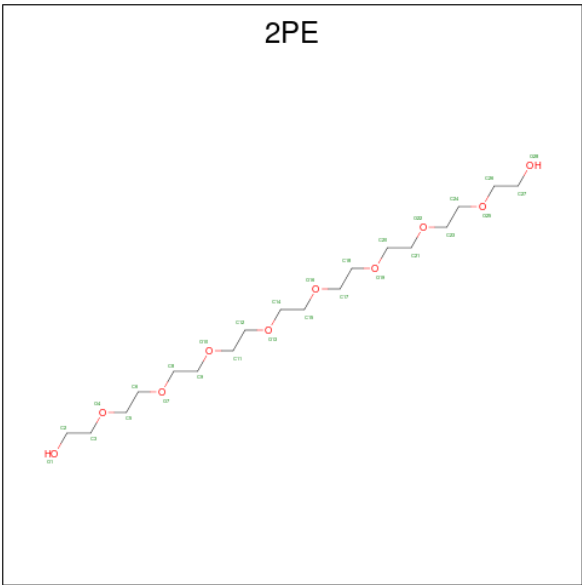
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			16	10	6		
3	C	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			16	10	6		
3	C	1	Total	C	O	0	1
			32	20	12		
3	E	1	Total	C	O	0	0
			16	10	6		
3	E	1	Total	C	O	0	0
			10	6	4		
3	F	1	Total	C	O	0	0
			13	8	5		
3	F	1	Total	C	O	0	0
			16	10	6		
3	F	1	Total	C	O	0	0
			13	8	5		
3	F	1	Total	C	O	0	1
			32	20	12		
3	G	1	Total	C	O	0	0
			10	6	4		
3	H	1	Total	C	O	0	0
			16	10	6		
3	H	1	Total	C	O	0	1
			20	12	8		
3	H	1	Total	C	O	0	0
			10	6	4		
3	I	1	Total	C	O	0	0
			16	10	6		
3	I	1	Total	C	O	0	0
			10	6	4		
3	I	1	Total	C	O	0	0
			10	6	4		
3	J	1	Total	C	O	0	0
			10	6	4		
3	J	1	Total	C	O	0	0
			16	10	6		
3	K	1	Total	C	O	0	0
			10	6	4		

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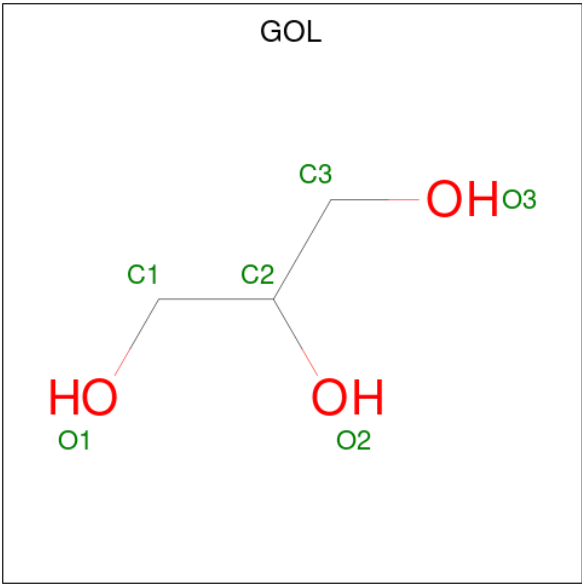
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	K	1	Total	C	O	0	0
			13	8	5		
3	L	1	Total	C	O	0	0
			16	10	6		
3	L	1	Total	C	O	0	0
			13	8	5		
3	L	1	Total	C	O	0	1
			32	20	12		
3	N	1	Total	C	O	0	0
			10	6	4		
3	N	1	Total	C	O	0	0
			10	6	4		
3	N	1	Total	C	O	0	0
			13	8	5		
3	O	1	Total	C	O	0	0
			10	6	4		
3	P	1	Total	C	O	0	0
			13	8	5		
3	P	1	Total	C	O	0	0
			13	8	5		
3	Q	1	Total	C	O	0	0
			16	10	6		
3	Q	1	Total	C	O	0	0
			10	6	4		
3	R	1	Total	C	O	0	0
			10	6	4		
3	R	1	Total	C	O	0	0
			7	4	3		
3	R	1	Total	C	O	0	0
			13	8	5		
3	T	1	Total	C	O	0	0
			16	10	6		
3	T	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is NONAETHYLENE GLYCOL (CCD ID: 2PE) (formula: C₁₈H₃₈O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	H	1	Total	C	O	0	0
			25	16	9		
4	H	1	Total	C	O	0	0
			22	14	8		
4	J	1	Total	C	O	0	0
			16	10	6		
4	L	1	Total	C	O	0	0
			25	16	9		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	G	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		
5	I	1	Total	C	O	0	0
			6	3	3		
5	I	1	Total	C	O	0	0
			6	3	3		
5	I	1	Total	C	O	0	0
			6	3	3		
5	I	1	Total	C	O	0	0
			6	3	3		
5	I	1	Total	C	O	0	0
			6	3	3		
5	J	1	Total	C	O	0	0
			6	3	3		
5	J	1	Total	C	O	0	0
			6	3	3		
5	J	1	Total	C	O	0	0
			6	3	3		
5	J	1	Total	C	O	0	0
			6	3	3		
5	K	1	Total	C	O	0	0
			6	3	3		
5	K	1	Total	C	O	0	0
			6	3	3		
5	K	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	K	1	Total	C	O	0	0
			6	3	3		
5	K	1	Total	C	O	0	0
			6	3	3		
5	K	1	Total	C	O	0	0
			6	3	3		
5	L	1	Total	C	O	0	0
			6	3	3		
5	L	1	Total	C	O	0	0
			6	3	3		
5	L	1	Total	C	O	0	0
			6	3	3		
5	L	1	Total	C	O	0	0
			6	3	3		
5	M	1	Total	C	O	0	0
			6	3	3		
5	M	1	Total	C	O	0	0
			6	3	3		
5	M	1	Total	C	O	0	0
			6	3	3		
5	N	1	Total	C	O	0	0
			6	3	3		
5	N	1	Total	C	O	0	0
			6	3	3		
5	O	1	Total	C	O	0	0
			6	3	3		
5	O	1	Total	C	O	0	0
			6	3	3		
5	O	1	Total	C	O	0	0
			6	3	3		
5	O	1	Total	C	O	0	0
			6	3	3		
5	O	1	Total	C	O	0	0
			6	3	3		
5	Q	1	Total	C	O	0	0
			6	3	3		
5	Q	1	Total	C	O	0	0
			6	3	3		
5	Q	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	R	1	Total 6	C 3	O 3	0	0
5	R	1	Total 6	C 3	O 3	0	0
5	R	1	Total 6	C 3	O 3	0	0
5	R	1	Total 6	C 3	O 3	0	0
5	S	1	Total 6	C 3	O 3	0	0
5	S	1	Total 6	C 3	O 3	0	0
5	S	1	Total 6	C 3	O 3	0	0
5	S	1	Total 6	C 3	O 3	0	0
5	S	1	Total 6	C 3	O 3	0	0
5	S	1	Total 6	C 3	O 3	0	0
5	T	1	Total 6	C 3	O 3	0	0
5	T	1	Total 6	C 3	O 3	0	0
5	T	1	Total 6	C 3	O 3	0	0
5	T	1	Total 6	C 3	O 3	0	0

- Molecule 6 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

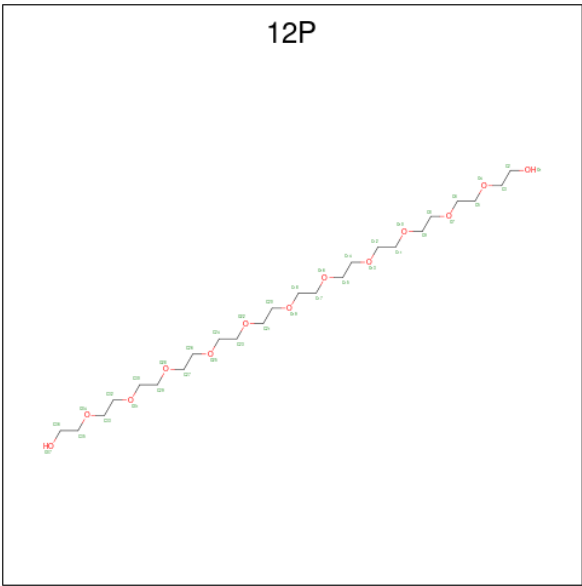
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	Ni 1	0	0
6	C	4	Total 4	Ni 4	0	0
6	D	2	Total 2	Ni 2	0	0
6	E	2	Total 2	Ni 2	0	0
6	F	2	Total 2	Ni 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	2	Total 2	Ni 2	0	0
6	I	2	Total 2	Ni 2	0	0
6	J	2	Total 2	Ni 2	0	0
6	K	1	Total 1	Ni 1	0	0
6	L	2	Total 2	Ni 2	0	0
6	M	1	Total 1	Ni 1	0	0
6	N	1	Total 1	Ni 1	0	0
6	O	3	Total 3	Ni 3	0	0
6	P	2	Total 2	Ni 2	0	0
6	Q	2	Total 2	Ni 2	0	0
6	R	1	Total 1	Ni 1	0	0
6	S	3	Total 3	Ni 3	0	0

- Molecule 7 is DODECAETHYLENE GLYCOL (CCD ID: 12P) (formula: C₂₄H₅₀O₁₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	T	1	Total	C	O	0	0
			13	8	5		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	25	Total	O		0	0
			25	25			
8	B	14	Total	O		0	0
			14	14			
8	C	15	Total	O		0	0
			15	15			
8	D	16	Total	O		0	0
			16	16			
8	E	14	Total	O		0	0
			14	14			
8	F	24	Total	O		0	0
			24	24			
8	G	12	Total	O		0	0
			12	12			
8	H	23	Total	O		0	0
			23	23			
8	I	29	Total	O		0	0
			29	29			
8	J	30	Total	O		0	0
			30	30			
8	K	24	Total	O		0	0
			24	24			
8	L	28	Total	O		0	0
			28	28			
8	M	18	Total	O		0	0
			18	18			
8	N	17	Total	O		0	0
			17	17			
8	O	16	Total	O		0	0
			16	16			
8	P	14	Total	O		0	0
			14	14			
8	Q	18	Total	O		0	0
			18	18			
8	R	19	Total	O		0	0
			19	19			
8	S	24	Total	O		0	0
			24	24			

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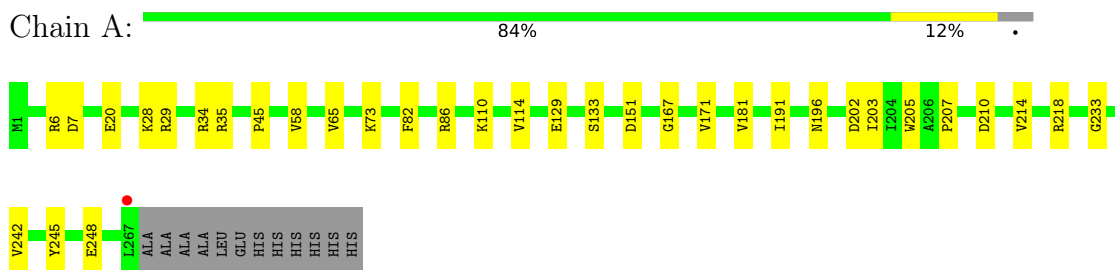
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	T	12	Total	O	0	0
			12	12		

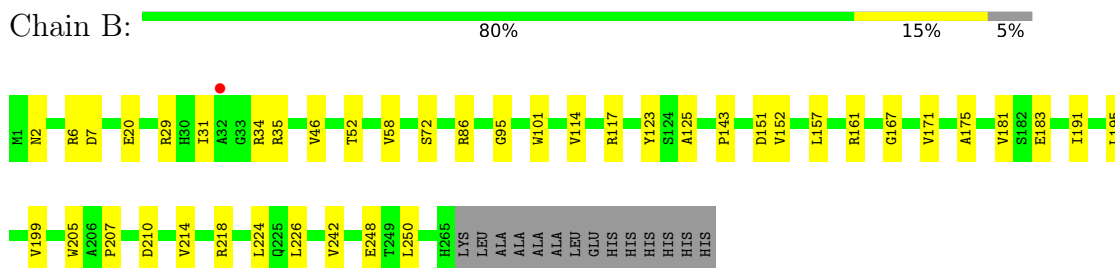
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

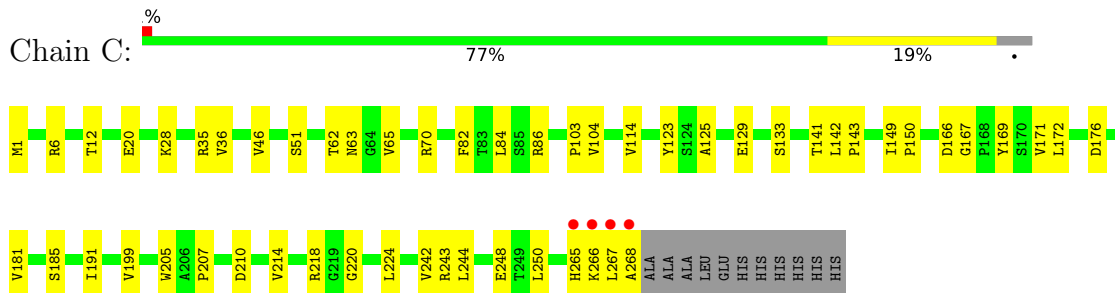
- Molecule 1: Type 1 encapsulin shell protein



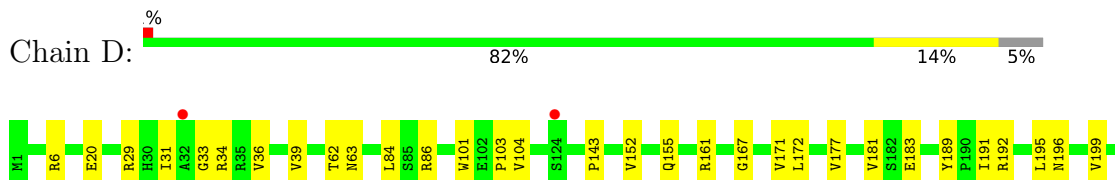
- Molecule 1: Type 1 encapsulin shell protein

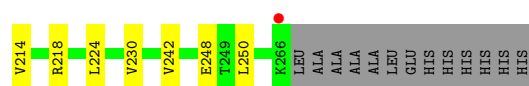


- Molecule 1: Type 1 encapsulin shell protein



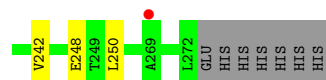
- Molecule 1: Type 1 encapsulin shell protein





- Molecule 1: Type 1 encapsulin shell protein

Chain E: 85% 12% .



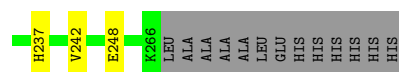
- Molecule 1: Type 1 encapsulin shell protein

Chain F: 78% 17% 5%



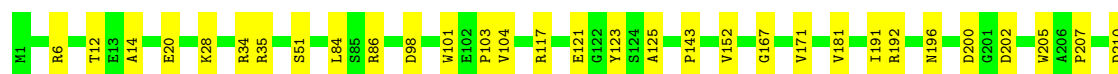
- Molecule 1: Type 1 encapsulin shell protein

Chain G: 84% 12% 5%



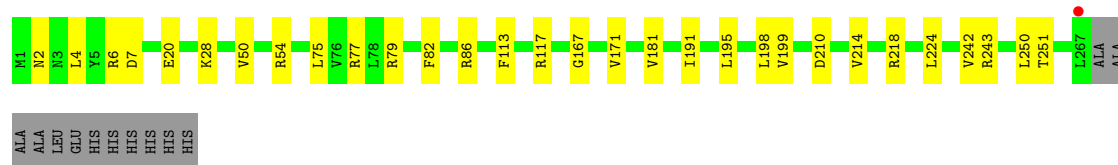
- Molecule 1: Type 1 encapsulin shell protein

Chain H: 81% 15% .

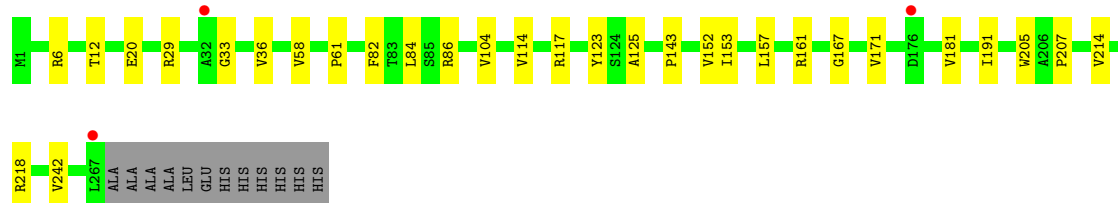
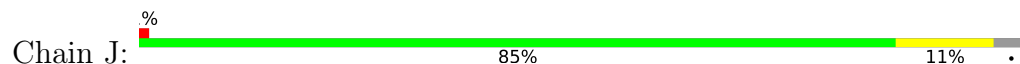


- Molecule 1: Type 1 encapsulin shell protein

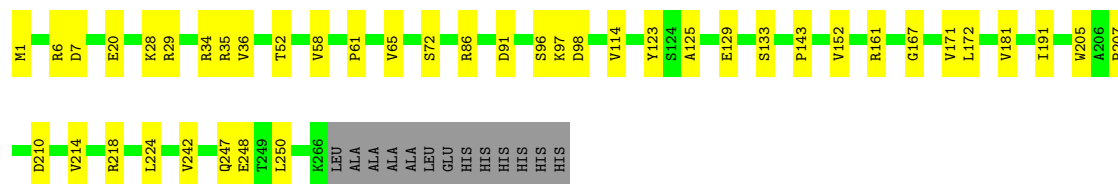
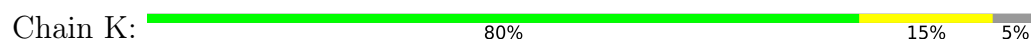
Chain I: 85% 11% .



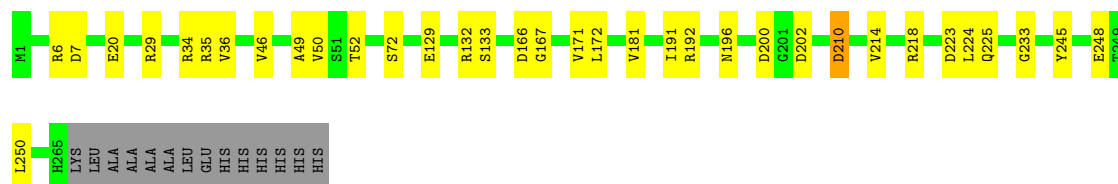
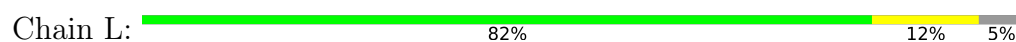
- Molecule 1: Type 1 encapsulin shell protein



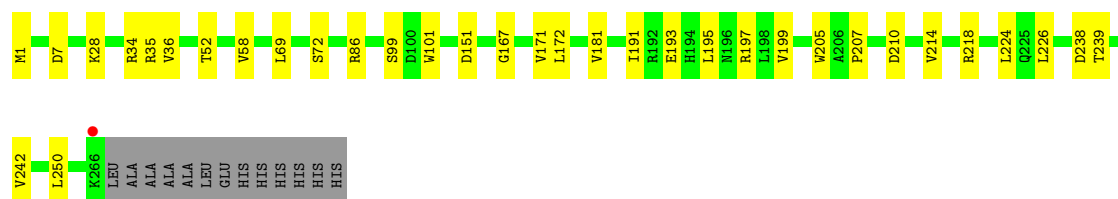
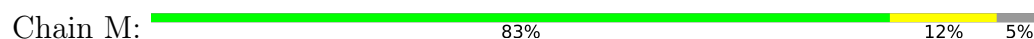
- Molecule 1: Type 1 encapsulin shell protein



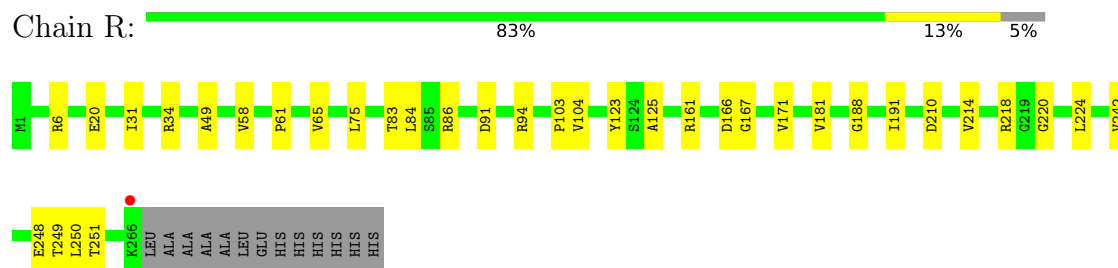
- Molecule 1: Type 1 encapsulin shell protein



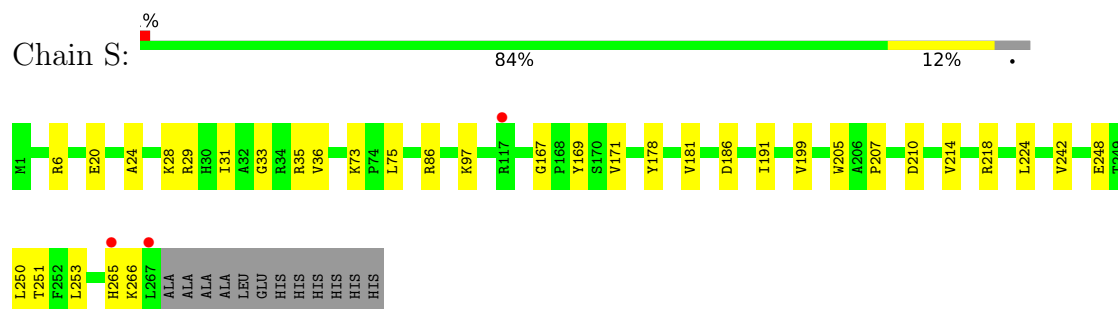
- Molecule 1: Type 1 encapsulin shell protein



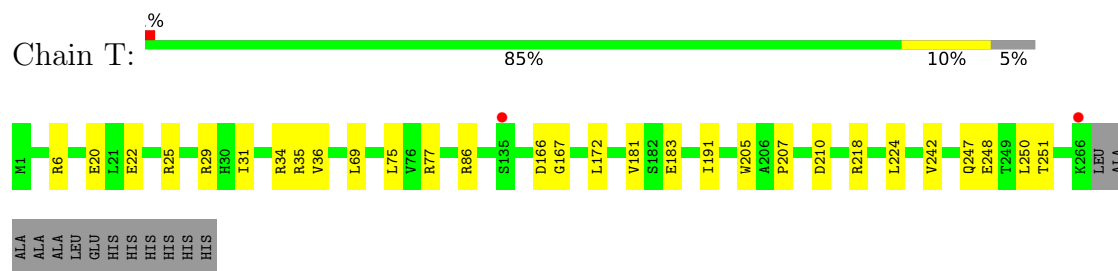
- Molecule 1: Type 1 encapsulin shell protein



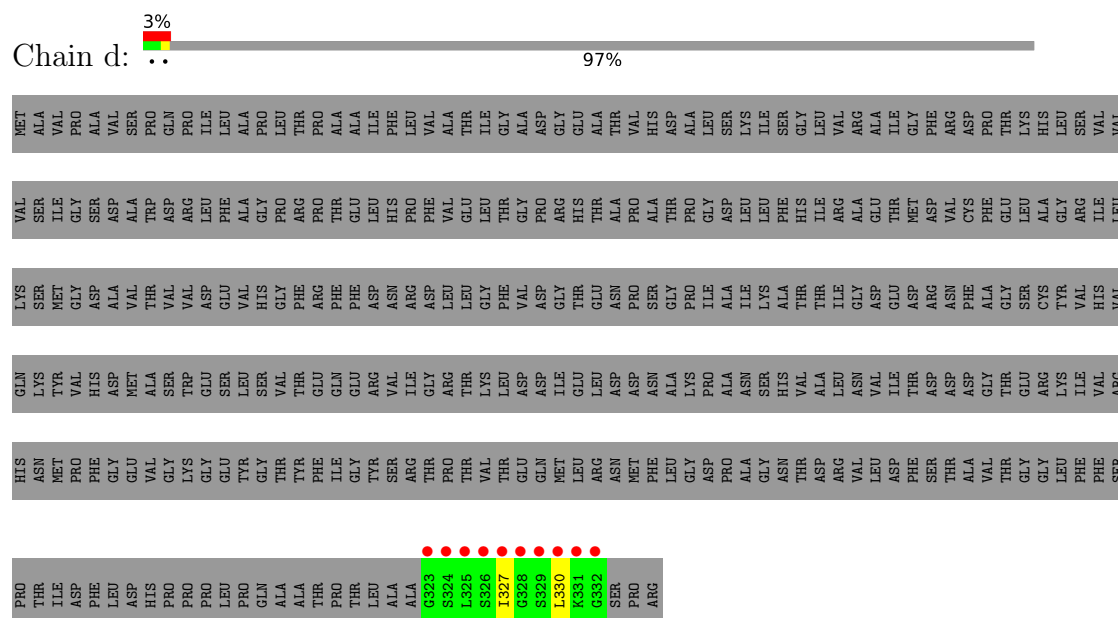
• Molecule 1: Type 1 encapsulin shell protein



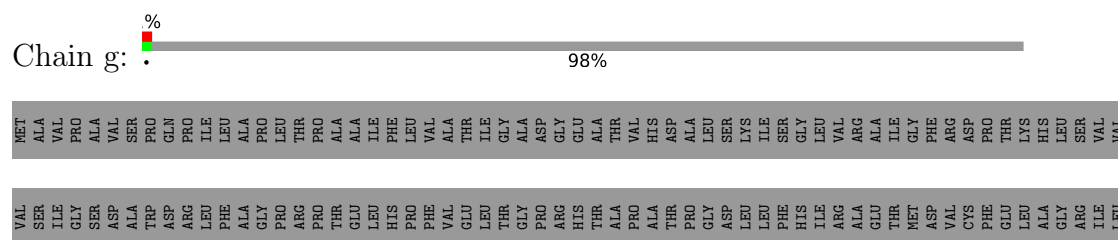
• Molecule 1: Type 1 encapsulin shell protein



• Molecule 2: Dye-decolorizing peroxidase



• Molecule 2: Dye-decolorizing peroxidase



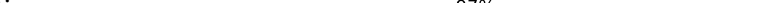
LYS SER MET MET GLY ASP ALA VAL THR VAL VAL VAL ASP ASP GLU VAL HIS GLY PHE PHE PHE ASP ASP ASN ARG ARG ASP ASP LEU LEU PHE PHE VAL ASP ASP GLY THR GLU GLU ASN ASN PRO PRO SER SER PRO PRO ILE ILE ALA ALA ILE ILE LYS LYS ALA ALA THR THR ILE ILE GLY GLY ASP ASP GLU ASP ARG ASN ASN PHE PHE ALA ALA GLY SER CYS TYR VAL THR HIS HIS VAL VAL

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HIS	ASN	MET	PRO	PHE	GLY	GLU	VAL	GLY	LYS	GLY	GLU	TYR	GLY	THR	TYR	PHE	ILE	GLY	GLY	SER	ARG	THR	PRO	THR	VAL	GLU	GLN	MET	LEU	LEU	ASP	PRO	ALA	GLY	ASN	THR	ASP	ARG	VAL	LEU	ASP	PHE	SER	THR	ALA	VAL	THR	GLY	GLY	LEU	PHE	PHE	THR
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PRO	THR	ILE	ASP	PHE	LEU	ASP	HIS	PRO	PRO	PRO	LEU	LEU	GLN	ALA	ALA	THR	THR	THR	LEU	ALA	ALA	GLY	GLY	SER	L325	L326	L327	G328	G329	L330	LYS	GLY	SER	PRO	ARG
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- Molecule 2: Dye-decolorizing peroxidase

Chain h: 

NET	ALA	VAL	PRO	ALA	VAL	SER	PRO	PRO	GLN	PRO	ILE	LEU	ALA	ALA	PRO	PRO	ALA	ALA	ILE	PHE	LEU	VAL	VAL	ASP	GLY	GLU	ALA	THR	THR	VAL	HIS	ASP	ALA	SER	LEU	SER	LYS	ILE	SER	GLY	LEU	VAL	ARG	ALA	ILE	ALA	GLY	PHE	ARG	ASP	PRO	THR	LYS	HIS	LEU	VAL	VAL
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VAL	SER	ILE	GLY	ASP	ALA	TRP	ASP	ARG	LEU	PHE	ALA	GLY	PRO	PRO	ARG	PRO	THR	GLU	LEU	HIS	PHE	VAL	GLU	LEU	THR	PRO	GLY	ARG	HIS	THR	ALA	ALA	ALA	THR	PRO	PRO	GLY	ASP	LEU	LEU	PHE	HIS	ILE	ARG	ALA	ALA	GLU	THR	MET	ASP	VAL	CYS	PHE	GLU	LEU	ALA	GLY	ILE	LEU
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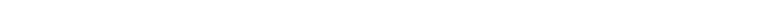
LYS SER MET NET GLY ASP ALA VAL THR VAL VAL VAL ASP ASP GLU VAL HIS GLY PHE ARG ARG PHE PHE ASP ASN ARG ASP LEU LEU GLY PHE VAL VAL ASP GLY THR GLU GLU ASN PRO SER SER PRO ILE ILE LYS LYS ALA THR THR ILE GLY GLY ASP GLU ASP ARG ASN PHE PHE ALA GLY SER CYS TYR VAL VAL HIS VAL

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HIS	ASN	MET	PHE	GLY	GLU	VAL	GLY	LYS	GLY	GLU	TYR	GLY	THR	TYR	PHE	ILE	GLY	TYR	SER	ARG	THR	PRO	THR	VAL	THR	THR	GLU	GLN	MET	LEU	ARG	ASN	MET	PHE	LEU	GLY	ASP	PRO	ALA	ALA	GLY	ASN	THR	ASP	THR	SER	THR	ALA	VAL	THR	GLY	LEU	PHE	PHE	PER
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PRO	THR	ILE	ASP	PHE	LEU	ASP	HIS	PRO	PRO	PRO	LEU	LEU	GLN	ALA	ALA	THR	THR	THR	LEU	ALA	ALA	G323	G324	L325	G326	L327	G328	G329	L330	K331	GLY	SER	PRO	ARG
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- Molecule 2: Dye-decolorizing peroxidase

Chain i: 

MET	VAL	ALA	VAL	PRO	ALA	SER	PRO	GLN	PRO	ILE	LEU	ALA	PRO	THR	PRO	ALA	ALA	ILE	PHE	LEU	VAL	VAL	ASP	GLY	GLU	ALA	THR	VAL	HIS	ASP	ALA	LEU	SER	LYS	ILE	SER	GLY	LEU	VAL	ARG	ALA	ILE	GLY	PHE	ARG	ASP	PRO	THR	LYS	HIS	LEU	SER	VAL
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VAL	SER	ILE	GLY	SER	ASP	ALA	TRP	ASP	ARG	ASP	ARG	LEU	PHE	ALA	GLY	PRO	ARG	PRO	THR	GLU	LEU	HIS	PHE	VAL	GLY	LEU	THR	PRO	ARG	HIS	THR	ALA	PRO	ALA	ALA	THR	PRO	GLY	ASP	LEU	PHE	HIS	ILE	ARG	GLU	THR	MET	ASP	VAL	CYS	PHE	GLU	LEU	ALA	GLY	ILE	ARG	LEU
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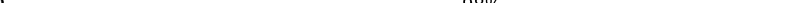
LYS SER MET MET GLY ASP ALA VAL THR VAL VAL ASP GLU VAL VAL HIS GLY PHE ARG ARG ARG ASP LEU LEU GLY PHE VAL ASP GLY THR GLU GLU ASN ASN PRO PRO SER SER PRO PRO ILE ILE ILE ILE LYS LYS ALA THR THR THR THR ILE ILE GLY GLY ASP ASP GLU ASP ARG ASN ASN PHE PHE GLY GLY SER CYS TYR VAL VAL HIS VAL

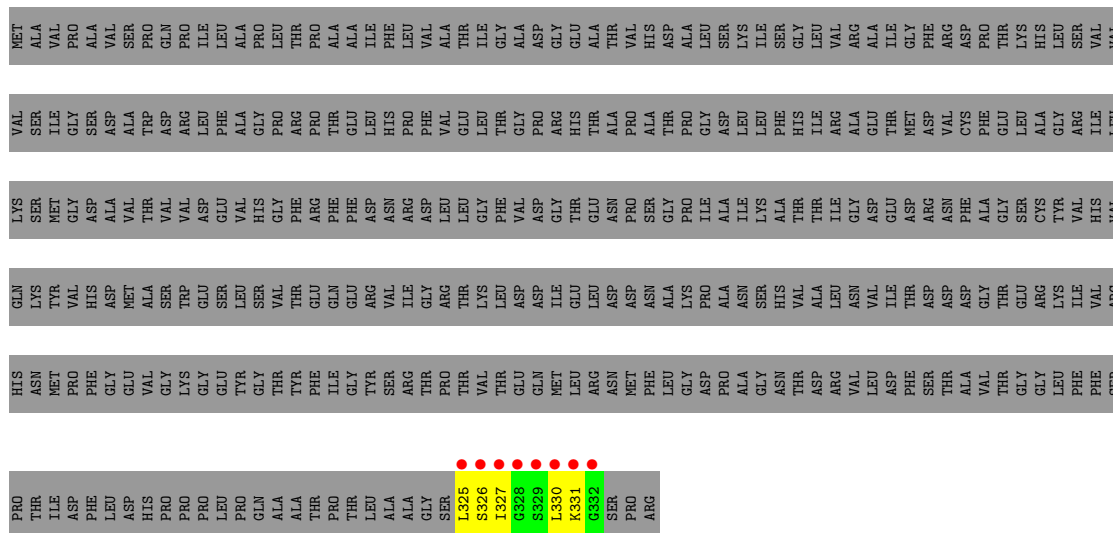
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VAL
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HIS	ASN	MET	PRO	PHE	GLY	GLU	VAL	GLY	LYS	GLY	GLU	TYR	GLY	THR	THR	PHE	PHE	ILE	GLY	TYR	ARG	SER	THR	PRO	THR	VAL	THR	THR	GLU	GLN	GLY	MET	LEU	LEU	ASP	ASN	ASN	MET	MET	PHE	LEU	GLY	ASP	PRO	PRO	ALA	ALA	GLY	GLY	ASN	THR	ASP	ASP	ARG	VAL	VAL	LEU	ASP	PHE	PHE	SER	THR	THR	ALA	ALA	VAL	THR	GLY	GLY	LEU	PHE	PHE	SER
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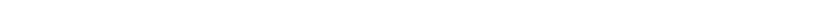
PRO	THR	ILE	ASP	PHE	LEU	ASP	HIS	PRO	PRO	PRO	LEU	LEU	GLN	ALA	ALA	THR	PRO	L319	L320	A321	A322	G323	S324	L325	S326	L327	G328	S329	L330	LYS	GLY	SER	PRO	ARG
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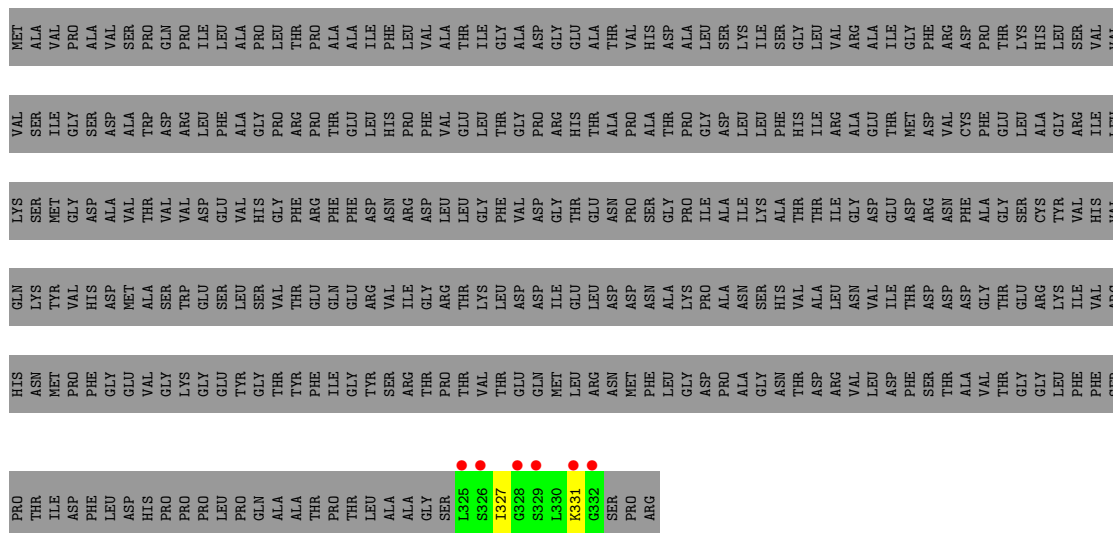
- Molecule 2: Dye-decolorizing peroxidase

Chain p: 

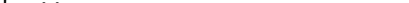


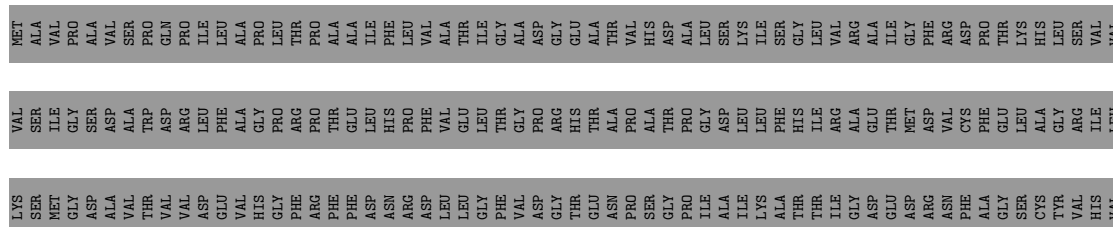
- Molecule 2: Dye-decolorizing peroxidase

Chain q:  2% 98%



- Molecule 2: Dye-decolorizing peroxidase

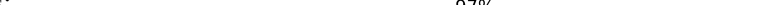
Chain r:  98%



[illegible]

PRO	THR	ILE	ASP	PHE	LEU	ASP	HIS	PRO	PRO	PRO	LEU	PRO	GLN	ALA	ALA	THR	PRO	THR	LEU	ALA	ALA	G232	S324	L325	S326	I327	G328	S329	L330	LYS	GLY	SER	PRO	ARG
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- Molecule 2: Dye-decolorizing peroxidase

Chain s: 

NET	ALA	VAL	PRO	PRO	GLN	ILE	LEU	ALA	PRO	THR	PRO	ALA	ALA	ILE	PHE	LEU	VAL	VAL	ASP	GLY	GLU	ALA	THR	THR	VAL	HIS	ASP	ALA	LEU	SER	LEU	LYS	ILE	SER	GLY	LEU	VAL	ARG	ALA	ILE	GLY	PHE	ARG	ASP	PRO	THR	LYS	HIS	LEU	SER	VAL
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VAL	SER	ILE	GLY	GLY	ASP	ALA	TRP	ASP	ARG	LEU	PHE	ALA	GLY	PRO	ARG	THR	LEU	GLU	HIS	PRO	PHE	VAL	GLY	THR	PRO	ARG	HIS	THR	ALA	ALA	PRO	THR	PRO	GLY	ASP	LEU	PHE	HIS	ILE	ARG	ALA	GLU	THR	NET	ASP	VAL	CYS	PHE	GLU	LEU	ALA	GLY	ARG	ILE
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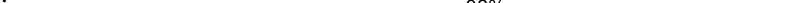
LYS SER MET GLY ASP ALA VAL THR VAL VAL ASP GLU VAL HIS GLY PHE ARG PHE ASP PHE ASN ARG ASP LEU LEU GLY PHE VAL VAL ASP GLY THR GLU GLU ASN PRO PRO SER SER GLY PRO PRO ILE ILE ILE LYS ALA THR THR ILE ILE GLY ASP GLU ASP ARG ASN PHE ALA CYS TYR VAL HIS

GLN	LYS	TYR	VAL	HIS	ASP	MET	ALA	SER	TRP	SER	GLU	SER	LEU	SER	VAL	THR	GLU	GLN	GLU	ARG	VAL	ILE	GLY	ARG	THR	LYS	LEU	ASP	ASP	ILE	GLU	LEU	ASP	ASN	ALA	LYS	PRO	ALA	ASN	SER	HIS	VAL	ALA	LEU	LEU	VAL	VAL	ASN	THR	THR	GLU	ARG	LYS	ILE	VAL
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HIS ASN MET MET PRO PHE GLY GLU VAL GLY GLY LYS GLY TYR THR GLY THR TYR PHE ILE GLY TYR SER ARG SER THR THR PRO THR VAL THR GLU GLN MET LEU LEU ASP ASP PRO PRO ALA ALA GLY ASN THR ASP ASP ARG VAL VAL LEU ASP PHE SER THR ALA ALA VAL THR GLY GLY LEU PHE PHE

PRO	THR	ILE	ASP	PHE	LEU	ASP	HIS	PRO	PRO	PRO	LEU	LEU	GLN	ALA	ALA	THR	LEU	ALA	G323	G324	G325	G326	G327	G328	G329	L330	G331	G332	SER	ARG
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- Molecule 2: Dye-decolorizing peroxidase

Chain t:  2% 2% 98%

NET	ALA	VAL	PRO	ALA	VAL	SER	PRO	SER	GLN	PRO	PRO	ILE	LEU	ALA	ALA	PRO	LEU	THR	PRO	ALA	ALA	ILE	PHE	LEU	VAL	VAL	ASP	GLY	GLU	ALA	ALA	THR	THR	VAL	HIS	ASP	ALA	ALA	LEU	SER	LYS	LYS	SER	GLY	LEU	VAL	VAL	ARG	ALA	ILE	GLY	PHE	ARG	ASP	PRO	THR	HIS	HIS	LEU	SER	VAL
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VAL	SER	ILE	GLY	SER	ASP	ALA	TRP	ASP	ARG	LEU	PHE	ALA	GLY	PRO	ARG	PRO	THR	GLU	LEU	HIS	PRO	PHE	VAL	GLU	THR	PRO	ARG	HIS	THR	ALA	PRO	THR	PRO	GLY	ASP	LEU	PHE	HIS	ILE	ARG	ALA	GLU	THR	THR	NET	ASP	VAL	CYS	PHE	GLU	LEU	ALA	GLY	ARG	ILE
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LYS SER MET LYS GLY ASP ALA VAL THR VAL VAL ASP GLU VAL HIS HIS PHE PHE PHE ASP ASN ARG ARG ASP LEU LEU GLY PHE VAL ASP GLY THR GLU GLU ASN PRO PRO SER SER GLY PRO PRO ILE ILE ILE ILE LYS ALA THR THR ILE ILE GLY ASP GLU ASP ARG ASN PHE ALA CYS TYR VAL HIS

GLN	LYS	TYR	VAL	HIS	ASP	MET	ALA	SER	TRP	TRP	GLU	SER	LEU	SER	VAL	THR	GLU	GLN	GLU	ARG	GLU	VAL	ILE	GLY	ARG	THR	LYS	LEU	ASP	ASP	ILE	GLU	LEU	ASP	ASN	ALA	LYS	PRO	ALA	ALA	ALA	ASN	SER	HIS	VAL	ALA	VAL	LEU	LEU	ASN	VAL	ILE	THR	GLY	THR	GLU	ARG	LYS	ILE	VAL
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HIS	ASN	MET	MET	PRO	PHE	GLY	GLU	VAL	GLY	GLY	LYS	GLY	GLU	TYR	GLY	THR	TYR	PHE	ILE	GLY	TYR	ARG	ARG	THR	PRO	THR	VAL	GLU	GLN	GLU	MET	LEU	ARG	ASN	ASN	PHE	LEU	GLY	ASP	PRO	PRO	ALA	GLY	ASN	THR	ASP	ASP	THR	THR	THR	THR	THR	GLY	GLY	LEU	PHE	PHE	PHE
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PRO	THR	ILE	ASP	PHE	LEU	ASP	HIS	PRO	PRO	PRO	PRO	GLN	ALA	ALA	THR	PRO	THR	LEU	ALA	GLY	S324	S326	S327	S329	L330	K331	GLY	SER	PRO	ARG
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	313.45Å 313.45Å 313.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.56 – 3.15 49.56 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.56-3.15) 99.3 (49.56-3.15)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.201 , 0.233 (Not available) , 0.194	Depositor DCC
R_{free} test set	8550 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	52.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	42837	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% 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: 1PE, NI, 12P, 2PE, GOL

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	0.08	0/2083	0.26	0/2842
1	B	0.09	0/2070	0.27	0/2823
1	C	0.12	0/2099	0.28	0/2863
1	D	0.10	0/2085	0.27	0/2843
1	E	0.11	0/2115	0.29	0/2885
1	F	0.10	0/2075	0.27	0/2830
1	G	0.09	0/2075	0.27	0/2830
1	H	0.09	0/2084	0.25	0/2842
1	I	0.10	0/2084	0.29	0/2842
1	J	0.09	0/2080	0.27	0/2837
1	K	0.09	0/2079	0.26	0/2835
1	L	0.09	0/2085	0.26	0/2844
1	M	0.08	0/2071	0.26	0/2825
1	N	0.09	0/2075	0.28	0/2831
1	O	0.08	0/2075	0.26	0/2830
1	P	0.08	0/2067	0.25	0/2821
1	Q	0.08	0/2063	0.26	0/2815
1	R	0.09	0/2075	0.26	0/2831
1	S	0.11	0/2115	0.32	1/2883 (0.0%)
1	T	0.09	0/2079	0.26	0/2835
2	d	0.19	0/53	0.59	0/70
2	g	0.13	0/34	0.29	0/45
2	h	0.19	0/49	0.55	0/65
2	i	0.15	0/73	0.43	0/98
2	p	0.11	0/43	0.63	0/57
2	q	0.18	0/42	0.68	0/55
2	r	0.10	0/47	0.25	0/62
2	s	0.18	0/59	0.89	0/77
2	t	0.14	0/49	0.44	0/65
All	All	0.09	0/42083	0.28	1/57381 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	S	266	LYS	CB-CA-C	-5.57	110.13	116.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2040	0	2011	26	0
1	B	2030	0	2009	31	0
1	C	2055	0	2034	38	0
1	D	2042	0	2019	23	0
1	E	2075	0	2057	23	0
1	F	2035	0	2011	35	0
1	G	2035	0	2009	25	0
1	H	2044	0	2017	30	0
1	I	2044	0	2017	23	0
1	J	2040	0	2013	23	0
1	K	2039	0	2015	31	0
1	L	2039	0	2015	29	0
1	M	2031	0	2007	20	0
1	N	2035	0	2004	25	0
1	O	2035	0	2011	35	0
1	P	2027	0	1996	25	0
1	Q	2023	0	1996	18	0
1	R	2035	0	2004	26	0
1	S	2065	0	2050	26	0
1	T	2039	0	2015	21	0
2	d	54	0	43	3	0
2	g	35	0	30	4	0
2	h	50	0	40	4	0
2	i	74	0	78	6	0
2	p	44	0	35	4	0
2	q	43	0	32	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	r	48	0	47	1	0
2	s	60	0	60	5	0
2	t	50	0	49	2	0
3	A	20	0	26	5	0
3	B	36	0	48	6	0
3	C	58	0	79	2	0
3	E	26	0	35	0	0
3	F	74	0	100	6	0
3	G	10	0	13	0	0
3	H	46	0	61	5	0
3	I	36	0	48	3	0
3	J	26	0	35	0	0
3	K	23	0	30	0	0
3	L	61	0	83	8	0
3	N	33	0	43	1	0
3	O	10	0	13	1	0
3	P	26	0	34	1	0
3	Q	26	0	35	2	0
3	R	30	0	39	2	0
3	T	26	0	35	2	0
4	A	10	0	13	1	0
4	H	47	0	62	1	0
4	J	16	0	21	1	0
4	L	25	0	33	7	0
5	A	30	0	40	5	0
5	B	30	0	40	2	0
5	C	12	0	16	1	0
5	D	30	0	40	2	0
5	E	24	0	32	2	0
5	F	18	0	24	1	0
5	G	6	0	8	0	0
5	H	30	0	40	2	0
5	I	36	0	48	3	0
5	J	24	0	32	1	0
5	K	36	0	48	5	0
5	L	24	0	32	3	0
5	M	18	0	24	0	0
5	N	12	0	16	0	0
5	O	36	0	48	1	0
5	Q	18	0	24	0	0
5	R	24	0	32	0	0
5	S	36	0	48	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	T	24	0	32	3	0
6	B	1	0	0	0	0
6	C	4	0	0	0	0
6	D	2	0	0	0	0
6	E	2	0	0	0	0
6	F	2	0	0	0	0
6	H	2	0	0	0	0
6	I	2	0	0	0	0
6	J	2	0	0	0	0
6	K	1	0	0	0	0
6	L	2	0	0	0	0
6	M	1	0	0	0	0
6	N	1	0	0	0	0
6	O	3	0	0	0	0
6	P	2	0	0	0	0
6	Q	2	0	0	0	0
6	R	1	0	0	0	0
6	S	3	0	0	0	0
7	T	13	0	16	1	0
8	A	25	0	0	0	0
8	B	14	0	0	0	0
8	C	15	0	0	0	0
8	D	16	0	0	0	0
8	E	14	0	0	1	0
8	F	24	0	0	0	0
8	G	12	0	0	0	0
8	H	23	0	0	0	0
8	I	29	0	0	0	0
8	J	30	0	0	1	0
8	K	24	0	0	0	0
8	L	28	0	0	0	0
8	M	18	0	0	0	0
8	N	17	0	0	0	0
8	O	16	0	0	0	0
8	P	14	0	0	0	0
8	Q	18	0	0	0	0
8	R	19	0	0	0	0
8	S	24	0	0	0	0
8	T	12	0	0	0	0
All	All	42837	0	42250	501	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 6.

All (501) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:VAL:HG22	1:C:214:VAL:HG22	1.63	0.79
1:J:171:VAL:HG22	1:J:214:VAL:HG22	1.67	0.76
1:L:171:VAL:HG22	1:L:214:VAL:HG22	1.67	0.76
1:O:147:ARG:HD2	1:O:186:ASP:HA	1.67	0.75
1:B:171:VAL:HG22	1:B:214:VAL:HG22	1.69	0.74
1:I:171:VAL:HG22	1:I:214:VAL:HG22	1.69	0.74
1:N:224:LEU:HD11	1:N:250:LEU:HD12	1.70	0.73
1:S:171:VAL:HG22	1:S:214:VAL:HG22	1.71	0.73
1:S:28:LYS:O	1:S:35:ARG:NH2	2.21	0.73
1:M:171:VAL:HG22	1:M:214:VAL:HG22	1.70	0.73
1:T:34:ARG:NH2	1:T:248:GLU:OE2	2.21	0.73
1:E:171:VAL:HG22	1:E:214:VAL:HG22	1.69	0.73
1:T:34:ARG:NH1	2:t:327:ILE:O	2.22	0.73
1:C:224:LEU:HD11	1:C:250:LEU:HD12	1.71	0.72
1:H:171:VAL:HG22	1:H:214:VAL:HG22	1.70	0.72
1:F:171:VAL:HG22	1:F:214:VAL:HG22	1.70	0.72
1:N:171:VAL:HG22	1:N:214:VAL:HG22	1.71	0.72
1:A:171:VAL:HG22	1:A:214:VAL:HG22	1.70	0.72
1:G:171:VAL:HG22	1:G:214:VAL:HG22	1.70	0.71
1:D:34:ARG:NH2	1:D:248:GLU:OE2	2.23	0.71
1:K:171:VAL:HG22	1:K:214:VAL:HG22	1.73	0.71
1:D:143:PRO:HD3	1:D:152:VAL:HG21	1.73	0.71
1:M:167:GLY:HA3	1:M:218:ARG:HB3	1.72	0.71
1:Q:171:VAL:HG22	1:Q:214:VAL:HG22	1.73	0.70
1:J:29:ARG:HH22	5:J:305:GOL:H2	1.54	0.70
1:E:224:LEU:HD11	1:E:250:LEU:HD12	1.73	0.70
1:R:171:VAL:HG22	1:R:214:VAL:HG22	1.73	0.69
1:L:29:ARG:HH22	5:L:306:GOL:H31	1.56	0.69
1:T:77:ARG:NH1	1:T:247:GLN:OE1	2.25	0.69
1:N:167:GLY:HA3	1:N:218:ARG:HB3	1.74	0.69
1:B:167:GLY:HA3	1:B:218:ARG:HB3	1.73	0.69
1:O:171:VAL:HG22	1:O:214:VAL:HG22	1.74	0.69
1:S:224:LEU:HD11	1:S:250:LEU:HD12	1.74	0.68
1:C:28:LYS:O	1:C:35:ARG:NH2	2.26	0.68
1:E:29:ARG:HH22	5:E:304:GOL:H2	1.58	0.68
1:P:171:VAL:HG22	1:P:214:VAL:HG22	1.74	0.68
1:N:28:LYS:O	1:N:35:ARG:NH2	2.27	0.68
1:O:181:VAL:HA	1:O:191:ILE:HD11	1.75	0.68
1:D:167:GLY:HA3	1:D:218:ARG:HB3	1.75	0.67
1:P:31:ILE:O	1:P:35:ARG:NH1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ARG:NH2	1:B:20:GLU:OE2	2.27	0.67
1:F:224:LEU:HD11	1:F:250:LEU:HD12	1.76	0.67
1:F:143:PRO:HD3	1:F:152:VAL:HG21	1.77	0.67
1:S:29:ARG:HH22	5:S:301:GOL:H32	1.60	0.67
1:C:220:GLY:HA3	3:F:304[B]:1PE:H152	1.77	0.66
1:K:6:ARG:NH2	1:K:20:GLU:OE2	2.28	0.66
1:D:171:VAL:HG22	1:D:214:VAL:HG22	1.76	0.66
1:I:6:ARG:NH2	1:I:20:GLU:OE2	2.27	0.66
1:K:28:LYS:O	1:K:35:ARG:NH2	2.28	0.66
1:R:6:ARG:NH2	1:R:20:GLU:OE2	2.26	0.66
1:F:34:ARG:NH2	1:F:248:GLU:OE2	2.29	0.65
1:G:230:VAL:HG11	2:g:327:ILE:HD12	1.77	0.65
1:L:6:ARG:NH2	1:L:20:GLU:OE2	2.30	0.65
1:S:24:ALA:HA	2:s:327:ILE:HD11	1.77	0.65
1:H:167:GLY:HA3	1:H:218:ARG:HB3	1.77	0.65
1:G:24:ALA:HA	2:g:327:ILE:HD11	1.79	0.65
1:H:143:PRO:HD3	1:H:152:VAL:HG21	1.79	0.65
1:J:167:GLY:HA3	1:J:218:ARG:HB3	1.78	0.65
1:N:62:THR:HG22	1:N:63:ASN:H	1.62	0.64
1:P:167:GLY:HA3	1:P:218:ARG:HB3	1.80	0.64
1:C:167:GLY:HA3	1:C:218:ARG:HB3	1.79	0.64
1:B:224:LEU:HD11	1:B:250:LEU:HD12	1.79	0.64
1:M:28:LYS:O	1:M:35:ARG:NH2	2.30	0.64
1:C:6:ARG:NH2	1:C:20:GLU:OE2	2.28	0.64
1:C:185:SER:H	5:C:305:GOL:H2	1.63	0.63
1:B:29:ARG:HH22	3:B:303:1PE:H251	1.61	0.63
1:A:167:GLY:HA3	1:A:218:ARG:HB3	1.81	0.63
1:L:35:ARG:NH1	5:L:306:GOL:O1	2.31	0.63
1:T:167:GLY:HA3	1:T:218:ARG:HB3	1.79	0.63
1:A:82:PHE:HA	5:A:305:GOL:H32	1.81	0.62
1:D:6:ARG:NH2	1:D:20:GLU:OE2	2.32	0.62
3:I:301:1PE:H132	1:J:161:ARG:HD3	1.81	0.62
1:E:167:GLY:HA3	1:E:218:ARG:HB3	1.80	0.62
1:I:167:GLY:HA3	1:I:218:ARG:HB3	1.80	0.62
1:R:167:GLY:HA3	1:R:218:ARG:HB3	1.80	0.62
1:I:113:PHE:HB3	5:I:307:GOL:H32	1.81	0.62
1:F:167:GLY:HA3	1:F:218:ARG:HB3	1.81	0.62
1:H:6:ARG:NH2	1:H:20:GLU:OE2	2.32	0.62
1:B:7:ASP:HB3	3:B:305:1PE:H141	1.82	0.62
1:O:167:GLY:HA3	1:O:218:ARG:HB3	1.82	0.61
1:G:181:VAL:HA	1:G:191:ILE:HD11	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:6:ARG:NH2	1:P:20:GLU:OE2	2.33	0.61
1:H:230:VAL:HB	2:h:326:SER:HB3	1.83	0.61
1:J:6:ARG:NH2	1:J:20:GLU:OE2	2.32	0.61
1:L:196:ASN:HB3	3:L:305[A]:1PE:H252	1.83	0.61
1:L:167:GLY:HA3	1:L:218:ARG:HB3	1.82	0.60
1:K:34:ARG:NH2	1:K:248:GLU:OE2	2.34	0.60
1:K:167:GLY:HA3	1:K:218:ARG:HB3	1.84	0.60
1:K:143:PRO:HD3	1:K:152:VAL:HG21	1.83	0.60
1:I:77:ARG:HH12	1:I:79:ARG:HD2	1.67	0.60
1:G:27:PHE:HB3	2:g:327:ILE:HD13	1.83	0.60
1:L:34:ARG:NH2	1:L:248:GLU:OE2	2.34	0.59
1:O:6:ARG:NH2	1:O:20:GLU:OE2	2.33	0.59
1:Q:167:GLY:HA3	1:Q:218:ARG:HB3	1.83	0.59
1:T:22:GLU:OE1	1:T:25:ARG:NH2	2.35	0.59
1:L:181:VAL:HA	1:L:191:ILE:HD11	1.84	0.59
1:L:192:ARG:HG2	1:L:196:ASN:HD21	1.68	0.59
1:D:101:TRP:O	1:D:104:VAL:HG12	2.03	0.59
1:L:36:VAL:HG11	1:L:172:LEU:HD11	1.83	0.59
1:T:166:ASP:HB2	5:T:304:GOL:H32	1.85	0.59
1:M:28:LYS:HD3	1:M:35:ARG:HH22	1.68	0.59
1:E:161:ARG:NH2	8:E:401:HOH:O	2.33	0.59
1:E:6:ARG:NH2	1:E:20:GLU:OE2	2.34	0.58
1:K:181:VAL:HA	1:K:191:ILE:HD11	1.86	0.58
1:S:167:GLY:HA3	1:S:218:ARG:HB3	1.84	0.58
1:B:248:GLU:HG2	1:B:250:LEU:HD22	1.86	0.58
1:G:167:GLY:HA3	1:G:218:ARG:HB3	1.85	0.58
1:J:58:VAL:HG22	1:R:125:ALA:HB1	1.85	0.58
1:K:36:VAL:HG11	1:K:172:LEU:HD11	1.85	0.58
1:H:28:LYS:HG3	2:h:330:LEU:HD13	1.86	0.58
1:B:205:TRP:H	3:B:303:1PE:H161	1.68	0.58
1:N:36:VAL:HG11	1:N:172:LEU:HD11	1.85	0.58
1:L:52:THR:HG23	1:L:72:SER:HA	1.86	0.57
1:D:39:VAL:HG11	2:d:330:LEU:HA	1.84	0.57
1:F:181:VAL:HA	1:F:191:ILE:HD11	1.86	0.57
1:P:79:ARG:NH2	1:P:247:GLN:OE1	2.30	0.57
1:S:35:ARG:HB3	2:s:331:LYS:HE3	1.86	0.57
1:J:125:ALA:HB1	1:R:58:VAL:HG22	1.87	0.57
1:S:20:GLU:HG2	2:s:325:LEU:CD2	2.35	0.57
1:Q:181:VAL:HA	1:Q:191:ILE:HD11	1.85	0.57
1:T:6:ARG:NH2	1:T:20:GLU:OE2	2.38	0.57
1:B:181:VAL:HA	1:B:191:ILE:HD11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6:ARG:NH2	1:G:20:GLU:OE2	2.36	0.56
1:H:117:ARG:HB3	5:H:309:GOL:H32	1.87	0.56
1:B:31:ILE:HG23	1:B:35:ARG:HH12	1.71	0.56
1:B:101:TRP:H	3:B:304:1PE:H141	1.70	0.56
1:N:181:VAL:HA	1:N:191:ILE:HD11	1.86	0.56
1:O:101:TRP:HB2	3:O:301:1PE:H141	1.87	0.56
3:B:305:1PE:H232	1:O:7:ASP:HB3	1.86	0.56
1:D:181:VAL:HA	1:D:191:ILE:HD11	1.85	0.56
1:G:28:LYS:O	1:G:35:ARG:NH2	2.38	0.56
1:C:181:VAL:HA	1:C:191:ILE:HD11	1.88	0.56
1:M:28:LYS:HE2	1:M:35:ARG:HH12	1.70	0.56
1:O:192:ARG:O	1:O:196:ASN:ND2	2.39	0.56
1:S:6:ARG:NH2	1:S:20:GLU:OE2	2.39	0.56
3:P:301:1PE:H241	1:Q:166:ASP:HB2	1.88	0.56
1:K:97:LYS:HG3	4:L:302:2PE:H61	1.86	0.56
1:L:192:ARG:HG2	1:L:196:ASN:ND2	2.20	0.56
1:J:143:PRO:HD3	1:J:152:VAL:HG21	1.87	0.56
1:H:192:ARG:O	1:H:196:ASN:ND2	2.39	0.55
1:A:34:ARG:NH2	1:A:248:GLU:OE2	2.39	0.55
1:R:84:LEU:HD23	1:R:103:PRO:HG2	1.88	0.55
1:E:248:GLU:HG2	1:E:250:LEU:HD22	1.89	0.55
1:F:192:ARG:HH11	1:F:196:ASN:HD21	1.54	0.55
1:B:114:VAL:HG21	1:P:65:VAL:HG21	1.89	0.55
1:H:34:ARG:HE	2:h:328:GLY:HA2	1.72	0.55
1:N:62:THR:HG22	1:N:63:ASN:N	2.21	0.55
1:N:58:VAL:HG21	1:N:69:LEU:HG	1.88	0.54
1:B:125:ALA:HB1	1:P:58:VAL:HG22	1.89	0.54
1:F:248:GLU:HG2	1:F:250:LEU:HD22	1.87	0.54
1:B:143:PRO:HD3	1:B:152:VAL:HG21	1.90	0.54
1:C:84:LEU:HD23	1:C:103:PRO:HG2	1.89	0.54
1:C:142:LEU:HD12	1:C:266:LYS:HA	1.88	0.54
1:J:117:ARG:NH1	8:J:401:HOH:O	2.40	0.54
1:M:181:VAL:HA	1:M:191:ILE:HD11	1.90	0.54
1:D:84:LEU:HD23	1:D:103:PRO:HG2	1.90	0.54
1:F:84:LEU:HD23	1:F:103:PRO:HG2	1.90	0.54
1:T:35:ARG:HG2	2:t:330:LEU:HB2	1.89	0.54
1:G:34:ARG:NH2	1:G:248:GLU:OE2	2.41	0.54
1:H:28:LYS:O	1:H:35:ARG:NH2	2.41	0.54
1:R:34:ARG:NH2	1:R:248:GLU:OE2	2.41	0.54
1:B:157:LEU:HD12	1:B:214:VAL:HG11	1.90	0.53
1:Q:84:LEU:HD21	1:Q:104:VAL:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:82:PHE:CE2	1:Q:104:VAL:HG22	2.43	0.53
1:S:248:GLU:HG2	1:S:250:LEU:HD22	1.89	0.53
1:N:6:ARG:NH2	1:N:20:GLU:OE2	2.40	0.53
1:O:62:THR:HG22	1:O:63:ASN:H	1.73	0.53
1:H:200:ASP:HB3	3:H:301:1PE:H221	1.91	0.53
1:O:157:LEU:HD12	1:O:214:VAL:HG11	1.91	0.53
1:A:181:VAL:HA	1:A:191:ILE:HD11	1.90	0.53
1:H:228:THR:HG21	3:H:305:1PE:H242	1.90	0.53
1:D:34:ARG:NH1	2:d:327:ILE:O	2.42	0.53
1:F:210:ASP:OD1	1:F:210:ASP:N	2.42	0.53
1:A:28:LYS:O	1:A:35:ARG:NH2	2.42	0.52
1:S:86:ARG:NH2	5:S:303:GOL:H11	2.24	0.52
1:F:114:VAL:HG21	1:K:65:VAL:HG21	1.91	0.52
1:M:1:MET:HE2	1:M:7:ASP:HB2	1.91	0.52
1:F:58:VAL:HG22	1:K:125:ALA:HB1	1.90	0.52
1:L:50:VAL:HG13	4:L:302:2PE:H111	1.90	0.52
1:H:98:ASP:OD1	1:I:54:ARG:NH1	2.42	0.52
1:F:6:ARG:NH2	1:F:20:GLU:OE2	2.41	0.52
1:F:192:ARG:O	1:F:196:ASN:ND2	2.43	0.52
1:E:86:ARG:HG2	1:E:242:VAL:HG23	1.92	0.52
1:R:181:VAL:HA	1:R:191:ILE:HD11	1.92	0.52
1:A:58:VAL:HG22	1:C:125:ALA:HB1	1.91	0.51
1:P:84:LEU:HD23	1:P:103:PRO:HG2	1.93	0.51
1:T:31:ILE:O	1:T:35:ARG:NH1	2.41	0.51
2:h:324:SER:O	2:h:326:SER:N	2.43	0.51
1:Q:157:LEU:HD12	1:Q:214:VAL:HG11	1.92	0.51
1:Q:86:ARG:HG2	1:Q:242:VAL:HG23	1.92	0.51
1:I:82:PHE:HA	3:I:302:1PE:H242	1.91	0.51
1:Q:6:ARG:NH1	1:Q:20:GLU:OE2	2.32	0.51
1:L:200:ASP:HA	3:L:305[A]:1PE:H232	1.91	0.51
1:L:7:ASP:HB3	3:L:304:1PE:H141	1.92	0.51
1:C:176:ASP:HB3	1:C:268:ALA:HB3	1.93	0.51
1:H:239:THR:HG23	4:H:303:2PE:H52	1.92	0.51
1:P:24:ALA:HB1	2:p:327:ILE:HD11	1.91	0.50
1:R:210:ASP:OD1	1:R:210:ASP:N	2.44	0.50
1:A:86:ARG:HG2	1:A:242:VAL:HG23	1.92	0.50
1:A:203:ILE:H	3:A:303:1PE:H121	1.76	0.50
1:L:52:THR:HB	4:L:302:2PE:H22	1.93	0.50
1:M:58:VAL:HG21	1:M:69:LEU:HG	1.93	0.50
5:A:306:GOL:H12	1:R:166:ASP:HB2	1.93	0.50
5:H:311:GOL:H32	1:I:50:VAL:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ASN:ND2	3:A:303:1PE:OH3	2.45	0.50
1:B:123:TYR:CZ	1:P:61:PRO:HG3	2.47	0.50
1:C:36:VAL:HG11	1:C:172:LEU:HD11	1.94	0.50
1:A:202:ASP:HA	3:A:303:1PE:H222	1.92	0.50
5:A:304:GOL:H31	1:R:161:ARG:HD3	1.94	0.50
1:G:58:VAL:HG22	1:O:125:ALA:HB1	1.93	0.50
1:M:224:LEU:HD11	1:M:250:LEU:HD22	1.94	0.50
1:P:34:ARG:NH2	1:P:248:GLU:OE2	2.45	0.50
1:F:202:ASP:HA	3:F:303:1PE:H252	1.94	0.50
1:C:86:ARG:HG2	1:C:242:VAL:HG23	1.93	0.49
1:S:73[B]:LYS:HD3	1:S:253:LEU:HG	1.94	0.49
1:P:84:LEU:HD21	1:P:104:VAL:HG23	1.93	0.49
1:P:117:ARG:HD3	1:P:121:GLU:HG3	1.94	0.49
3:A:301:1PE:H152	1:R:220:GLY:HA3	1.95	0.49
1:B:195:LEU:O	1:B:199:VAL:HG23	2.12	0.49
1:C:129:GLU:HG2	1:C:133:SER:HB3	1.93	0.49
1:O:86:ARG:HG2	1:O:242:VAL:HG23	1.94	0.49
1:P:181:VAL:HA	1:P:191:ILE:HD11	1.93	0.49
1:I:117:ARG:HB3	5:I:306:GOL:H32	1.94	0.49
1:N:248:GLU:HG2	1:N:250:LEU:HD22	1.94	0.49
1:R:86:ARG:HG2	1:R:242:VAL:HG23	1.93	0.49
1:H:86:ARG:HG2	1:H:242:VAL:HG23	1.93	0.49
1:P:129:GLU:HG2	1:P:133:SER:HB3	1.95	0.49
1:B:86:ARG:HG2	1:B:242:VAL:HG23	1.95	0.49
1:F:123:TYR:CZ	1:K:61:PRO:HG3	2.47	0.49
1:D:183:GLU:HB2	1:E:151:ASP:HA	1.93	0.49
1:K:205:TRP:CD1	1:K:207:PRO:HD3	2.48	0.49
2:i:321:ALA:O	2:i:323:GLY:N	2.45	0.49
1:F:125:ALA:HB1	1:K:58:VAL:HG22	1.94	0.49
1:R:91:ASP:OD1	1:R:94:ARG:NH1	2.45	0.49
1:S:33:GLY:HA2	1:S:36:VAL:HG22	1.95	0.49
1:I:195:LEU:O	1:I:199:VAL:HG23	2.13	0.48
1:E:29:ARG:HH21	1:F:161:ARG:HD3	1.78	0.48
1:A:114:VAL:HG21	1:C:65:VAL:HG21	1.95	0.48
1:J:86:ARG:HG2	1:J:242:VAL:HG23	1.94	0.48
1:J:123:TYR:CZ	1:R:61:PRO:HG3	2.49	0.48
1:M:36:VAL:HG11	1:M:172:LEU:HD11	1.96	0.48
1:M:238:ASP:CG	1:M:239:THR:H	2.21	0.48
1:C:84:LEU:HD21	1:C:104:VAL:HG23	1.95	0.48
1:G:123:TYR:CZ	1:O:61:PRO:HG3	2.48	0.48
1:L:202:ASP:HA	3:L:305[B]:1PE:H262	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ARG:NH2	1:A:20:GLU:OE2	2.46	0.48
1:C:248:GLU:HG2	1:C:250:LEU:HD22	1.95	0.48
1:K:167:GLY:N	5:K:303:GOL:O2	2.46	0.48
1:I:181:VAL:HA	1:I:191:ILE:HD11	1.94	0.48
1:L:46:VAL:HG12	4:L:302:2PE:H231	1.96	0.48
1:E:181:VAL:HA	1:E:191:ILE:HD11	1.96	0.47
5:E:306:GOL:O3	1:F:51:SER:O	2.31	0.47
1:A:65:VAL:HG21	1:C:114:VAL:HG21	1.95	0.47
1:H:192:ARG:HH11	1:H:196:ASN:HD21	1.62	0.47
1:N:86:ARG:HG2	1:N:242:VAL:HG23	1.94	0.47
1:N:205:TRP:CD1	1:N:207:PRO:HD3	2.50	0.47
1:O:153:ILE:O	1:O:157:LEU:HD13	2.14	0.47
1:Q:36:VAL:HG11	1:Q:172:LEU:HD11	1.95	0.47
1:E:143:PRO:HD3	1:E:152:VAL:HG21	1.95	0.47
1:I:7:ASP:HA	2:i:320:LEU:HD22	1.95	0.47
1:S:205:TRP:CD1	1:S:207:PRO:HD3	2.50	0.47
1:B:58:VAL:HG22	1:P:125:ALA:HB1	1.97	0.47
1:Q:205:TRP:CD1	1:Q:207:PRO:HD3	2.50	0.47
1:S:210:ASP:OD1	1:S:210:ASP:N	2.46	0.47
1:I:77:ARG:NH1	1:I:79:ARG:HD2	2.29	0.47
1:L:49:ALA:O	4:L:302:2PE:H182	2.14	0.47
3:L:305[B]:1PE:H152	3:L:305[B]:1PE:H161	1.65	0.47
1:J:114:VAL:HG21	1:R:65:VAL:HG21	1.97	0.47
1:C:51:SER:HB2	3:C:301:1PE:H141	1.97	0.46
1:E:82:PHE:CE2	1:E:104:VAL:HG22	2.50	0.46
1:L:129:GLU:HG2	1:L:133:SER:HB3	1.97	0.46
1:N:99:SER:HB2	1:N:101:TRP:CH2	2.50	0.46
1:H:247:GLN:HE22	3:H:305:1PE:H231	1.79	0.46
1:J:29:ARG:HH21	1:K:161:ARG:HD3	1.80	0.46
1:O:192:ARG:HE	1:O:203:ILE:HD12	1.79	0.46
1:H:12:THR:HG22	1:H:14:ALA:H	1.80	0.46
1:R:75:LEU:HA	1:R:251:THR:OG1	2.15	0.46
1:T:205:TRP:CD1	1:T:207:PRO:HD3	2.50	0.46
1:E:28:LYS:O	1:E:35:ARG:NH2	2.49	0.46
1:K:29:ARG:NH1	5:K:308:GOL:H11	2.29	0.46
1:K:86:ARG:HG2	1:K:242:VAL:HG23	1.96	0.46
1:Q:230:VAL:HA	1:Q:247:GLN:O	2.15	0.46
1:A:151:ASP:HA	1:B:183:GLU:HB2	1.97	0.46
1:C:62:THR:HG22	1:C:63:ASN:N	2.31	0.46
1:F:75:LEU:HA	1:F:251:THR:OG1	2.15	0.46
3:Q:301:1PE:H221	3:Q:301:1PE:H132	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:ASN:HA	1:O:12:THR:HG23	1.97	0.46
1:E:193:GLU:OE2	1:F:189:TYR:OH	2.31	0.46
1:A:129:GLU:HG2	1:A:133:SER:HB3	1.97	0.46
1:H:84:LEU:HD23	1:H:103:PRO:HG2	1.97	0.46
1:K:129:GLU:HG2	1:K:133:SER:HB3	1.98	0.46
1:N:101:TRP:HZ3	3:N:303:1PE:H122	1.80	0.46
1:Q:143:PRO:HD2	1:Q:149:ILE:HD13	1.97	0.46
1:C:169:TYR:O	1:C:199:VAL:HG13	2.16	0.46
1:M:193:GLU:O	1:M:197:ARG:HG3	2.16	0.46
1:O:84:LEU:HD21	1:O:104:VAL:HG23	1.98	0.46
1:O:205:TRP:CD1	1:O:207:PRO:HD3	2.51	0.46
1:S:86:ARG:HG2	1:S:242:VAL:HG23	1.98	0.46
1:A:210:ASP:OD1	1:A:210:ASP:N	2.46	0.46
1:I:2:ASN:HD21	2:i:322:ALA:HA	1.80	0.46
1:B:34:ARG:NH2	1:B:226:LEU:HD11	2.30	0.45
1:F:28:LYS:HE3	1:F:28:LYS:HB2	1.81	0.45
1:G:86:ARG:HG2	1:G:242:VAL:HG23	1.98	0.45
1:K:210:ASP:OD1	1:K:210:ASP:N	2.46	0.45
5:K:308:GOL:H12	1:L:166:ASP:HB2	1.98	0.45
1:C:205:TRP:CD1	1:C:207:PRO:HD3	2.52	0.45
1:C:210:ASP:OD1	1:C:210:ASP:N	2.48	0.45
1:H:123:TYR:CE1	1:H:125:ALA:HB3	2.51	0.45
1:I:4:LEU:HD12	2:i:322:ALA:O	2.15	0.45
1:L:192:ARG:O	1:L:196:ASN:ND2	2.49	0.45
1:M:195:LEU:O	1:M:199:VAL:HG22	2.16	0.45
1:M:151:ASP:HA	1:Q:183:GLU:HB2	1.98	0.45
1:D:230:VAL:HB	2:d:327:ILE:HD12	1.99	0.45
1:T:36:VAL:HG11	1:T:172:LEU:HD11	1.99	0.45
2:p:325:LEU:O	2:p:327:ILE:N	2.49	0.45
1:I:75:LEU:HA	1:I:251:THR:OG1	2.16	0.45
1:M:99:SER:HB2	1:M:101:TRP:CZ2	2.52	0.45
1:S:97:LYS:HE3	5:T:305:GOL:H32	1.98	0.45
3:B:305:1PE:H152	1:C:1:MET:HG3	1.97	0.45
1:C:141:THR:HG23	1:C:265[A]:HIS:HB3	1.99	0.45
1:M:205:TRP:CD1	1:M:207:PRO:HD3	2.52	0.45
1:P:224:LEU:HD11	1:P:250:LEU:HD22	1.99	0.45
1:G:34:ARG:NH1	2:g:327:ILE:O	2.49	0.45
1:H:233:GLY:HA3	1:H:245:TYR:CZ	2.52	0.45
1:J:153:ILE:O	1:J:157:LEU:HD23	2.16	0.45
1:B:117:ARG:NH2	1:B:210:ASP:OD2	2.47	0.45
1:C:166:ASP:HB2	3:F:302:1PE:H262	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:LEU:HD11	1:D:250:LEU:HD22	1.98	0.45
1:M:34:ARG:NH2	1:M:226:LEU:HD11	2.32	0.45
1:E:13:GLU:HG2	1:K:1:MET:H2	1.81	0.45
1:I:77:ARG:HH12	1:I:79:ARG:CD	2.30	0.45
4:J:302:2PE:H81	1:R:49:ALA:H	1.81	0.45
1:S:75:LEU:HA	1:S:251:THR:OG1	2.17	0.45
1:N:165:VAL:HG13	1:N:218:ARG:HE	1.82	0.44
1:P:205:TRP:CD1	1:P:207:PRO:HD3	2.52	0.44
1:T:167:GLY:N	5:T:304:GOL:O2	2.50	0.44
1:F:205:TRP:CD1	1:F:207:PRO:HD3	2.52	0.44
1:G:195:LEU:O	1:G:199:VAL:HG22	2.16	0.44
1:C:12:THR:HG23	1:O:2:ASN:HA	2.00	0.44
1:E:129:GLU:HG2	1:E:133:SER:HB3	1.98	0.44
1:G:234:TYR:OH	1:G:237:HIS:ND1	2.33	0.44
1:Q:153:ILE:O	1:Q:157:LEU:HD13	2.17	0.44
1:S:181:VAL:HA	1:S:191:ILE:HD11	1.98	0.44
1:A:7:ASP:HA	4:A:302:2PE:H61	1.99	0.44
1:G:65:VAL:HG21	1:O:114:VAL:HG21	1.99	0.44
1:O:193:GLU:HG3	1:P:197:ARG:NH2	2.32	0.44
3:Q:301:1PE:H251	3:Q:301:1PE:H241	1.77	0.44
1:T:181:VAL:HA	1:T:191:ILE:HD11	1.98	0.44
1:Q:195:LEU:O	1:Q:199:VAL:HG22	2.18	0.44
1:H:117:ARG:HD3	1:H:121:GLU:HG3	2.00	0.44
1:J:84:LEU:HD21	1:J:104:VAL:HG23	2.00	0.44
1:K:98:ASP:OD1	4:L:302:2PE:O1	2.36	0.44
3:L:304:1PE:H231	3:L:304:1PE:H242	1.74	0.44
1:P:86:ARG:HG2	1:P:242:VAL:HG23	2.00	0.44
1:R:31:ILE:HG21	2:r:330:LEU:HD12	1.99	0.44
1:B:95:GLY:HA3	1:C:46:VAL:HG13	1.99	0.44
1:F:25:ARG:NH1	3:F:304[A]:1PE:H162	2.33	0.44
1:N:192:ARG:O	1:N:196:ASN:ND2	2.51	0.44
1:J:205:TRP:CD1	1:J:207:PRO:HD3	2.52	0.44
1:K:224:LEU:HD11	1:K:250:LEU:HD22	2.00	0.44
1:L:200:ASP:HB3	3:L:305[A]:1PE:H221	2.00	0.44
1:O:192:ARG:HG3	1:O:196:ASN:HD21	1.82	0.44
1:A:45:PRO:O	1:C:70:ARG:NH2	2.49	0.43
1:F:2:ASN:HA	1:J:12:THR:HG23	1.99	0.43
1:P:34:ARG:NH1	2:p:327:ILE:O	2.51	0.43
1:P:69:LEU:HD23	1:P:69:LEU:HA	1.91	0.43
3:T:302:1PE:H141	3:T:302:1PE:H131	1.75	0.43
1:H:101:TRP:HB2	3:H:302[B]:1PE:H242	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:86:ARG:HG2	1:M:242:VAL:HG23	2.00	0.43
1:I:28:LYS:HE3	2:i:330:LEU:HD13	2.01	0.43
1:M:210:ASP:OD1	1:M:210:ASP:N	2.49	0.43
1:N:33:GLY:O	1:N:37:VAL:HG22	2.18	0.43
1:S:29:ARG:HA	1:S:29:ARG:HD2	1.84	0.43
3:A:301:1PE:H151	3:A:301:1PE:H142	1.68	0.43
1:D:177:VAL:HG22	5:D:304:GOL:H31	2.00	0.43
1:D:189:TYR:OH	1:G:193:GLU:OE2	2.32	0.43
1:P:210:ASP:OD1	1:P:210:ASP:N	2.49	0.43
1:I:224:LEU:HD11	1:I:250:LEU:HD22	2.01	0.43
3:I:302:1PE:H241	3:I:302:1PE:H232	1.69	0.43
1:J:33:GLY:HA2	1:J:36:VAL:HG22	2.01	0.43
1:D:195:LEU:O	1:D:199:VAL:HG22	2.18	0.43
1:E:205:TRP:CD1	1:E:207:PRO:HD3	2.54	0.43
1:N:29:ARG:HH21	1:O:161:ARG:CD	2.31	0.43
1:N:84:LEU:HD21	1:N:104:VAL:HG23	1.99	0.43
1:J:61:PRO:HG3	1:R:123:TYR:CZ	2.54	0.43
5:B:308:GOL:H2	1:T:25:ARG:HB3	2.01	0.43
1:F:73:LYS:HE3	1:F:127:SER:O	2.18	0.43
1:I:210:ASP:OD1	1:I:210:ASP:N	2.50	0.43
1:G:205:TRP:CD1	1:G:207:PRO:HD3	2.54	0.43
1:H:51:SER:O	5:L:301:GOL:O1	2.37	0.43
1:D:62:THR:HG22	1:D:63:ASN:H	1.84	0.42
1:F:86:ARG:HG2	1:F:242:VAL:HG23	2.01	0.42
1:L:52:THR:HA	4:L:302:2PE:H52	2.00	0.42
3:L:305[A]:1PE:H232	3:L:305[A]:1PE:H241	1.88	0.42
1:T:75:LEU:HA	1:T:251:THR:OG1	2.19	0.42
1:T:210:ASP:OD1	1:T:210:ASP:N	2.50	0.42
7:T:301:12P:H241	7:T:301:12P:H212	1.81	0.42
1:A:205:TRP:CD1	1:A:207:PRO:HD3	2.53	0.42
1:J:157:LEU:HD22	1:J:214:VAL:HG11	2.01	0.42
1:K:58:VAL:O	5:K:305:GOL:O1	2.35	0.42
1:L:223:ASP:CG	1:L:225:GLN:HE21	2.27	0.42
1:N:132:ARG:NH2	1:N:210:ASP:O	2.52	0.42
1:C:143:PRO:HG2	1:C:267:LEU:HD11	2.01	0.42
1:F:117:ARG:HD3	1:F:208:ALA:O	2.20	0.42
1:K:247:GLN:NE2	5:K:306:GOL:H2	2.34	0.42
1:P:35:ARG:HG2	2:p:330:LEU:HB2	2.00	0.42
1:R:83:THR:O	3:R:303:1PE:H251	2.20	0.42
1:S:24:ALA:HA	2:s:327:ILE:CD1	2.46	0.42
1:B:175:ALA:HB3	5:B:306:GOL:H2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ARG:CD	1:T:29:ARG:HH21	2.32	0.42
1:C:82:PHE:CZ	1:C:244:LEU:HB2	2.55	0.42
1:G:69:LEU:HD23	1:G:69:LEU:HA	1.92	0.42
1:G:114:VAL:HG21	1:O:65:VAL:HG21	2.00	0.42
1:O:123:TYR:CE1	1:O:125:ALA:HB3	2.55	0.42
1:A:233:GLY:HA3	1:A:245:TYR:CZ	2.55	0.42
1:D:29:ARG:NH2	5:D:302:GOL:O2	2.49	0.42
1:R:224:LEU:HD11	1:R:250:LEU:HD22	2.02	0.42
1:A:29:ARG:NH2	5:A:304:GOL:O2	2.47	0.42
1:A:73:LYS:HA	1:A:73:LYS:HD2	1.84	0.42
1:B:52:THR:HG23	1:B:72:SER:HA	2.02	0.42
1:S:28:LYS:HA	1:S:31:ILE:HG22	2.01	0.42
3:T:302:1PE:H222	3:T:302:1PE:H132	1.76	0.42
1:B:123:TYR:CE1	1:B:125:ALA:HB3	2.54	0.42
3:F:304[B]:1PE:H151	3:F:304[B]:1PE:H142	1.77	0.42
1:N:75:LEU:HA	1:N:251:THR:OG1	2.20	0.42
1:F:58:VAL:CG2	1:K:125:ALA:HB1	2.49	0.41
1:F:149:ILE:N	1:F:150:PRO:HD2	2.35	0.41
1:L:224:LEU:HD11	1:L:250:LEU:HD22	2.02	0.41
1:R:75:LEU:HD23	1:R:249:THR:HG22	2.02	0.41
1:T:86:ARG:HG2	1:T:242:VAL:HG23	2.02	0.41
1:B:46:VAL:HG13	1:O:95:GLY:HA3	2.03	0.41
1:F:65:VAL:HG21	1:K:114:VAL:HG21	2.01	0.41
1:H:224:LEU:HD11	1:H:250:LEU:HD22	2.02	0.41
1:T:224:LEU:HD11	1:T:250:LEU:HD22	2.01	0.41
1:A:29:ARG:NH1	5:A:306:GOL:H11	2.36	0.41
1:N:31:ILE:HD12	1:N:31:ILE:HA	1.93	0.41
1:A:58:VAL:CG2	1:C:125:ALA:HB1	2.50	0.41
1:E:29:ARG:NH2	1:F:161:ARG:HD3	2.35	0.41
1:G:61:PRO:HG3	1:O:123:TYR:CZ	2.56	0.41
1:J:181:VAL:HA	1:J:191:ILE:HD11	2.02	0.41
1:O:224:LEU:HD11	1:O:250:LEU:HD22	2.01	0.41
2:i:321:ALA:O	2:i:322:ALA:C	2.63	0.41
1:H:205:TRP:CD1	1:H:207:PRO:HD3	2.55	0.41
1:K:52:THR:HG23	1:K:72:SER:HA	2.03	0.41
1:K:91:ASP:HB3	1:K:96:SER:CB	2.50	0.41
1:D:31:ILE:HD12	1:D:31:ILE:HA	1.97	0.41
1:H:181:VAL:HA	1:H:191:ILE:HD11	2.01	0.41
1:J:123:TYR:CE1	1:J:125:ALA:HB3	2.56	0.41
1:L:233:GLY:HA3	1:L:245:TYR:CZ	2.56	0.41
1:M:52:THR:HG23	1:M:72:SER:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:ARG:HG2	1:D:242:VAL:HG23	2.02	0.41
1:S:178:TYR:OH	5:S:301:GOL:O2	2.23	0.41
1:A:110:LYS:HE3	1:A:110:LYS:HB2	1.92	0.41
1:B:205:TRP:CD1	1:B:207:PRO:HD3	2.55	0.41
1:D:192:ARG:NH1	1:D:196:ASN:OD1	2.54	0.41
1:E:123:TYR:CE1	1:E:125:ALA:HB3	2.56	0.41
1:O:210:ASP:OD1	1:O:210:ASP:N	2.52	0.41
2:s:324:SER:C	2:s:326:SER:H	2.28	0.41
1:C:149:ILE:N	1:C:150:PRO:HD2	2.36	0.41
1:G:125:ALA:HB1	1:O:58:VAL:HG22	2.03	0.41
1:G:191:ILE:O	1:G:195:LEU:HD13	2.21	0.41
1:G:210:ASP:OD1	1:G:210:ASP:N	2.53	0.41
1:N:123:TYR:CE1	1:N:125:ALA:HB3	2.56	0.41
1:N:143:PRO:HD3	1:N:152:VAL:HG11	2.03	0.41
1:B:151:ASP:HA	1:T:183:GLU:HB2	2.03	0.41
1:C:123:TYR:CE1	1:C:125:ALA:HB3	2.55	0.41
1:O:201:GLY:O	5:O:305:GOL:H2	2.20	0.41
1:R:84:LEU:HD21	1:R:104:VAL:HG23	2.03	0.41
1:R:188:GLY:HA3	1:S:186:ASP:O	2.21	0.41
1:T:69:LEU:HD23	1:T:69:LEU:HA	1.96	0.41
1:F:233:GLY:HA3	1:F:245:TYR:CZ	2.56	0.40
1:H:84:LEU:HD21	1:H:104:VAL:HG23	2.03	0.40
1:I:198:LEU:HD23	1:I:198:LEU:HA	1.91	0.40
1:O:52:THR:HG23	1:O:72:SER:HA	2.03	0.40
1:S:169:TYR:O	1:S:199:VAL:HG13	2.21	0.40
1:H:202:ASP:HA	3:H:301:1PE:H262	2.03	0.40
1:K:7:ASP:N	1:K:7:ASP:OD1	2.54	0.40
1:O:59:LYS:HD3	1:O:60:ALA:O	2.20	0.40
1:P:36:VAL:HG11	1:P:172:LEU:HD11	2.02	0.40
1:Q:123:TYR:CE1	1:Q:125:ALA:HB3	2.56	0.40
1:E:146:PRO:HG3	1:E:180:LYS:NZ	2.36	0.40
1:E:188:GLY:HA3	1:F:186:ASP:O	2.21	0.40
3:F:304[A]:1PE:H121	3:F:304[A]:1PE:H232	1.88	0.40
1:I:86:ARG:HG2	1:I:242:VAL:HG23	2.02	0.40
1:O:31:ILE:HD12	1:O:31:ILE:HA	1.94	0.40
1:D:36:VAL:HG11	1:D:172:LEU:HD11	2.02	0.40
1:J:82:PHE:CE2	1:J:104:VAL:HG22	2.56	0.40
1:O:62:THR:HG22	1:O:63:ASN:N	2.37	0.40
1:Q:11:VAL:HB	1:Q:16:TRP:NE1	2.37	0.40
1:S:28:LYS:HE2	1:S:28:LYS:HB3	1.90	0.40
1:C:243:ARG:HH12	3:C:302:1PE:H141	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:ARG:CD	1:G:29:ARG:HH21	2.35	0.40
1:E:185:SER:OG	5:F:306:GOL:H12	2.22	0.40
1:F:61:PRO:HG3	1:K:123:TYR:CZ	2.56	0.40
1:H:210:ASP:OD1	1:H:210:ASP:N	2.54	0.40
1:I:243:ARG:HB2	5:I:309:GOL:H11	2.02	0.40
1:R:83:THR:H	3:R:303:1PE:H141	1.86	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	266/279 (95%)	258 (97%)	8 (3%)	0	100	100
1	B	263/279 (94%)	256 (97%)	7 (3%)	0	100	100
1	C	267/279 (96%)	258 (97%)	9 (3%)	0	100	100
1	D	265/279 (95%)	257 (97%)	7 (3%)	1 (0%)	30	59
1	E	270/279 (97%)	261 (97%)	9 (3%)	0	100	100
1	F	264/279 (95%)	258 (98%)	6 (2%)	0	100	100
1	G	264/279 (95%)	255 (97%)	9 (3%)	0	100	100
1	H	265/279 (95%)	257 (97%)	8 (3%)	0	100	100
1	I	265/279 (95%)	256 (97%)	9 (3%)	0	100	100
1	J	265/279 (95%)	257 (97%)	8 (3%)	0	100	100
1	K	264/279 (95%)	256 (97%)	8 (3%)	0	100	100
1	L	265/279 (95%)	258 (97%)	7 (3%)	0	100	100
1	M	264/279 (95%)	256 (97%)	8 (3%)	0	100	100
1	N	264/279 (95%)	257 (97%)	7 (3%)	0	100	100
1	O	264/279 (95%)	257 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	264/279 (95%)	256 (97%)	8 (3%)	0	100	100
1	Q	263/279 (94%)	255 (97%)	8 (3%)	0	100	100
1	R	264/279 (95%)	258 (98%)	6 (2%)	0	100	100
1	S	268/279 (96%)	260 (97%)	8 (3%)	0	100	100
1	T	264/279 (95%)	257 (97%)	7 (3%)	0	100	100
2	d	8/335 (2%)	6 (75%)	2 (25%)	0	100	100
2	g	4/335 (1%)	4 (100%)	0	0	100	100
2	h	7/335 (2%)	4 (57%)	2 (29%)	1 (14%)	0	1
2	i	10/335 (3%)	7 (70%)	2 (20%)	1 (10%)	0	2
2	p	6/335 (2%)	4 (67%)	0	2 (33%)	0	0
2	q	6/335 (2%)	3 (50%)	1 (17%)	2 (33%)	0	0
2	r	6/335 (2%)	5 (83%)	0	1 (17%)	0	0
2	s	8/335 (2%)	3 (38%)	3 (38%)	2 (25%)	0	0
2	t	6/335 (2%)	6 (100%)	0	0	100	100
All	All	5359/8595 (62%)	5185 (97%)	164 (3%)	10 (0%)	43	71

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	i	322	ALA
2	q	327	ILE
2	h	325	LEU
2	q	331	LYS
2	s	329	SER
2	p	326	SER
2	p	331	LYS
2	r	327	ILE
2	s	331	LYS
1	D	33	GLY

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	216/228 (95%)	216 (100%)	0	100	100
1	B	217/228 (95%)	217 (100%)	0	100	100
1	C	219/228 (96%)	219 (100%)	0	100	100
1	D	218/228 (96%)	216 (99%)	2 (1%)	70	77
1	E	220/228 (96%)	220 (100%)	0	100	100
1	F	217/228 (95%)	217 (100%)	0	100	100
1	G	217/228 (95%)	217 (100%)	0	100	100
1	H	218/228 (96%)	218 (100%)	0	100	100
1	I	218/228 (96%)	218 (100%)	0	100	100
1	J	217/228 (95%)	217 (100%)	0	100	100
1	K	218/228 (96%)	218 (100%)	0	100	100
1	L	218/228 (96%)	216 (99%)	2 (1%)	70	77
1	M	216/228 (95%)	216 (100%)	0	100	100
1	N	217/228 (95%)	217 (100%)	0	100	100
1	O	217/228 (95%)	217 (100%)	0	100	100
1	P	215/228 (94%)	215 (100%)	0	100	100
1	Q	215/228 (94%)	215 (100%)	0	100	100
1	R	217/228 (95%)	217 (100%)	0	100	100
1	S	221/228 (97%)	219 (99%)	2 (1%)	70	77
1	T	218/228 (96%)	218 (100%)	0	100	100
2	d	3/275 (1%)	3 (100%)	0	100	100
2	g	2/275 (1%)	2 (100%)	0	100	100
2	h	3/275 (1%)	3 (100%)	0	100	100
2	i	7/275 (2%)	7 (100%)	0	100	100
2	p	2/275 (1%)	2 (100%)	0	100	100
2	q	3/275 (1%)	3 (100%)	0	100	100
2	r	4/275 (2%)	4 (100%)	0	100	100
2	s	4/275 (2%)	4 (100%)	0	100	100
2	t	5/275 (2%)	5 (100%)	0	100	100
All	All	4382/7035 (62%)	4376 (100%)	6 (0%)	88	89

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	155[A]	GLN
1	D	155[B]	GLN
1	L	210[A]	ASP
1	L	210[B]	ASP
1	S	265[A]	HIS
1	S	265[B]	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	87	ASN
1	D	265	HIS
1	E	265	HIS
1	F	225	GLN
1	H	63	ASN
1	H	265	HIS
1	K	196	ASN
1	M	225	GLN
1	M	265	HIS
1	N	265	HIS
1	O	196	ASN
1	O	225	GLN
1	P	87	ASN
1	R	265	HIS
1	T	225	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 162 ligands modelled in this entry, 33 are monoatomic - leaving 129 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GOL	J	305	-	5,5,5	0.34	0	5,5,5	0.37	0
5	GOL	Q	305	-	5,5,5	0.34	0	5,5,5	0.36	0
5	GOL	S	301	-	5,5,5	0.36	0	5,5,5	0.41	0
3	1PE	Q	301	-	15,15,15	0.30	0	14,14,14	0.20	0
5	GOL	A	308	-	5,5,5	0.33	0	5,5,5	0.40	0
5	GOL	D	302	-	5,5,5	0.36	0	5,5,5	0.32	0
3	1PE	E	301	-	15,15,15	0.30	0	14,14,14	0.16	0
5	GOL	H	308	-	5,5,5	0.35	0	5,5,5	0.42	0
5	GOL	L	306	-	5,5,5	0.35	0	5,5,5	0.43	0
5	GOL	K	306	-	5,5,5	0.33	0	5,5,5	0.35	0
5	GOL	R	306	-	5,5,5	0.34	0	5,5,5	0.40	0
5	GOL	H	311	-	5,5,5	0.33	0	5,5,5	0.41	0
3	1PE	L	305[A]	-	15,15,15	0.30	0	14,14,14	0.19	0
3	1PE	N	303	-	12,12,15	0.29	0	11,11,14	0.18	0
5	GOL	O	307	-	5,5,5	0.33	0	5,5,5	0.36	0
3	1PE	A	301	-	12,12,15	0.29	0	11,11,14	0.21	0
5	GOL	K	304	-	5,5,5	0.34	0	5,5,5	0.40	0
3	1PE	K	301	-	9,9,15	0.28	0	8,8,14	0.20	0
5	GOL	H	310	-	5,5,5	0.34	0	5,5,5	0.34	0
3	1PE	O	301	-	9,9,15	0.28	0	8,8,14	0.19	0
5	GOL	B	306	-	5,5,5	0.34	0	5,5,5	0.37	0
5	GOL	R	307	-	5,5,5	0.34	0	5,5,5	0.39	0
5	GOL	A	306	-	5,5,5	0.33	0	5,5,5	0.37	0
5	GOL	I	305	-	5,5,5	0.36	0	5,5,5	0.30	0
5	GOL	B	307	-	5,5,5	0.32	0	5,5,5	0.41	0
5	GOL	L	301	-	5,5,5	0.33	0	5,5,5	0.50	0
3	1PE	H	301	-	15,15,15	0.30	0	14,14,14	0.19	0
5	GOL	J	306	-	5,5,5	0.35	0	5,5,5	0.47	0
3	1PE	B	305	-	15,15,15	0.30	0	14,14,14	0.19	0
5	GOL	N	305	-	5,5,5	0.34	0	5,5,5	0.39	0
5	GOL	E	303	-	5,5,5	0.34	0	5,5,5	0.36	0
3	1PE	N	301	-	9,9,15	0.29	0	8,8,14	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	1PE	H	302[A]	-	9,9,15	0.28	0	8,8,14	0.19	0
3	1PE	C	301	-	9,9,15	0.28	0	8,8,14	0.17	0
5	GOL	M	303	-	5,5,5	0.34	0	5,5,5	0.38	0
5	GOL	S	304	-	5,5,5	0.33	0	5,5,5	0.39	0
4	2PE	H	303	-	24,24,27	0.30	0	23,23,26	0.15	0
5	GOL	G	302	-	5,5,5	0.34	0	5,5,5	0.36	0
3	1PE	R	303	-	12,12,15	0.29	0	11,11,14	0.16	0
4	2PE	A	302	-	9,9,27	0.28	0	8,8,26	0.22	0
3	1PE	H	302[B]	-	9,9,15	0.28	0	8,8,14	0.20	0
3	1PE	P	301	-	12,12,15	0.29	0	11,11,14	0.18	0
3	1PE	L	303	-	15,15,15	0.30	0	14,14,14	0.19	0
5	GOL	F	306	-	5,5,5	0.34	0	5,5,5	0.46	0
3	1PE	A	303	-	6,6,15	0.27	0	5,5,14	0.23	0
5	GOL	I	307	-	5,5,5	0.33	0	5,5,5	0.40	0
5	GOL	K	305	-	5,5,5	0.35	0	5,5,5	0.49	0
5	GOL	B	302	-	5,5,5	0.34	0	5,5,5	0.39	0
5	GOL	D	301	-	5,5,5	0.34	0	5,5,5	0.35	0
3	1PE	H	305	-	9,9,15	0.30	0	8,8,14	0.35	0
5	GOL	D	305	-	5,5,5	0.33	0	5,5,5	0.37	0
5	GOL	C	305	-	5,5,5	0.33	0	5,5,5	0.41	0
3	1PE	R	301	-	9,9,15	0.29	0	8,8,14	0.19	0
3	1PE	G	301	-	9,9,15	0.28	0	8,8,14	0.26	0
5	GOL	L	307	-	5,5,5	0.34	0	5,5,5	0.39	0
5	GOL	L	308	-	5,5,5	0.33	0	5,5,5	0.44	0
3	1PE	L	305[B]	-	15,15,15	0.30	0	14,14,14	0.17	0
5	GOL	O	306	-	5,5,5	0.33	0	5,5,5	0.33	0
5	GOL	R	305	-	5,5,5	0.36	0	5,5,5	0.39	0
5	GOL	K	308	-	5,5,5	0.34	0	5,5,5	0.33	0
3	1PE	F	302	-	15,15,15	0.30	0	14,14,14	0.21	0
5	GOL	J	304	-	5,5,5	0.33	0	5,5,5	0.44	0
5	GOL	Q	304	-	5,5,5	0.34	0	5,5,5	0.44	0
3	1PE	E	302	-	9,9,15	0.28	0	8,8,14	0.30	0
5	GOL	B	308	-	5,5,5	0.34	0	5,5,5	0.40	0
5	GOL	F	307	-	5,5,5	0.34	0	5,5,5	0.37	0
4	2PE	L	302	-	24,24,27	0.31	0	23,23,26	0.35	0
3	1PE	I	303	-	9,9,15	0.28	0	8,8,14	0.26	0
5	GOL	N	304	-	5,5,5	0.34	0	5,5,5	0.39	0
3	1PE	C	302	-	15,15,15	0.30	0	14,14,14	0.17	0
5	GOL	K	303	-	5,5,5	0.34	0	5,5,5	0.37	0
5	GOL	A	305	-	5,5,5	0.34	0	5,5,5	0.37	0
5	GOL	O	304	-	5,5,5	0.34	0	5,5,5	0.39	0
3	1PE	I	301	-	15,15,15	0.29	0	14,14,14	0.16	0
3	1PE	J	301	-	9,9,15	0.28	0	8,8,14	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	1PE	P	302	-	12,12,15	0.29	0	11,11,14	0.20	0
5	GOL	B	301	-	5,5,5	0.35	0	5,5,5	0.30	0
5	GOL	M	302	-	5,5,5	0.35	0	5,5,5	0.36	0
5	GOL	D	303	-	5,5,5	0.34	0	5,5,5	0.31	0
5	GOL	S	306	-	5,5,5	0.33	0	5,5,5	0.35	0
3	1PE	N	302	-	9,9,15	0.29	0	8,8,14	0.19	0
3	1PE	L	304	-	12,12,15	0.29	0	11,11,14	0.19	0
3	1PE	B	303	-	9,9,15	0.29	0	8,8,14	0.26	0
5	GOL	H	307	-	5,5,5	0.35	0	5,5,5	0.39	0
5	GOL	M	301	-	5,5,5	0.39	0	5,5,5	0.34	0
5	GOL	T	306	-	5,5,5	0.33	0	5,5,5	0.38	0
5	GOL	T	305	-	5,5,5	0.33	0	5,5,5	0.39	0
5	GOL	T	307	-	5,5,5	0.34	0	5,5,5	0.38	0
4	2PE	H	304	-	21,21,27	0.30	0	20,20,26	0.17	0
3	1PE	F	303	-	12,12,15	0.30	0	11,11,14	0.20	0
5	GOL	Q	303	-	5,5,5	0.34	0	5,5,5	0.36	0
5	GOL	I	310	-	5,5,5	0.33	0	5,5,5	0.37	0
5	GOL	A	307	-	5,5,5	0.33	0	5,5,5	0.39	0
4	2PE	J	302	-	15,15,27	0.30	0	14,14,26	0.18	0
5	GOL	O	302	-	5,5,5	0.33	0	5,5,5	0.38	0
3	1PE	T	302	-	15,15,15	0.30	0	14,14,14	0.22	0
5	GOL	S	302	-	5,5,5	0.34	0	5,5,5	0.34	0
5	GOL	J	307	-	5,5,5	0.34	0	5,5,5	0.40	0
3	1PE	K	302	-	12,12,15	0.31	0	11,11,14	0.24	0
5	GOL	O	305	-	5,5,5	0.34	0	5,5,5	0.37	0
5	GOL	I	309	-	5,5,5	0.36	0	5,5,5	0.39	0
5	GOL	F	305	-	5,5,5	0.34	0	5,5,5	0.34	0
5	GOL	K	307	-	5,5,5	0.35	0	5,5,5	0.33	0
3	1PE	F	301	-	12,12,15	0.30	0	11,11,14	0.17	0
5	GOL	S	303	-	5,5,5	0.33	0	5,5,5	0.41	0
3	1PE	I	302	-	9,9,15	0.28	0	8,8,14	0.21	0
5	GOL	E	306	-	5,5,5	0.34	0	5,5,5	0.43	0
5	GOL	D	304	-	5,5,5	0.33	0	5,5,5	0.39	0
3	1PE	C	303[A]	-	15,15,15	0.30	0	14,14,14	0.18	0
3	1PE	C	303[B]	-	15,15,15	0.30	0	14,14,14	0.18	0
3	1PE	J	303	-	15,15,15	0.30	0	14,14,14	0.18	0
5	GOL	E	305	-	5,5,5	0.34	0	5,5,5	0.38	0
3	1PE	B	304	-	9,9,15	0.29	0	8,8,14	0.18	0
5	GOL	S	305	-	5,5,5	0.33	0	5,5,5	0.41	0
5	GOL	C	306	-	5,5,5	0.36	0	5,5,5	0.37	0
5	GOL	I	306	-	5,5,5	0.34	0	5,5,5	0.40	0
5	GOL	R	304	-	5,5,5	0.33	0	5,5,5	0.42	0
5	GOL	O	303	-	5,5,5	0.34	0	5,5,5	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	1PE	T	303	-	9,9,15	0.29	0	8,8,14	0.20	0
3	1PE	F	304[A]	-	15,15,15	0.29	0	14,14,14	0.25	0
5	GOL	A	304	-	5,5,5	0.35	0	5,5,5	0.33	0
7	12P	T	301	-	12,12,36	0.30	0	11,11,35	0.15	0
3	1PE	F	304[B]	-	15,15,15	0.29	0	14,14,14	0.23	0
5	GOL	H	309	-	5,5,5	0.34	0	5,5,5	0.41	0
5	GOL	I	308	-	5,5,5	0.34	0	5,5,5	0.40	0
5	GOL	E	304	-	5,5,5	0.32	0	5,5,5	0.41	0
3	1PE	R	302	-	6,6,15	0.27	0	5,5,14	0.21	0
3	1PE	Q	302	-	9,9,15	0.28	0	8,8,14	0.23	0
5	GOL	T	304	-	5,5,5	0.34	0	5,5,5	0.36	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	J	305	-	-	0/4/4/4	-
5	GOL	Q	305	-	-	0/4/4/4	-
5	GOL	S	301	-	-	2/4/4/4	-
3	1PE	Q	301	-	-	8/13/13/13	-
5	GOL	A	308	-	-	0/4/4/4	-
5	GOL	D	302	-	-	0/4/4/4	-
3	1PE	E	301	-	-	5/13/13/13	-
5	GOL	H	308	-	-	0/4/4/4	-
5	GOL	L	306	-	-	0/4/4/4	-
5	GOL	K	306	-	-	0/4/4/4	-
5	GOL	R	306	-	-	0/4/4/4	-
5	GOL	H	311	-	-	0/4/4/4	-
3	1PE	L	305[A]	-	-	4/13/13/13	-
3	1PE	N	303	-	-	6/10/10/13	-
5	GOL	O	307	-	-	0/4/4/4	-
3	1PE	A	301	-	-	5/10/10/13	-
5	GOL	K	304	-	-	0/4/4/4	-
3	1PE	K	301	-	-	4/7/7/13	-
5	GOL	H	310	-	-	0/4/4/4	-
3	1PE	O	301	-	-	1/7/7/13	-
5	GOL	B	306	-	-	0/4/4/4	-
5	GOL	R	307	-	-	0/4/4/4	-
5	GOL	A	306	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	I	305	-	-	2/4/4/4	-
5	GOL	B	307	-	-	0/4/4/4	-
5	GOL	L	301	-	-	0/4/4/4	-
3	1PE	H	301	-	-	4/13/13/13	-
5	GOL	J	306	-	-	0/4/4/4	-
3	1PE	B	305	-	-	6/13/13/13	-
5	GOL	N	305	-	-	0/4/4/4	-
5	GOL	E	303	-	-	0/4/4/4	-
3	1PE	N	301	-	-	3/7/7/13	-
3	1PE	H	302[A]	-	-	4/7/7/13	-
3	1PE	C	301	-	-	2/7/7/13	-
5	GOL	M	303	-	-	0/4/4/4	-
5	GOL	S	304	-	-	0/4/4/4	-
4	2PE	H	303	-	-	11/22/22/25	-
5	GOL	G	302	-	-	0/4/4/4	-
3	1PE	R	303	-	-	0/10/10/13	-
4	2PE	A	302	-	-	1/7/7/25	-
3	1PE	H	302[B]	-	-	3/7/7/13	-
3	1PE	P	301	-	-	5/10/10/13	-
3	1PE	L	303	-	-	5/13/13/13	-
5	GOL	F	306	-	-	0/4/4/4	-
3	1PE	A	303	-	-	0/4/4/13	-
5	GOL	I	307	-	-	0/4/4/4	-
5	GOL	K	305	-	-	0/4/4/4	-
5	GOL	B	302	-	-	0/4/4/4	-
5	GOL	D	301	-	-	0/4/4/4	-
3	1PE	H	305	-	-	5/7/7/13	-
5	GOL	D	305	-	-	0/4/4/4	-
5	GOL	C	305	-	-	1/4/4/4	-
3	1PE	R	301	-	-	4/7/7/13	-
3	1PE	G	301	-	-	1/7/7/13	-
5	GOL	L	307	-	-	0/4/4/4	-
5	GOL	L	308	-	-	0/4/4/4	-
3	1PE	L	305[B]	-	-	4/13/13/13	-
5	GOL	O	306	-	-	0/4/4/4	-
5	GOL	R	305	-	-	0/4/4/4	-
5	GOL	K	308	-	-	0/4/4/4	-
3	1PE	F	302	-	-	3/13/13/13	-
5	GOL	J	304	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	Q	304	-	-	0/4/4/4	-
3	1PE	E	302	-	-	1/7/7/13	-
5	GOL	B	308	-	-	0/4/4/4	-
5	GOL	F	307	-	-	0/4/4/4	-
4	2PE	L	302	-	-	12/22/22/25	-
3	1PE	I	303	-	-	2/7/7/13	-
5	GOL	N	304	-	-	0/4/4/4	-
3	1PE	C	302	-	-	4/13/13/13	-
5	GOL	K	303	-	-	0/4/4/4	-
5	GOL	A	305	-	-	0/4/4/4	-
5	GOL	O	304	-	-	0/4/4/4	-
3	1PE	I	301	-	-	5/13/13/13	-
3	1PE	J	301	-	-	3/7/7/13	-
3	1PE	P	302	-	-	3/10/10/13	-
5	GOL	B	301	-	-	0/4/4/4	-
5	GOL	M	302	-	-	0/4/4/4	-
5	GOL	D	303	-	-	2/4/4/4	-
5	GOL	S	306	-	-	2/4/4/4	-
3	1PE	N	302	-	-	2/7/7/13	-
3	1PE	L	304	-	-	3/10/10/13	-
3	1PE	B	303	-	-	3/7/7/13	-
5	GOL	H	307	-	-	0/4/4/4	-
5	GOL	M	301	-	-	0/4/4/4	-
5	GOL	T	306	-	-	0/4/4/4	-
5	GOL	T	305	-	-	2/4/4/4	-
5	GOL	T	307	-	-	0/4/4/4	-
4	2PE	H	304	-	-	4/19/19/25	-
3	1PE	F	303	-	-	2/10/10/13	-
5	GOL	Q	303	-	-	2/4/4/4	-
5	GOL	I	310	-	-	0/4/4/4	-
5	GOL	A	307	-	-	0/4/4/4	-
4	2PE	J	302	-	-	4/13/13/25	-
5	GOL	O	302	-	-	0/4/4/4	-
3	1PE	T	302	-	-	10/13/13/13	-
5	GOL	S	302	-	-	0/4/4/4	-
5	GOL	J	307	-	-	0/4/4/4	-
3	1PE	K	302	-	-	8/10/10/13	-
5	GOL	O	305	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	I	309	-	-	0/4/4/4	-
5	GOL	F	305	-	-	2/4/4/4	-
5	GOL	K	307	-	-	1/4/4/4	-
3	1PE	F	301	-	-	2/10/10/13	-
5	GOL	S	303	-	-	2/4/4/4	-
3	1PE	I	302	-	-	3/7/7/13	-
5	GOL	E	306	-	-	0/4/4/4	-
5	GOL	D	304	-	-	0/4/4/4	-
3	1PE	C	303[A]	-	-	6/13/13/13	-
3	1PE	C	303[B]	-	-	6/13/13/13	-
3	1PE	J	303	-	-	6/13/13/13	-
5	GOL	E	305	-	-	0/4/4/4	-
3	1PE	B	304	-	-	1/7/7/13	-
5	GOL	S	305	-	-	0/4/4/4	-
5	GOL	C	306	-	-	0/4/4/4	-
5	GOL	I	306	-	-	0/4/4/4	-
5	GOL	R	304	-	-	0/4/4/4	-
5	GOL	O	303	-	-	0/4/4/4	-
3	1PE	T	303	-	-	1/7/7/13	-
3	1PE	F	304[A]	-	-	6/13/13/13	-
5	GOL	A	304	-	-	2/4/4/4	-
7	12P	T	301	-	-	3/10/10/34	-
3	1PE	F	304[B]	-	-	5/13/13/13	-
5	GOL	H	309	-	-	0/4/4/4	-
5	GOL	I	308	-	-	0/4/4/4	-
5	GOL	E	304	-	-	0/4/4/4	-
3	1PE	R	302	-	-	1/4/4/13	-
3	1PE	Q	302	-	-	5/7/7/13	-
5	GOL	T	304	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (229) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	305	GOL	C1-C2-C3-O3
5	Q	303	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	S	301	GOL	C1-C2-C3-O3
3	K	302	1PE	OH4-C13-C23-OH3
3	L	303	1PE	OH5-C14-C24-OH4
3	L	303	1PE	OH6-C15-C25-OH5
3	C	302	1PE	OH6-C15-C25-OH5
3	F	302	1PE	OH4-C13-C23-OH3
3	C	303[A]	1PE	OH4-C13-C23-OH3
3	C	302	1PE	OH4-C13-C23-OH3
3	E	302	1PE	OH7-C16-C26-OH6
3	F	301	1PE	OH6-C15-C25-OH5
3	R	301	1PE	OH5-C14-C24-OH4
3	A	301	1PE	OH5-C14-C24-OH4
3	B	305	1PE	OH5-C14-C24-OH4
3	I	303	1PE	OH6-C15-C25-OH5
3	B	303	1PE	C15-C25-OH5-C14
3	C	303[A]	1PE	OH5-C14-C24-OH4
3	B	305	1PE	OH4-C13-C23-OH3
3	J	303	1PE	OH4-C13-C23-OH3
3	E	301	1PE	OH5-C14-C24-OH4
3	J	303	1PE	OH5-C14-C24-OH4
3	L	305[B]	1PE	OH6-C15-C25-OH5
5	Q	303	GOL	O1-C1-C2-O2
5	T	304	GOL	O2-C2-C3-O3
3	F	304[B]	1PE	OH5-C14-C24-OH4
3	B	305	1PE	C15-C25-OH5-C14
3	K	302	1PE	OH6-C15-C25-OH5
3	R	301	1PE	OH7-C16-C26-OH6
4	L	302	2PE	O7-C8-C9-O10
3	T	302	1PE	OH6-C15-C25-OH5
3	H	305	1PE	OH4-C13-C23-OH3
3	N	303	1PE	OH5-C14-C24-OH4
3	I	302	1PE	C23-C13-OH4-C24
3	E	301	1PE	OH6-C15-C25-OH5
3	I	302	1PE	OH4-C13-C23-OH3
3	P	302	1PE	OH4-C13-C23-OH3
4	H	303	2PE	O4-C5-C6-O7
3	T	302	1PE	C14-C24-OH4-C13
3	A	301	1PE	OH4-C13-C23-OH3
3	B	303	1PE	OH5-C14-C24-OH4
3	B	305	1PE	OH7-C16-C26-OH6
3	H	301	1PE	OH7-C16-C26-OH6
3	I	303	1PE	OH5-C14-C24-OH4

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Mol	Chain	Res	Type	Atoms
3	J	301	1PE	OH5-C14-C24-OH4
3	J	303	1PE	OH7-C16-C26-OH6
3	L	305[A]	1PE	OH7-C16-C26-OH6
3	P	301	1PE	OH4-C13-C23-OH3
3	I	301	1PE	OH6-C15-C25-OH5
3	L	304	1PE	OH5-C14-C24-OH4
3	T	302	1PE	OH4-C13-C23-OH3
3	F	304[A]	1PE	OH5-C14-C24-OH4
3	P	302	1PE	OH5-C14-C24-OH4
4	L	302	2PE	O16-C17-C18-O19
3	B	305	1PE	C25-C15-OH6-C26
3	P	301	1PE	OH5-C14-C24-OH4
3	F	301	1PE	OH4-C13-C23-OH3
5	A	304	GOL	C1-C2-C3-O3
5	D	303	GOL	C1-C2-C3-O3
5	F	305	GOL	C1-C2-C3-O3
5	O	305	GOL	C1-C2-C3-O3
5	S	303	GOL	C1-C2-C3-O3
5	S	306	GOL	C1-C2-C3-O3
5	T	304	GOL	C1-C2-C3-O3
5	T	305	GOL	C1-C2-C3-O3
3	C	301	1PE	OH5-C14-C24-OH4
3	E	301	1PE	OH7-C16-C26-OH6
3	G	301	1PE	OH5-C14-C24-OH4
3	H	302[A]	1PE	OH7-C16-C26-OH6
3	H	305	1PE	OH5-C14-C24-OH4
3	I	302	1PE	OH5-C14-C24-OH4
3	Q	301	1PE	OH7-C16-C26-OH6
3	T	302	1PE	OH7-C16-C26-OH6
4	H	303	2PE	O19-C20-C21-O22
3	C	301	1PE	OH4-C13-C23-OH3
3	L	303	1PE	OH4-C13-C23-OH3
3	F	303	1PE	OH6-C15-C25-OH5
3	H	302[A]	1PE	OH5-C14-C24-OH4
3	K	301	1PE	OH7-C16-C26-OH6
3	L	303	1PE	OH7-C16-C26-OH6
3	J	303	1PE	OH6-C15-C25-OH5
3	C	303[B]	1PE	OH4-C13-C23-OH3
3	A	301	1PE	OH6-C15-C25-OH5
3	C	303[B]	1PE	OH5-C14-C24-OH4
3	Q	302	1PE	OH4-C13-C23-OH3
3	L	305[B]	1PE	C16-C26-OH6-C15

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Mol	Chain	Res	Type	Atoms
3	B	303	1PE	OH7-C16-C26-OH6
3	K	301	1PE	OH5-C14-C24-OH4
3	N	303	1PE	OH6-C15-C25-OH5
3	Q	302	1PE	OH2-C12-C22-OH3
5	F	305	GOL	O2-C2-C3-O3
5	I	305	GOL	O2-C2-C3-O3
5	S	301	GOL	O2-C2-C3-O3
3	N	301	1PE	OH4-C13-C23-OH3
3	L	304	1PE	C23-C13-OH4-C24
3	N	303	1PE	OH4-C13-C23-OH3
4	L	302	2PE	O4-C5-C6-O7
5	D	303	GOL	O2-C2-C3-O3
3	C	303[A]	1PE	C23-C13-OH4-C24
3	I	301	1PE	OH4-C13-C23-OH3
3	C	302	1PE	OH5-C14-C24-OH4
3	R	301	1PE	OH6-C15-C25-OH5
3	A	301	1PE	C15-C25-OH5-C14
3	N	301	1PE	OH2-C12-C22-OH3
3	A	301	1PE	C23-C13-OH4-C24
3	H	305	1PE	C12-C22-OH3-C23
3	K	302	1PE	C14-C24-OH4-C13
3	Q	301	1PE	C13-C23-OH3-C22
3	C	303[A]	1PE	C16-C26-OH6-C15
5	C	305	GOL	O1-C1-C2-C3
3	N	303	1PE	C24-C14-OH5-C25
3	K	302	1PE	C15-C25-OH5-C14
3	E	301	1PE	C15-C25-OH5-C14
3	B	305	1PE	C12-C22-OH3-C23
4	J	302	2PE	C6-C5-O4-C3
4	L	302	2PE	C9-C8-O7-C6
3	N	302	1PE	OH7-C16-C26-OH6
3	P	302	1PE	OH6-C15-C25-OH5
3	Q	301	1PE	OH6-C15-C25-OH5
4	L	302	2PE	O19-C20-C21-O22
5	T	305	GOL	O2-C2-C3-O3
3	P	301	1PE	C23-C13-OH4-C24
3	F	302	1PE	OH7-C16-C26-OH6
3	H	301	1PE	OH2-C12-C22-OH3
4	H	303	2PE	C11-C12-O13-C14
3	E	301	1PE	C23-C13-OH4-C24
3	I	301	1PE	C25-C15-OH6-C26
3	C	303[B]	1PE	C24-C14-OH5-C25

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Mol	Chain	Res	Type	Atoms
3	F	303	1PE	OH5-C14-C24-OH4
7	T	301	12P	C24-C23-O22-C21
3	T	303	1PE	OH4-C13-C23-OH3
4	H	303	2PE	C20-C21-O22-C23
3	C	303[B]	1PE	OH7-C16-C26-OH6
3	H	305	1PE	OH2-C12-C22-OH3
4	H	303	2PE	O7-C8-C9-O10
3	I	301	1PE	C15-C25-OH5-C14
3	Q	301	1PE	C14-C24-OH4-C13
5	A	304	GOL	O2-C2-C3-O3
5	O	305	GOL	O2-C2-C3-O3
5	K	307	GOL	C1-C2-C3-O3
3	K	302	1PE	C23-C13-OH4-C24
3	F	304[B]	1PE	C12-C22-OH3-C23
3	F	304[B]	1PE	C15-C25-OH5-C14
3	L	305[A]	1PE	C24-C14-OH5-C25
3	L	304	1PE	C12-C22-OH3-C23
3	H	302[B]	1PE	OH6-C15-C25-OH5
3	L	305[B]	1PE	C23-C13-OH4-C24
3	Q	302	1PE	OH5-C14-C24-OH4
3	Q	301	1PE	C24-C14-OH5-C25
4	H	303	2PE	C9-C8-O7-C6
3	C	303[A]	1PE	OH7-C16-C26-OH6
3	H	302[B]	1PE	OH7-C16-C26-OH6
3	C	303[B]	1PE	C23-C13-OH4-C24
3	F	302	1PE	C12-C22-OH3-C23
3	T	302	1PE	C13-C23-OH3-C22
3	Q	301	1PE	OH5-C14-C24-OH4
3	T	302	1PE	OH5-C14-C24-OH4
3	H	301	1PE	C16-C26-OH6-C15
3	Q	301	1PE	OH4-C13-C23-OH3
3	H	301	1PE	OH4-C13-C23-OH3
3	P	301	1PE	C15-C25-OH5-C14
3	F	304[A]	1PE	C15-C25-OH5-C14
3	N	302	1PE	C25-C15-OH6-C26
3	P	301	1PE	OH6-C15-C25-OH5
3	F	304[B]	1PE	OH4-C13-C23-OH3
3	L	303	1PE	C13-C23-OH3-C22
3	J	301	1PE	C25-C15-OH6-C26
3	F	304[A]	1PE	C12-C22-OH3-C23
3	O	301	1PE	C15-C25-OH5-C14
3	C	303[B]	1PE	C25-C15-OH6-C26

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Mol	Chain	Res	Type	Atoms
3	H	305	1PE	C14-C24-OH4-C13
4	H	303	2PE	C8-C9-O10-C11
4	J	302	2PE	C9-C8-O7-C6
3	N	303	1PE	C15-C25-OH5-C14
4	L	302	2PE	C8-C9-O10-C11
3	J	303	1PE	C16-C26-OH6-C15
3	F	304[A]	1PE	OH4-C13-C23-OH3
4	H	303	2PE	O16-C17-C18-O19
7	T	301	12P	C30-C29-O28-C27
4	J	302	2PE	C11-C12-O13-C14
4	A	302	2PE	C2-C3-O4-C5
4	J	302	2PE	O4-C5-C6-O7
5	S	303	GOL	O2-C2-C3-O3
5	S	306	GOL	O2-C2-C3-O3
4	H	303	2PE	C15-C14-O13-C12
3	L	305[B]	1PE	OH7-C16-C26-OH6
3	H	302[A]	1PE	C16-C26-OH6-C15
3	Q	302	1PE	C12-C22-OH3-C23
3	Q	301	1PE	C15-C25-OH5-C14
3	H	302[A]	1PE	C24-C14-OH5-C25
3	T	302	1PE	C23-C13-OH4-C24
3	C	302	1PE	C13-C23-OH3-C22
3	B	304	1PE	C23-C13-OH4-C24
3	J	303	1PE	C23-C13-OH4-C24
3	H	302[B]	1PE	C24-C14-OH5-C25
4	L	302	2PE	C14-C15-O16-C17
3	N	301	1PE	C13-C23-OH3-C22
3	K	302	1PE	OH5-C14-C24-OH4
4	L	302	2PE	C18-C17-O16-C15
3	F	304[A]	1PE	OH6-C15-C25-OH5
3	F	304[B]	1PE	OH6-C15-C25-OH5
3	C	303[A]	1PE	C14-C24-OH4-C13
3	R	302	1PE	C12-C22-OH3-C23
3	N	303	1PE	OH2-C12-C22-OH3
3	Q	302	1PE	C23-C13-OH4-C24
3	R	301	1PE	C25-C15-OH6-C26
3	L	305[A]	1PE	C12-C22-OH3-C23
3	I	301	1PE	OH2-C12-C22-OH3
3	T	302	1PE	C24-C14-OH5-C25
3	K	301	1PE	C24-C14-OH5-C25
4	H	304	2PE	O16-C17-C18-O19
3	T	302	1PE	C12-C22-OH3-C23

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Mol	Chain	Res	Type	Atoms
3	K	301	1PE	C16-C26-OH6-C15
3	L	305[A]	1PE	C23-C13-OH4-C24
4	L	302	2PE	C5-C6-O7-C8
3	K	302	1PE	C13-C23-OH3-C22
3	F	304[A]	1PE	C14-C24-OH4-C13
4	H	304	2PE	O7-C8-C9-O10
4	L	302	2PE	O13-C14-C15-O16
7	T	301	12P	O25-C26-C27-O28
4	L	302	2PE	C17-C18-O19-C20
4	L	302	2PE	O10-C11-C12-O13
3	T	302	1PE	C16-C26-OH6-C15
4	H	303	2PE	C17-C18-O19-C20
4	H	304	2PE	C14-C15-O16-C17
4	H	303	2PE	C18-C17-O16-C15
4	H	304	2PE	O4-C5-C6-O7
3	J	301	1PE	OH6-C15-C25-OH5
3	K	302	1PE	C12-C22-OH3-C23

There are no ring outliers.

58 monomers are involved in 89 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	305	GOL	1	0
5	S	301	GOL	2	0
3	Q	301	1PE	2	0
5	D	302	GOL	1	0
5	L	306	GOL	2	0
5	K	306	GOL	1	0
5	H	311	GOL	1	0
3	L	305[A]	1PE	4	0
3	N	303	1PE	1	0
3	A	301	1PE	2	0
3	O	301	1PE	1	0
5	B	306	GOL	1	0
5	A	306	GOL	2	0
5	L	301	GOL	1	0
3	H	301	1PE	2	0
3	B	305	1PE	3	0
3	C	301	1PE	1	0
4	H	303	2PE	1	0
3	R	303	1PE	2	0
4	A	302	2PE	1	0

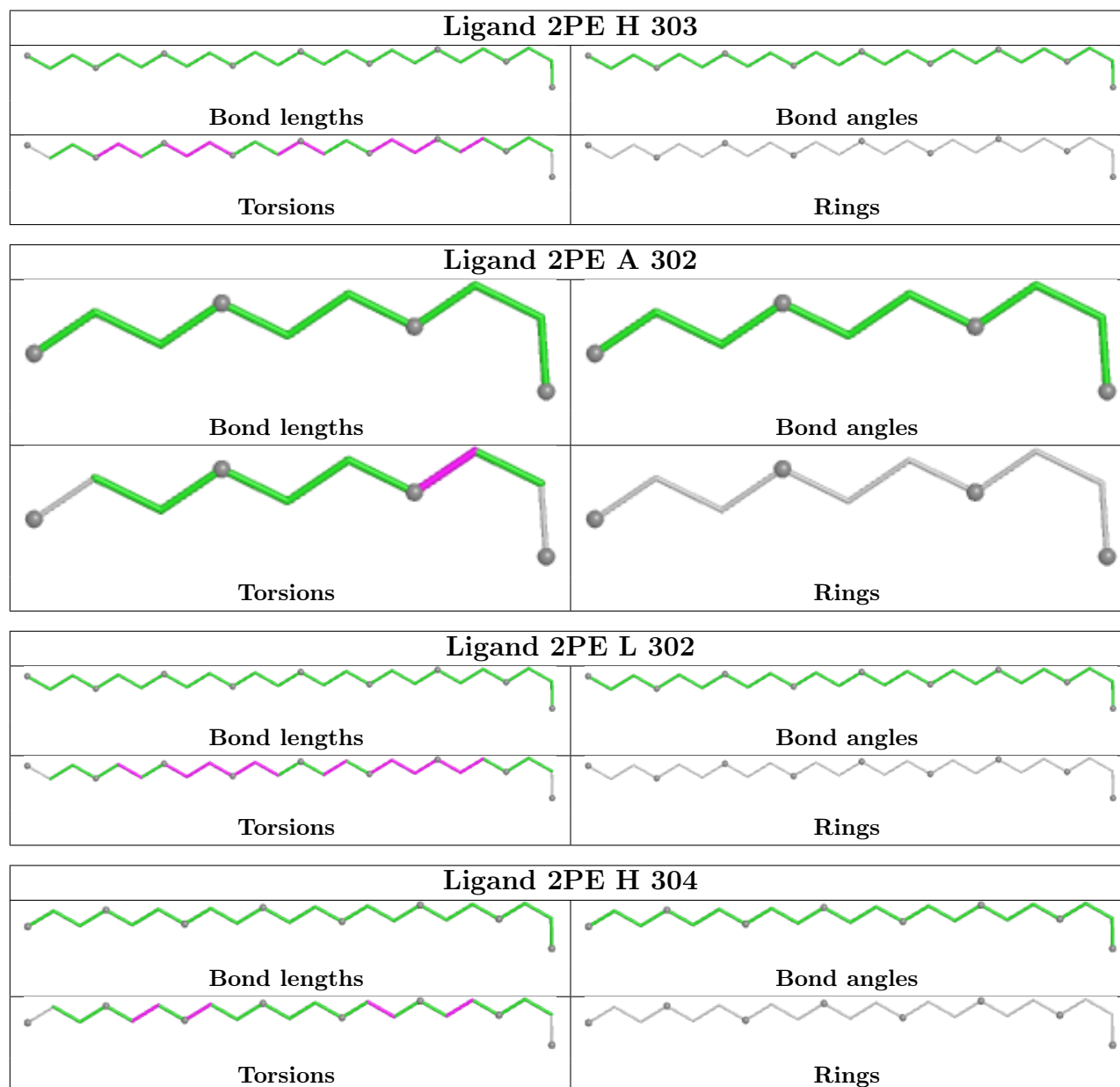
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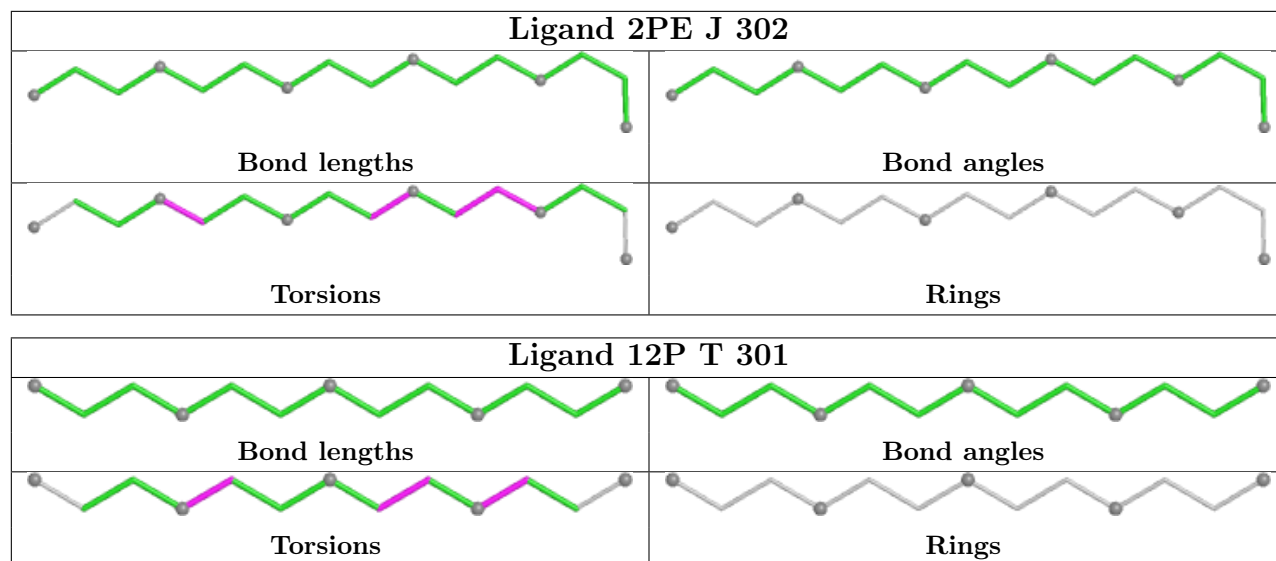
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	302[B]	1PE	1	0
3	P	301	1PE	1	0
5	F	306	GOL	1	0
3	A	303	1PE	3	0
5	I	307	GOL	1	0
5	K	305	GOL	1	0
3	H	305	1PE	2	0
5	C	305	GOL	1	0
3	L	305[B]	1PE	2	0
5	K	308	GOL	2	0
3	F	302	1PE	1	0
5	B	308	GOL	1	0
4	L	302	2PE	7	0
3	C	302	1PE	1	0
5	K	303	GOL	1	0
5	A	305	GOL	1	0
3	I	301	1PE	1	0
3	L	304	1PE	2	0
3	B	303	1PE	2	0
5	T	305	GOL	1	0
3	F	303	1PE	1	0
4	J	302	2PE	1	0
3	T	302	1PE	2	0
5	O	305	GOL	1	0
5	I	309	GOL	1	0
5	S	303	GOL	1	0
3	I	302	1PE	2	0
5	E	306	GOL	1	0
5	D	304	GOL	1	0
3	B	304	1PE	1	0
5	I	306	GOL	1	0
3	F	304[A]	1PE	2	0
5	A	304	GOL	2	0
7	T	301	12P	1	0
3	F	304[B]	1PE	2	0
5	H	309	GOL	1	0
5	E	304	GOL	1	0
5	T	304	GOL	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	267/279 (95%)	-0.27	1 (0%) 88 78	22, 38, 53, 64	1 (0%)
1	B	265/279 (94%)	-0.25	1 (0%) 88 78	26, 41, 55, 70	0
1	C	268/279 (96%)	-0.19	4 (1%) 72 52	26, 40, 57, 95	1 (0%)
1	D	266/279 (95%)	-0.17	3 (1%) 78 60	27, 43, 56, 69	1 (0%)
1	E	272/279 (97%)	-0.25	1 (0%) 88 78	22, 38, 56, 63	0
1	F	266/279 (95%)	-0.28	1 (0%) 88 78	24, 38, 53, 63	0
1	G	266/279 (95%)	-0.16	1 (0%) 88 78	27, 44, 57, 74	0
1	H	267/279 (95%)	-0.41	1 (0%) 88 78	21, 33, 49, 65	0
1	I	267/279 (95%)	-0.39	1 (0%) 88 78	24, 33, 50, 74	0
1	J	267/279 (95%)	-0.34	3 (1%) 78 60	22, 35, 50, 75	0
1	K	266/279 (95%)	-0.37	0 100 100	23, 36, 51, 68	0
1	L	265/279 (94%)	-0.40	0 100 100	21, 35, 51, 63	2 (0%)
1	M	266/279 (95%)	-0.01	1 (0%) 88 78	36, 50, 65, 75	0
1	N	266/279 (95%)	0.04	1 (0%) 88 78	34, 49, 61, 79	0
1	O	266/279 (95%)	-0.10	1 (0%) 88 78	30, 44, 59, 74	0
1	P	266/279 (95%)	-0.19	1 (0%) 88 78	30, 43, 58, 64	0
1	Q	265/279 (94%)	-0.09	1 (0%) 88 78	32, 46, 61, 84	0
1	R	266/279 (95%)	-0.34	1 (0%) 88 78	23, 36, 53, 68	0
1	S	267/279 (95%)	-0.30	3 (1%) 78 60	22, 37, 52, 78	3 (1%)
1	T	266/279 (95%)	-0.22	2 (0%) 82 66	28, 39, 54, 75	0
2	d	10/335 (2%)	4.93	10 (100%) 0 0	48, 57, 73, 74	10 (100%)
2	g	6/335 (1%)	4.50	5 (83%) 0 0	49, 50, 52, 65	6 (100%)
2	h	9/335 (2%)	3.64	8 (88%) 0 0	40, 47, 53, 55	9 (100%)
2	i	12/335 (3%)	4.30	11 (91%) 0 0	47, 52, 60, 61	12 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	p	8/335 (2%)	4.22	8 (100%) 0 0	43, 57, 60, 60	8 (100%)
2	q	8/335 (2%)	3.33	6 (75%) 0 0	44, 56, 59, 60	8 (100%)
2	r	8/335 (2%)	4.03	8 (100%) 0 0	48, 50, 57, 70	8 (100%)
2	s	10/335 (2%)	3.95	8 (80%) 0 0	39, 52, 58, 64	10 (100%)
2	t	8/335 (2%)	3.94	8 (100%) 0 0	49, 58, 60, 67	8 (100%)
All	All	5409/8595 (62%)	-0.17	100 (1%) 67 47	21, 40, 58, 95	87 (1%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	g	326	SER	9.1
2	d	325	LEU	9.1
2	r	326	SER	8.8
2	d	326	SER	8.4
2	p	326	SER	8.4
2	i	322	ALA	8.0
1	C	265[A]	HIS	7.4
2	s	326	SER	7.0
2	i	321	ALA	6.5
2	q	329	SER	6.1
2	h	324	SER	5.8
2	s	329	SER	5.6
2	r	329	SER	5.5
2	h	327	ILE	5.4
2	s	328	GLY	5.4
2	s	324	SER	5.3
2	i	326	SER	5.2
2	i	319	THR	5.2
2	t	331	LYS	5.2
2	h	329	SER	5.2
2	p	331	LYS	5.1
2	t	326	SER	5.0
2	i	324	SER	4.9
2	d	332	GLY	4.9
2	d	331	LYS	4.9
2	g	325	LEU	4.7
2	d	330	LEU	4.6
2	q	326	SER	4.6
2	d	328	GLY	4.3
1	N	266	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
2	g	329	SER	4.3
1	C	266	LYS	4.1
2	q	325	LEU	4.1
2	p	325	LEU	4.1
2	t	328	GLY	4.0
2	d	324	SER	3.9
2	s	331	LYS	3.9
2	t	329	SER	3.9
2	r	323	GLY	3.8
2	p	329	SER	3.8
2	s	327	ILE	3.8
2	i	323	GLY	3.7
2	t	330	LEU	3.7
2	h	326	SER	3.7
2	q	328	GLY	3.7
2	d	327	ILE	3.6
2	i	328	GLY	3.5
2	g	327	ILE	3.5
2	g	330	LEU	3.5
2	d	329	SER	3.4
2	i	325	LEU	3.4
2	t	324	SER	3.3
2	p	327	ILE	3.3
2	i	320	LEU	3.3
2	t	327	ILE	3.3
2	p	332	GLY	3.3
2	r	328	GLY	3.3
2	i	327	ILE	3.2
2	p	328	GLY	3.2
2	s	323	GLY	3.2
1	D	32	ALA	3.2
2	t	325	LEU	3.1
2	h	330	LEU	3.1
2	s	325	LEU	3.1
2	i	330	LEU	3.0
1	C	268	ALA	3.0
1	T	266	LYS	3.0
1	D	266	LYS	2.9
2	h	328	GLY	2.8
2	r	327	ILE	2.8
2	r	330	LEU	2.8
1	Q	265	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
2	p	330	LEU	2.6
2	r	324	SER	2.6
1	R	266	LYS	2.6
1	S	265[A]	HIS	2.6
2	q	332	GLY	2.6
1	A	267	LEU	2.6
1	J	267	LEU	2.6
2	r	325	LEU	2.6
1	I	267	LEU	2.5
2	h	331	LYS	2.5
1	P	167	GLY	2.5
1	J	32	ALA	2.5
1	B	32	ALA	2.4
1	S	267	LEU	2.4
1	M	266	LYS	2.4
2	h	325	LEU	2.4
1	C	267	LEU	2.4
1	F	266	LYS	2.3
1	J	176	ASP	2.3
1	H	266	LYS	2.2
1	E	269	ALA	2.2
2	q	331	LYS	2.2
2	d	323	GLY	2.1
1	D	124	SER	2.1
1	T	135	SER	2.1
1	G	13	GLU	2.1
1	S	117[A]	ARG	2.0
1	O	266	LYS	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
6	NI	C	309	1/1	0.62	0.28	191,191,191,191	0
5	GOL	M	303	6/6	0.66	0.21	61,65,68,73	0
5	GOL	A	308	6/6	0.68	0.20	60,71,77,85	0
5	GOL	M	301	6/6	0.71	0.27	32,68,75,78	0
5	GOL	G	302	6/6	0.72	0.19	51,52,55,64	0
3	1PE	P	302	13/16	0.72	0.30	63,77,87,88	0
5	GOL	F	306	6/6	0.73	0.22	63,67,74,78	0
3	1PE	E	302	10/16	0.73	0.27	54,68,72,84	0
5	GOL	H	307	6/6	0.73	0.21	37,52,57,60	0
4	2PE	H	304	22/28	0.74	0.26	58,73,76,79	22
5	GOL	S	304	6/6	0.74	0.16	55,71,77,78	0
5	GOL	S	306	6/6	0.74	0.22	46,62,77,78	0
5	GOL	B	302	6/6	0.74	0.20	47,58,71,76	0
3	1PE	P	301	13/16	0.76	0.24	38,62,80,81	0
5	GOL	D	305	6/6	0.76	0.23	43,58,70,72	0
5	GOL	Q	303	6/6	0.76	0.19	41,65,69,87	0
5	GOL	A	305	6/6	0.76	0.22	43,56,65,66	0
5	GOL	A	307	6/6	0.76	0.19	43,52,57,70	0
3	1PE	F	301	13/16	0.76	0.25	60,68,78,93	0
3	1PE	O	301	10/16	0.77	0.25	54,65,76,78	0
5	GOL	L	306	6/6	0.77	0.19	39,50,57,61	0
5	GOL	O	302	6/6	0.77	0.22	46,66,73,79	0
5	GOL	O	305	6/6	0.77	0.17	52,63,65,69	0
3	1PE	B	305	16/16	0.78	0.26	62,73,79,90	0
5	GOL	D	303	6/6	0.79	0.22	33,54,69,75	0
3	1PE	Q	301	16/16	0.79	0.24	47,77,86,87	0
3	1PE	F	304[B]	16/16	0.80	0.30	33,62,72,73	16
5	GOL	N	304	6/6	0.80	0.18	63,66,72,77	0
3	1PE	N	301	10/16	0.80	0.22	59,70,85,86	0
3	1PE	F	304[A]	16/16	0.80	0.30	38,62,73,73	16
5	GOL	O	303	6/6	0.81	0.20	39,67,74,77	0
3	1PE	B	304	10/16	0.81	0.22	45,56,74,77	0
3	1PE	C	302	16/16	0.81	0.22	62,74,86,86	0
3	1PE	J	303	16/16	0.81	0.24	41,67,84,92	0
3	1PE	F	302	16/16	0.81	0.22	46,58,78,87	0
3	1PE	R	301	10/16	0.81	0.21	47,62,69,72	0
3	1PE	H	301	16/16	0.82	0.21	52,63,76,78	0
3	1PE	L	305[A]	16/16	0.82	0.46	55,73,85,87	16
4	2PE	L	302	25/28	0.82	0.21	36,46,57,60	25
5	GOL	Q	304	6/6	0.82	0.13	57,61,65,68	0
5	GOL	S	303	6/6	0.82	0.23	47,56,61,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	1PE	L	305[B]	16/16	0.82	0.46	48,72,84,93	16
5	GOL	A	306	6/6	0.82	0.17	37,46,52,58	6
3	1PE	I	301	16/16	0.82	0.19	26,50,66,67	0
5	GOL	E	303	6/6	0.83	0.20	44,60,65,73	0
5	GOL	E	305	6/6	0.83	0.15	52,59,68,82	0
4	2PE	H	303	25/28	0.83	0.27	44,51,62,65	25
3	1PE	J	301	10/16	0.83	0.24	51,60,70,77	0
5	GOL	O	307	6/6	0.83	0.19	53,63,66,73	0
5	GOL	B	301	6/6	0.83	0.19	26,51,57,58	0
5	GOL	I	308	6/6	0.83	0.19	38,46,54,54	6
5	GOL	R	306	6/6	0.83	0.20	45,52,64,82	6
5	GOL	K	304	6/6	0.83	0.18	52,64,69,70	0
3	1PE	E	301	16/16	0.83	0.20	44,60,79,80	0
5	GOL	S	305	6/6	0.83	0.20	41,61,63,69	0
3	1PE	R	302	7/16	0.83	0.24	29,34,49,55	7
5	GOL	T	305	6/6	0.83	0.22	44,52,56,68	0
3	1PE	R	303	13/16	0.83	0.20	57,65,80,82	0
6	NI	O	308	1/1	0.83	0.18	120,120,120,120	0
3	1PE	I	303	10/16	0.84	0.21	54,65,74,74	0
3	1PE	N	302	10/16	0.84	0.20	61,74,78,78	0
3	1PE	T	302	16/16	0.84	0.22	58,73,82,84	0
5	GOL	J	304	6/6	0.84	0.18	59,60,72,74	0
5	GOL	J	307	6/6	0.84	0.12	48,57,62,64	0
4	2PE	A	302	10/28	0.84	0.18	53,64,74,84	0
5	GOL	B	308	6/6	0.84	0.17	45,57,68,75	0
3	1PE	C	301	10/16	0.84	0.22	38,48,58,62	0
3	1PE	H	302[A]	10/16	0.84	0.20	38,51,58,58	10
3	1PE	L	304	13/16	0.84	0.21	51,68,79,83	0
3	1PE	H	302[B]	10/16	0.84	0.20	39,48,55,57	10
6	NI	F	309	1/1	0.84	0.24	150,150,150,150	0
3	1PE	G	301	10/16	0.84	0.24	50,61,76,80	0
3	1PE	C	303[B]	16/16	0.85	0.30	36,67,79,80	16
5	GOL	C	306	6/6	0.85	0.16	41,59,63,63	0
3	1PE	T	303	10/16	0.85	0.21	54,61,72,72	0
5	GOL	T	304	6/6	0.85	0.17	44,45,60,61	0
3	1PE	A	301	13/16	0.85	0.22	51,64,76,78	0
5	GOL	R	307	6/6	0.85	0.16	56,58,69,73	0
5	GOL	S	301	6/6	0.85	0.17	39,55,64,79	0
3	1PE	C	303[A]	16/16	0.85	0.30	27,64,79,80	16
5	GOL	C	305	6/6	0.86	0.16	65,70,75,76	0
5	GOL	I	310	6/6	0.86	0.18	43,54,57,58	0
5	GOL	F	307	6/6	0.86	0.15	58,62,68,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	1PE	K	302	13/16	0.86	0.22	26,53,68,69	0
3	1PE	A	303	7/16	0.86	0.18	51,54,73,75	0
6	NI	J	309	1/1	0.86	0.30	135,135,135,135	0
5	GOL	R	304	6/6	0.86	0.15	50,65,67,71	0
5	GOL	I	306	6/6	0.87	0.17	50,53,64,65	0
5	GOL	K	308	6/6	0.87	0.20	35,46,74,85	0
5	GOL	B	306	6/6	0.87	0.15	44,56,62,65	0
5	GOL	T	307	6/6	0.87	0.14	42,57,62,63	0
6	NI	B	309	1/1	0.87	0.21	130,130,130,130	0
3	1PE	Q	302	10/16	0.87	0.20	62,73,80,85	0
3	1PE	F	303	13/16	0.87	0.17	57,68,79,80	0
5	GOL	H	310	6/6	0.87	0.16	38,42,52,62	0
5	GOL	Q	305	6/6	0.87	0.18	36,45,51,53	6
7	12P	T	301	13/37	0.87	0.17	45,51,58,67	0
5	GOL	T	306	6/6	0.88	0.14	37,49,54,59	0
5	GOL	J	306	6/6	0.88	0.21	22,40,48,50	6
3	1PE	B	303	10/16	0.88	0.17	41,59,68,69	0
6	NI	C	304	1/1	0.88	0.10	95,95,95,95	0
5	GOL	K	303	6/6	0.88	0.18	40,49,56,69	0
3	1PE	L	303	16/16	0.88	0.19	49,61,77,78	0
5	GOL	H	311	6/6	0.88	0.15	32,50,53,63	0
5	GOL	O	304	6/6	0.88	0.16	48,59,64,67	0
5	GOL	I	305	6/6	0.88	0.20	39,46,58,63	0
5	GOL	A	304	6/6	0.89	0.11	23,42,50,54	0
3	1PE	I	302	10/16	0.89	0.18	40,57,70,71	0
5	GOL	K	305	6/6	0.89	0.15	50,57,67,73	0
5	GOL	K	307	6/6	0.89	0.14	41,47,51,53	0
5	GOL	S	302	6/6	0.89	0.18	47,66,77,86	0
3	1PE	N	303	13/16	0.89	0.17	49,64,82,83	0
5	GOL	L	301	6/6	0.89	0.15	32,45,48,49	6
6	NI	I	311	1/1	0.89	0.10	86,86,86,86	0
5	GOL	J	305	6/6	0.89	0.14	34,46,55,57	0
5	GOL	F	305	6/6	0.89	0.19	34,39,54,62	6
5	GOL	I	307	6/6	0.89	0.20	47,52,56,66	0
5	GOL	D	302	6/6	0.90	0.11	33,47,54,56	0
4	2PE	J	302	16/28	0.90	0.18	32,42,51,52	16
3	1PE	H	305	10/16	0.90	0.17	33,44,54,54	0
5	GOL	B	307	6/6	0.90	0.19	47,52,61,62	0
5	GOL	L	307	6/6	0.90	0.17	41,50,58,69	0
5	GOL	E	304	6/6	0.90	0.12	37,43,51,56	0
5	GOL	O	306	6/6	0.90	0.14	46,50,56,59	0
6	NI	P	304	1/1	0.90	0.11	106,106,106,106	0

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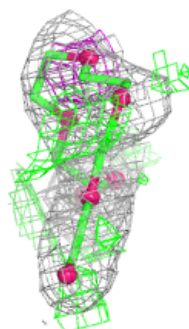
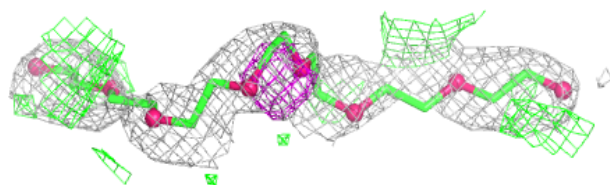
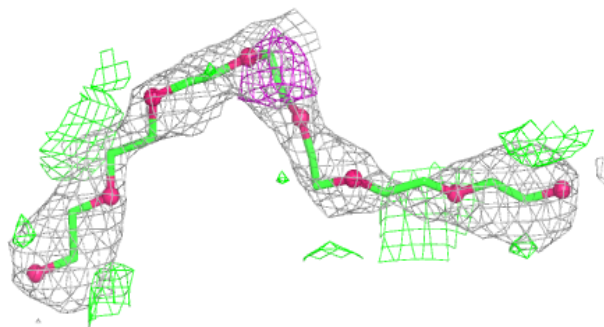
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	M	302	6/6	0.90	0.12	46,50,51,53	0
6	NI	L	310	1/1	0.91	0.15	99,99,99,99	0
6	NI	M	304	1/1	0.91	0.11	102,102,102,102	0
6	NI	H	312	1/1	0.91	0.11	87,87,87,87	0
5	GOL	H	309	6/6	0.91	0.15	40,49,53,57	0
6	NI	R	308	1/1	0.91	0.16	108,108,108,108	0
5	GOL	L	308	6/6	0.91	0.16	47,50,56,60	0
3	1PE	K	301	10/16	0.92	0.15	42,56,59,60	0
6	NI	J	308	1/1	0.92	0.10	94,94,94,94	0
5	GOL	D	301	6/6	0.92	0.13	32,49,58,66	0
5	GOL	D	304	6/6	0.92	0.15	51,53,66,70	0
5	GOL	R	305	6/6	0.92	0.13	37,50,52,58	0
5	GOL	K	306	6/6	0.92	0.18	35,47,52,56	0
6	NI	E	308	1/1	0.92	0.14	94,94,94,94	1
5	GOL	N	305	6/6	0.92	0.10	44,55,64,70	0
5	GOL	H	308	6/6	0.92	0.16	32,49,50,65	0
5	GOL	I	309	6/6	0.93	0.12	33,35,41,42	6
6	NI	L	309	1/1	0.93	0.12	90,90,90,90	0
6	NI	O	310	1/1	0.94	0.10	101,101,101,101	0
6	NI	D	307	1/1	0.94	0.11	99,99,99,99	0
6	NI	E	307	1/1	0.94	0.13	81,81,81,81	0
6	NI	S	307	1/1	0.94	0.09	106,106,106,106	0
5	GOL	E	306	6/6	0.94	0.11	39,51,57,62	0
6	NI	S	308	1/1	0.95	0.07	95,95,95,95	0
6	NI	F	308	1/1	0.95	0.10	104,104,104,104	0
6	NI	C	308	1/1	0.96	0.07	98,98,98,98	0
6	NI	O	309	1/1	0.96	0.08	110,110,110,110	0
6	NI	Q	306	1/1	0.97	0.10	96,96,96,96	0
6	NI	Q	307	1/1	0.97	0.10	74,74,74,74	1
6	NI	I	304	1/1	0.97	0.06	88,88,88,88	0
6	NI	N	306	1/1	0.97	0.06	89,89,89,89	0
6	NI	P	303	1/1	0.97	0.08	84,84,84,84	1
6	NI	H	306	1/1	0.97	0.08	92,92,92,92	0
6	NI	D	306	1/1	0.98	0.06	77,77,77,77	0
6	NI	C	307	1/1	0.98	0.09	88,88,88,88	0
6	NI	S	309	1/1	0.98	0.06	109,109,109,109	0
6	NI	K	309	1/1	0.98	0.08	86,86,86,86	0

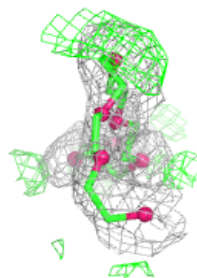
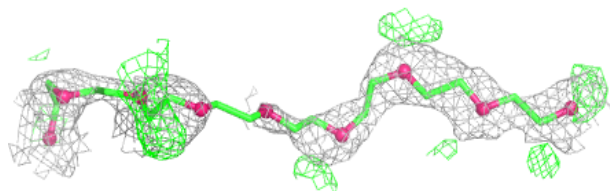
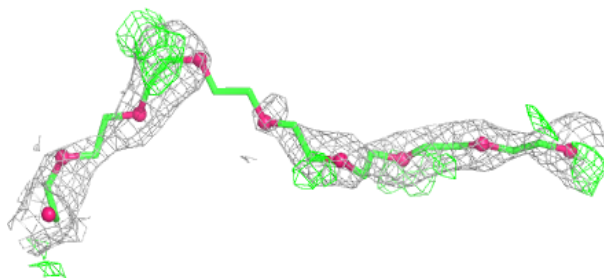
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 2PE H 304:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

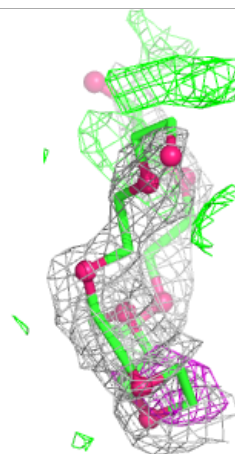
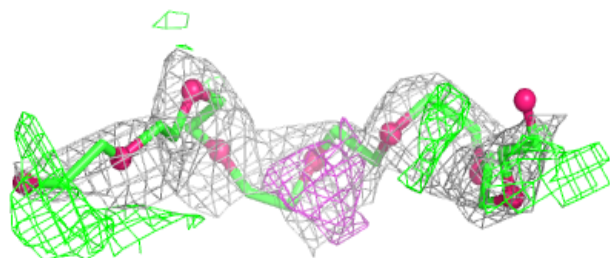
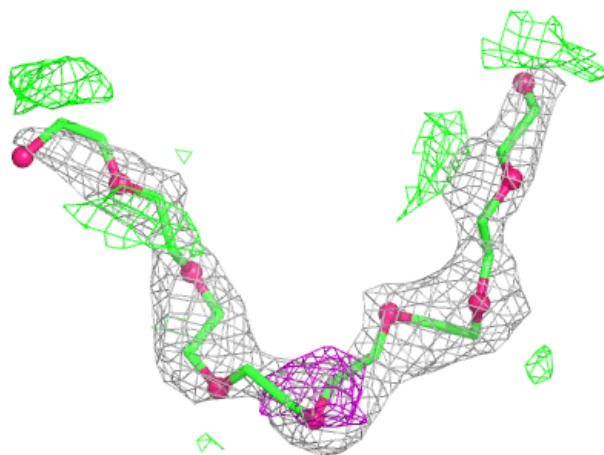
**Electron density around 2PE L 302:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



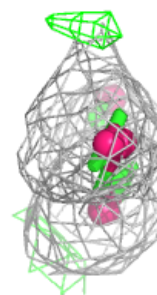
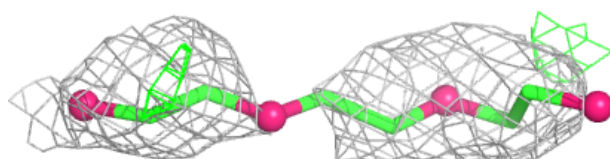
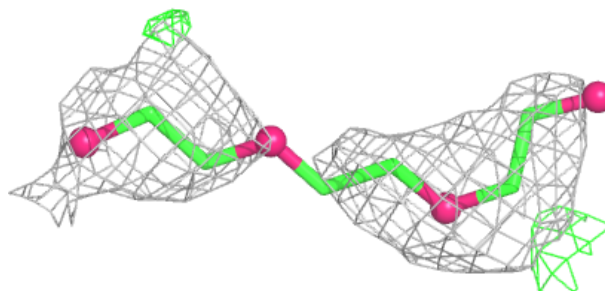
Electron density around 2PE H 303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

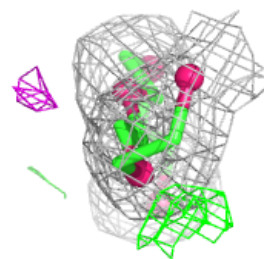
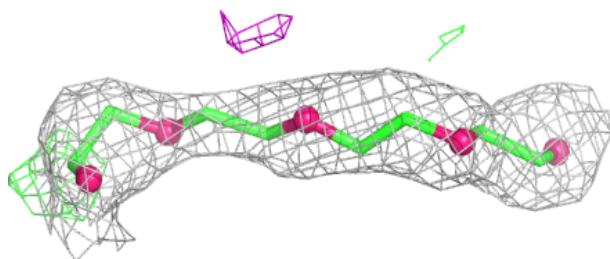
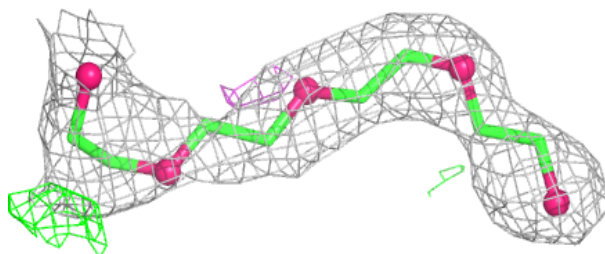


Electron density around 2PE A 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

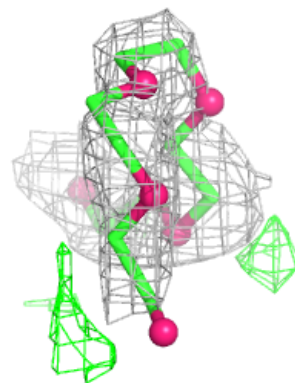
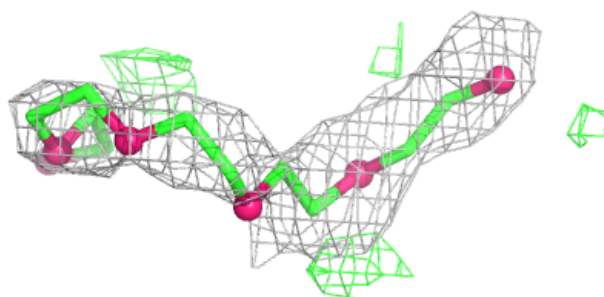
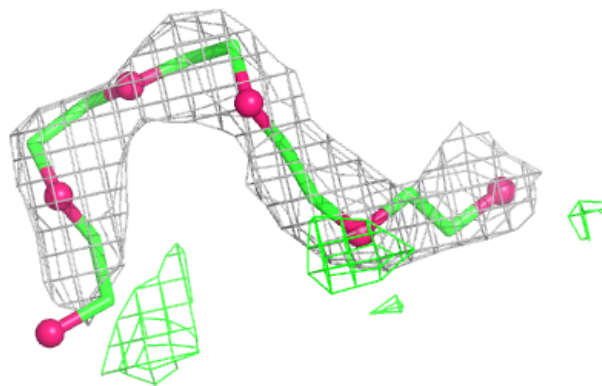
**Electron density around 12P T 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 2PE J 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.