



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2023 – 11:18 AM EDT

PDB ID : 8EIF
Title : Crystal structure of unmodified Pseudomonas aeruginosa protein PA0709
Authors : Cuthbert, B.J.; Goulding, C.W.
Deposited on : 2022-09-14
Resolution : 2.10 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

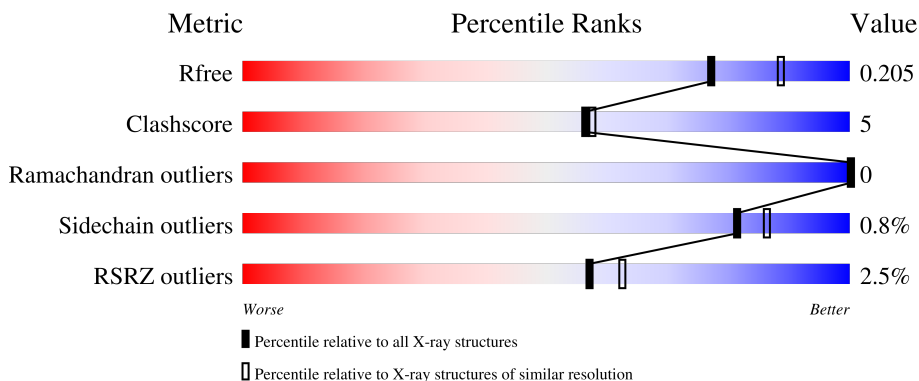
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	102	 87% 9% .
1	B	102	 3% 84% 11% 5%
1	C	102	 3% 85% 10% . .
1	D	102	 2% 83% 12% 5%
1	E	102	 2% 86% 10% .

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Mol	Chain	Length	Quality of chain
1	F	102	
1	G	102	
1	H	102	
1	I	102	
1	J	102	
1	K	102	
1	L	102	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PPI	B	1201	-	-	X	-
3	GOL	A	409	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 10805 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 Antibiotic biosynthesis monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	98	802	514	137	149	2	0	0	0
1	B	97	811	519	139	152	1	0	1	0
1	C	98	818	523	140	153	2	0	1	0
1	D	97	806	516	136	152	2	0	0	0
1	E	98	818	523	140	153	2	0	1	0
1	F	99	808	517	139	150	2	0	1	0
1	G	98	810	518	137	153	2	0	0	0
1	H	98	818	524	143	149	2	0	2	0
1	I	98	823	526	141	154	2	0	2	0
1	J	98	804	516	137	149	2	0	1	0
1	K	98	787	506	130	150	1	0	0	0
1	L	98	798	512	135	149	2	0	1	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	SER	-	expression tag	UNP A0A072ZNL3
A	-2	GLY	-	expression tag	UNP A0A072ZNL3
A	-1	GLY	-	expression tag	UNP A0A072ZNL3
A	0	GLY	-	expression tag	UNP A0A072ZNL3
B	-3	SER	-	expression tag	UNP A0A072ZNL3

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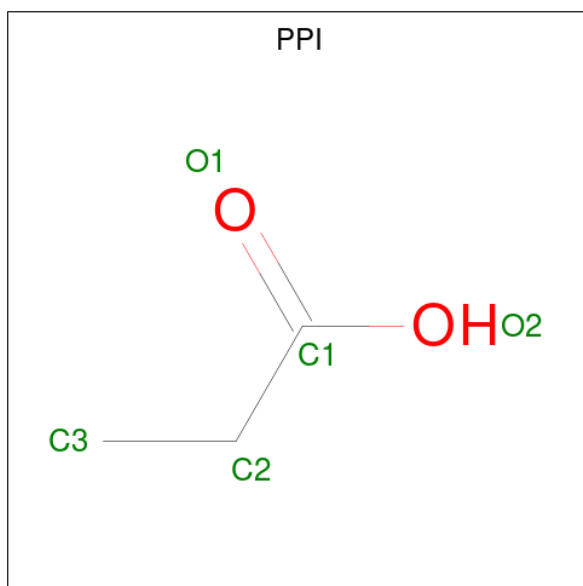
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP A0A072ZNL3
B	-1	GLY	-	expression tag	UNP A0A072ZNL3
B	0	GLY	-	expression tag	UNP A0A072ZNL3
C	-3	SER	-	expression tag	UNP A0A072ZNL3
C	-2	GLY	-	expression tag	UNP A0A072ZNL3
C	-1	GLY	-	expression tag	UNP A0A072ZNL3
C	0	GLY	-	expression tag	UNP A0A072ZNL3
D	-3	SER	-	expression tag	UNP A0A072ZNL3
D	-2	GLY	-	expression tag	UNP A0A072ZNL3
D	-1	GLY	-	expression tag	UNP A0A072ZNL3
D	0	GLY	-	expression tag	UNP A0A072ZNL3
E	-3	SER	-	expression tag	UNP A0A072ZNL3
E	-2	GLY	-	expression tag	UNP A0A072ZNL3
E	-1	GLY	-	expression tag	UNP A0A072ZNL3
E	0	GLY	-	expression tag	UNP A0A072ZNL3
F	-3	SER	-	expression tag	UNP A0A072ZNL3
F	-2	GLY	-	expression tag	UNP A0A072ZNL3
F	-1	GLY	-	expression tag	UNP A0A072ZNL3
F	0	GLY	-	expression tag	UNP A0A072ZNL3
G	-3	SER	-	expression tag	UNP A0A072ZNL3
G	-2	GLY	-	expression tag	UNP A0A072ZNL3
G	-1	GLY	-	expression tag	UNP A0A072ZNL3
G	0	GLY	-	expression tag	UNP A0A072ZNL3
H	-3	SER	-	expression tag	UNP A0A072ZNL3
H	-2	GLY	-	expression tag	UNP A0A072ZNL3
H	-1	GLY	-	expression tag	UNP A0A072ZNL3
H	0	GLY	-	expression tag	UNP A0A072ZNL3
I	-3	SER	-	expression tag	UNP A0A072ZNL3
I	-2	GLY	-	expression tag	UNP A0A072ZNL3
I	-1	GLY	-	expression tag	UNP A0A072ZNL3
I	0	GLY	-	expression tag	UNP A0A072ZNL3
J	-3	SER	-	expression tag	UNP A0A072ZNL3
J	-2	GLY	-	expression tag	UNP A0A072ZNL3
J	-1	GLY	-	expression tag	UNP A0A072ZNL3
J	0	GLY	-	expression tag	UNP A0A072ZNL3
K	-3	SER	-	expression tag	UNP A0A072ZNL3
K	-2	GLY	-	expression tag	UNP A0A072ZNL3
K	-1	GLY	-	expression tag	UNP A0A072ZNL3
K	0	GLY	-	expression tag	UNP A0A072ZNL3
L	-3	SER	-	expression tag	UNP A0A072ZNL3
L	-2	GLY	-	expression tag	UNP A0A072ZNL3
L	-1	GLY	-	expression tag	UNP A0A072ZNL3

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Chain	Residue	Modelled	Actual	Comment	Reference
L	0	GLY	-	expression tag	UNP A0A072ZNL3

- Molecule 2 is PROPANOIC ACID (three-letter code: PPI) (formula: $C_3H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	5	3	2	0	0
2	A	1	5	3	2	0	0
2	A	1	5	3	2	0	0
2	A	1	5	3	2	0	0
2	A	1	5	3	2	0	0
2	A	1	5	3	2	0	0
2	A	1	5	3	2	0	0
2	A	1	5	3	2	0	0
2	B	1	5	3	2	0	0
2	B	1	5	3	2	0	0
2	B	1	5	3	2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 5	C 3	O 2	0	0
2	B	1	Total 5	C 3	O 2	0	0
2	C	1	Total 5	C 3	O 2	0	0
2	C	1	Total 5	C 3	O 2	0	0
2	C	1	Total 5	C 3	O 2	0	0
2	C	1	Total 5	C 3	O 2	0	0
2	C	1	Total 5	C 3	O 2	0	0
2	D	1	Total 5	C 3	O 2	0	0
2	D	1	Total 5	C 3	O 2	0	0
2	D	1	Total 5	C 3	O 2	0	0
2	D	1	Total 5	C 3	O 2	0	0
2	E	1	Total 5	C 3	O 2	0	0
2	E	1	Total 5	C 3	O 2	0	0
2	E	1	Total 5	C 3	O 2	0	0
2	E	1	Total 5	C 3	O 2	0	0
2	F	1	Total 5	C 3	O 2	0	0
2	F	1	Total 5	C 3	O 2	0	0
2	F	1	Total 5	C 3	O 2	0	0
2	F	1	Total 5	C 3	O 2	0	0
2	G	1	Total 5	C 3	O 2	0	0
2	G	1	Total 5	C 3	O 2	0	0

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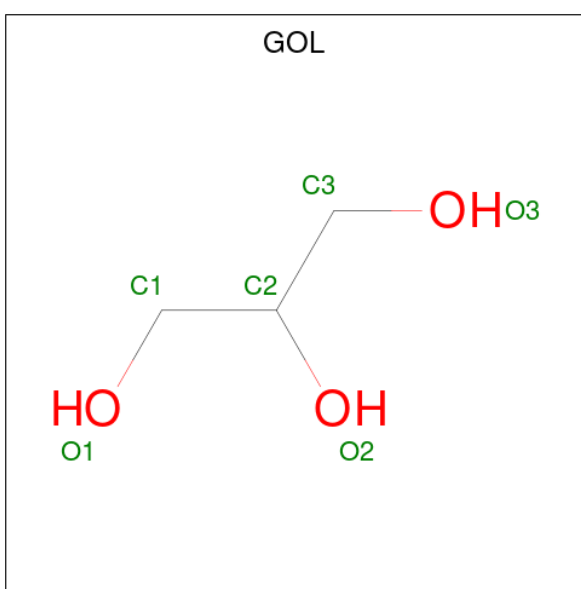
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	G	1	Total 5	C 3	O 2	0	0
2	G	1	Total 5	C 3	O 2	0	0
2	G	1	Total 5	C 3	O 2	0	0
2	H	1	Total 5	C 3	O 2	0	0
2	H	1	Total 5	C 3	O 2	0	0
2	H	1	Total 5	C 3	O 2	0	0
2	H	1	Total 5	C 3	O 2	0	0
2	I	1	Total 5	C 3	O 2	0	0
2	I	1	Total 5	C 3	O 2	0	0
2	I	1	Total 5	C 3	O 2	0	0
2	I	1	Total 5	C 3	O 2	0	0
2	J	1	Total 5	C 3	O 2	0	0
2	J	1	Total 5	C 3	O 2	0	0
2	J	1	Total 5	C 3	O 2	0	0
2	K	1	Total 5	C 3	O 2	0	0
2	K	1	Total 5	C 3	O 2	0	0
2	K	1	Total 5	C 3	O 2	0	0
2	K	1	Total 5	C 3	O 2	0	0
2	K	1	Total 5	C 3	O 2	0	0
2	L	1	Total 5	C 3	O 2	0	0
2	L	1	Total 5	C 3	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	L	1	Total	C	O	0	0
			5	3	2		
2	L	1	Total	C	O	0	0
			5	3	2		
2	L	1	Total	C	O	0	0
			5	3	2		
2	L	1	Total	C	O	0	0
			5	3	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



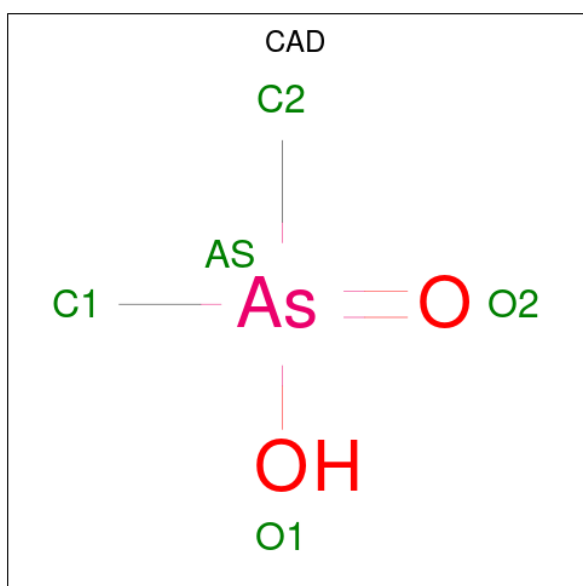
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is CACODYLIC ACID (three-letter code: CAD) (formula: C₂H₇AsO₂).



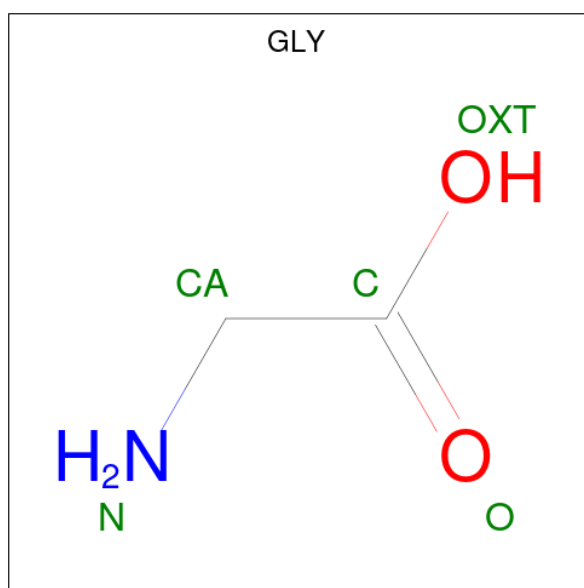
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	As	C	O	0	0
			5	1	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	As	C	O		
4	B	1	Total 5	As 1	C 2	O 2	0	0
4	E	1	Total 5	As 1	C 2	O 2	0	0
4	F	1	Total 5	As 1	C 2	O 2	0	0
4	G	1	Total 5	As 1	C 2	O 2	0	0
4	H	1	Total 5	As 1	C 2	O 2	0	0
4	I	1	Total 5	As 1	C 2	O 2	0	0
4	L	1	Total 5	As 1	C 2	O 2	0	0

- Molecule 5 is GLYCINE (three-letter code: GLY) (formula: C₂H₅NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	B	1	Total 4	C 2	N 1	O 1	0	0

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			13	8	5		
6	C	1	Total	C	O	0	0
			7	4	3		
6	D	1	Total	C	O	0	0
			13	8	5		
6	E	1	Total	C	O	0	0
			13	8	5		
6	F	1	Total	C	O	0	0
			10	6	4		
6	H	1	Total	C	O	0	0
			13	8	5		
6	I	1	Total	C	O	0	0
			16	10	6		
6	K	1	Total	C	O	0	0
			16	10	6		
6	L	1	Total	C	O	0	0
			16	10	6		

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	C O	0	1
			26	16 10		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	53	Total	O	0	0
			53	53		
8	B	56	Total	O	0	0
			56	56		
8	C	49	Total	O	0	0
			49	49		
8	D	40	Total	O	0	0
			40	40		
8	E	45	Total	O	0	0
			45	45		
8	F	50	Total	O	0	0
			50	50		
8	G	47	Total	O	0	0
			47	47		
8	H	45	Total	O	0	0
			45	45		
8	I	42	Total	O	0	0
			42	42		
8	J	32	Total	O	0	0
			32	32		
8	K	36	Total	O	0	0
			36	36		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	33	Total	O	0	0
			33	33		

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: Antibiotic biosynthesis monooxygenase

Chain A:  87% 9%




- Molecule 1: Antibiotic biosynthesis monooxygenase

Chain B:  84% 11% 5%




- Molecule 1: Antibiotic biosynthesis monooxygenase

Chain C:  85% 10%




- Molecule 1: Antibiotic biosynthesis monooxygenase

Chain D:  83% 12% 5%

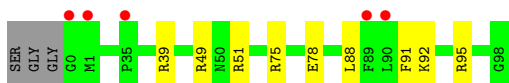
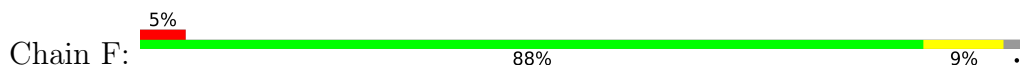


- Molecule 1: Antibiotic biosynthesis monooxygenase

Chain E:  86% 10%



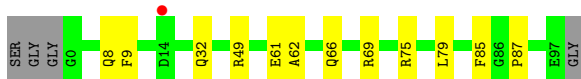
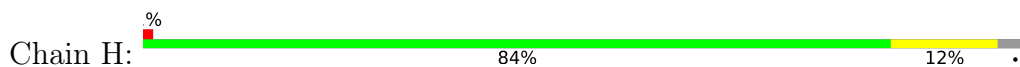
- Molecule 1: Antibiotic biosynthesis monooxygenase



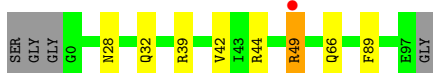
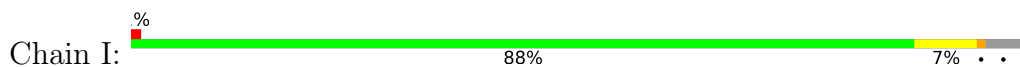
- Molecule 1: Antibiotic biosynthesis monooxygenase



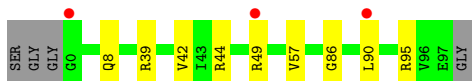
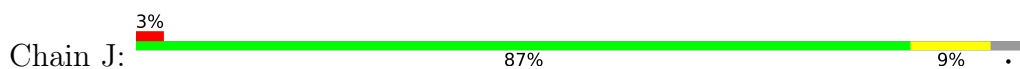
- Molecule 1: Antibiotic biosynthesis monooxygenase



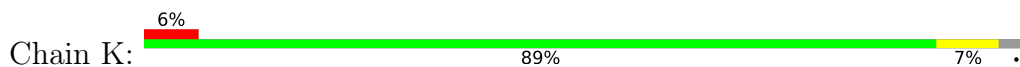
- Molecule 1: Antibiotic biosynthesis monooxygenase



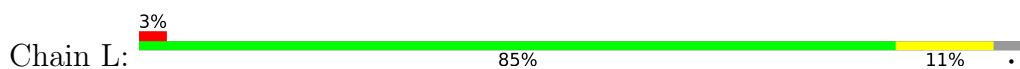
- Molecule 1: Antibiotic biosynthesis monooxygenase



- Molecule 1: Antibiotic biosynthesis monooxygenase



- Molecule 1: Antibiotic biosynthesis monooxygenase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.41Å 187.41Å 60.42Å 90.00° 99.19° 90.00°	Depositor
Resolution (Å)	39.16 – 2.10 39.16 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.8 (39.16-2.10) 98.7 (39.16-2.10)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.171 , 0.208 0.170 , 0.205	Depositor DCC
R_{free} test set	7630 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtrriage
Anisotropy	0.508	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 78.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.036 for l,-k,h	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10805	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, GOL, CAD, 1PE, PPI

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	0.26	0/822	0.51	0/1111
1	B	0.26	0/834	0.52	0/1127
1	C	0.26	0/841	0.53	0/1135
1	D	0.26	0/826	0.51	0/1116
1	E	0.26	0/841	0.53	0/1135
1	F	0.26	0/828	0.53	0/1119
1	G	0.26	0/830	0.51	0/1121
1	H	0.27	0/844	0.54	0/1139
1	I	0.29	0/849	0.54	0/1146
1	J	0.25	0/827	0.55	0/1118
1	K	0.25	0/807	0.51	0/1094
1	L	0.26	0/818	0.50	0/1107
All	All	0.26	0/9967	0.52	0/13468

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	802	0	750	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	811	0	761	12	0
1	C	818	0	771	9	0
1	D	806	0	755	10	0
1	E	818	0	771	11	0
1	F	808	0	753	9	0
1	G	810	0	758	3	0
1	H	818	0	776	11	0
1	I	823	0	777	8	0
1	J	804	0	752	7	0
1	K	787	0	719	6	0
1	L	798	0	739	11	0
2	A	40	0	40	2	0
2	B	25	0	25	5	0
2	C	25	0	25	5	0
2	D	20	0	20	5	0
2	E	20	0	20	1	0
2	F	20	0	20	4	0
2	G	25	0	25	2	0
2	H	20	0	20	1	0
2	I	20	0	20	2	0
2	J	15	0	15	2	0
2	K	25	0	25	2	0
2	L	30	0	30	2	0
3	A	12	0	16	6	0
3	B	30	0	40	2	0
3	C	12	0	16	0	0
3	E	12	0	16	0	0
3	F	12	0	16	0	0
3	G	6	0	8	1	0
3	H	12	0	16	2	0
3	L	6	0	8	1	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	H	5	0	0	1	0
4	I	5	0	0	0	0
4	L	5	0	0	0	0
5	B	4	0	2	0	0
6	B	13	0	17	0	0
6	C	7	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	13	0	17	2	0
6	E	13	0	17	2	0
6	F	10	0	13	1	0
6	H	13	0	17	0	0
6	I	16	0	22	1	0
6	K	16	0	22	1	0
6	L	16	0	22	4	0
7	D	26	0	36	3	0
8	A	53	0	0	1	0
8	B	56	0	0	0	0
8	C	49	0	0	0	0
8	D	40	0	0	1	0
8	E	45	0	0	1	0
8	F	50	0	0	1	0
8	G	47	0	0	0	0
8	H	45	0	0	1	0
8	I	42	0	0	2	0
8	J	32	0	0	0	0
8	K	36	0	0	0	0
8	L	33	0	0	1	0
All	All	10805	0	9696	100	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 5.

All (100) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:49[A]:ARG:HD3	1:I:49[A]:ARG:H	1.37	0.88
1:C:95:ARG:HH21	2:C:406:PPI:H21	1.43	0.83
2:A:408:PPI:H33	1:B:51:ARG:HH11	1.44	0.83
1:H:49[B]:ARG:HH11	1:H:49[B]:ARG:HG3	1.46	0.79
1:K:5:VAL:HG22	1:K:92:LYS:HG2	1.66	0.78
1:H:32:GLN:NE2	4:H:507:CAD:O1	2.19	0.76
1:A:81:ASP:HA	2:A:410:PPI:H32	1.67	0.74
1:H:66:GLN:HB3	3:H:506:GOL:H32	1.70	0.73
1:C:81:ASP:OD2	2:C:404:PPI:H31	1.88	0.73
1:F:51:ARG:HH12	6:F:506:1PE:H141	1.55	0.72
1:D:8:GLN:HG2	2:D:102:PPI:H31	1.72	0.71
1:D:81:ASP:HA	2:D:103:PPI:H33	1.73	0.69
1:I:49[A]:ARG:H	1:I:49[A]:ARG:CD	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:VAL:O	3:A:409:GOL:O3	2.13	0.67
1:J:8:GLN:HG2	2:J:301:PPI:H31	1.78	0.65
1:E:61:GLU:OE1	8:E:701:HOH:O	2.15	0.64
1:L:39:ARG:HD3	2:L:609:PPI:H31	1.81	0.62
1:H:49[B]:ARG:HG3	1:H:49[B]:ARG:NH1	2.14	0.62
1:D:69:ARG:NH1	8:D:201:HOH:O	2.33	0.61
1:I:28[B]:ASN:ND2	1:I:32:GLN:OE1	2.33	0.61
1:J:44:ARG:NH1	1:J:49:ARG:HG2	2.17	0.60
3:A:409:GOL:H31	1:B:42:VAL:H	1.68	0.59
3:A:409:GOL:H31	1:B:41:GLU:HA	1.84	0.59
1:A:42:VAL:H	2:B:1201:PPI:H31	1.67	0.58
1:L:15:LYS:HE3	6:L:607:1PE:H141	1.86	0.58
1:K:92:LYS:NZ	1:L:46:GLU:OE2	2.37	0.57
1:E:25:PHE:CE2	1:E:75[A]:ARG:HG2	2.39	0.57
1:I:42:VAL:H	1:J:95[B]:ARG:NH2	2.03	0.57
1:K:49:ARG:H	2:K:203:PPI:H31	1.70	0.57
1:H:62:ALA:O	1:H:66:GLN:HG3	2.06	0.56
1:B:49:ARG:HH21	2:F:503:PPI:H32	1.69	0.56
1:H:85:PHE:HB3	2:H:502:PPI:H33	1.88	0.55
1:B:81:ASP:HA	1:C:49:ARG:HH12	1.71	0.55
1:F:39:ARG:HD3	2:F:508:PPI:O1	2.07	0.54
1:A:41:GLU:HA	2:B:1201:PPI:H32	1.91	0.52
1:D:92:LYS:NZ	6:D:106:1PE:OH3	2.37	0.52
1:B:44:ARG:HD3	1:B:52:PHE:CZ	2.45	0.52
1:J:86:GLY:O	2:J:303:PPI:H32	2.10	0.52
1:H:61:GLU:OE1	8:H:601:HOH:O	2.18	0.51
1:L:15:LYS:HZ1	6:L:607:1PE:H242	1.75	0.51
1:L:66:GLN:NE2	8:L:701:HOH:O	2.37	0.51
2:C:408:PPI:H31	1:F:49:ARG:H	1.75	0.51
3:A:406:GOL:H32	1:E:51:ARG:NH2	2.26	0.50
3:B:1212:GOL:H32	1:F:88:LEU:HA	1.92	0.50
1:C:71:GLU:OE1	1:C:75[A]:ARG:NH1	2.44	0.50
1:F:78:GLU:OE2	2:F:505:PPI:H33	2.11	0.50
1:A:42:VAL:H	2:B:1201:PPI:C3	2.24	0.49
1:D:10:ASP:OD2	2:D:102:PPI:H21	2.13	0.49
1:D:77:TYR:HD1	2:D:103:PPI:H31	1.77	0.49
1:K:44:ARG:HD3	2:K:206:PPI:H21	1.94	0.49
1:K:15:LYS:HZ3	6:K:201:1PE:H121	1.76	0.49
1:F:78:GLU:OE2	1:I:39:ARG:HD3	2.13	0.49
1:L:68:CYS:HB3	2:L:608:PPI:H31	1.96	0.47
1:D:59:GLU:OE2	7:D:101[B]:PG4:H11	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:69:ARG:HH11	1:H:69:ARG:HG2	1.78	0.47
1:E:92:LYS:NZ	6:E:601:1PE:OH6	2.48	0.47
1:I:66:GLN:NE2	8:I:202:HOH:O	2.48	0.47
1:C:82:SER:HA	2:C:404:PPI:H33	1.97	0.47
1:L:88:LEU:HD22	3:L:603:GOL:H32	1.96	0.47
1:F:75:ARG:HD3	2:F:505:PPI:H31	1.97	0.47
2:I:106:PPI:C3	1:J:42:VAL:H	2.28	0.47
1:G:77:TYR:CG	2:G:604:PPI:H22	2.49	0.46
2:D:104:PPI:H31	1:E:81:ASP:HA	1.97	0.46
1:E:6:LEU:HD21	1:F:91:PHE:HE2	1.80	0.46
1:G:88:LEU:HB2	3:G:602:GOL:H11	1.97	0.46
2:C:406:PPI:H22	1:D:40:PHE:O	2.16	0.45
1:A:32:GLN:OE1	8:A:501:HOH:O	2.21	0.45
1:E:92:LYS:HZ3	6:E:601:1PE:H241	1.81	0.45
1:C:49:ARG:HD3	1:C:49:ARG:H	1.82	0.45
1:A:95:ARG:NH2	3:A:409:GOL:O2	2.49	0.45
1:I:89:PHE:CE2	6:I:103:1PE:H262	2.52	0.45
1:E:46:GLU:OE2	1:F:92:LYS:HE3	2.17	0.44
1:A:46:GLU:OE2	1:B:92:LYS:NZ	2.49	0.44
1:J:8:GLN:HB2	1:J:90:LEU:HD21	1.99	0.44
1:E:39:ARG:HH11	2:E:604:PPI:H21	1.83	0.44
1:L:15:LYS:CE	6:L:607:1PE:H131	2.48	0.44
1:L:77:TYR:OH	1:L:87:PRO:HG3	2.18	0.43
1:K:3:TYR:OH	1:K:92:LYS:HD2	2.18	0.43
1:L:44:ARG:HG3	1:L:52:PHE:CE2	2.53	0.43
1:B:81:ASP:HA	1:C:49:ARG:HH22	1.84	0.43
1:G:77:TYR:HB3	2:G:604:PPI:H31	2.00	0.43
7:D:101[B]:PG4:H82	7:D:101[B]:PG4:H61	1.60	0.43
1:B:39[A]:ARG:HH11	2:B:1206:PPI:H32	1.83	0.43
1:E:3:TYR:OH	1:E:92:LYS:HD2	2.19	0.42
1:B:95:ARG:NH2	2:B:1201:PPI:O2	2.44	0.42
1:B:70:ASN:HB3	3:B:1207:GOL:H11	2.01	0.42
1:E:25:PHE:CE2	1:E:75[B]:ARG:HG2	2.54	0.42
1:I:44:ARG:HD2	8:I:234:HOH:O	2.19	0.42
3:A:409:GOL:C3	1:B:42:VAL:H	2.32	0.42
8:F:607:HOH:O	2:I:102:PPI:H31	2.20	0.42
1:L:15:LYS:HZ1	6:L:607:1PE:H131	1.85	0.42
1:H:75:ARG:NH2	1:H:79:LEU:HD21	2.35	0.41
1:H:9:PHE:CZ	1:H:87:PRO:HB3	2.55	0.41
1:C:29:GLY:O	1:C:33:ASN:ND2	2.54	0.41
1:H:8:GLN:OE1	3:H:508:GOL:H32	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:39:ARG:HB3	1:J:57:VAL:HB	2.02	0.41
1:C:77:TYR:OH	1:C:87:PRO:HG3	2.20	0.40
1:A:47:ASN:OD1	6:D:106:1PE:H221	2.21	0.40
1:D:1:MET:HG3	1:D:94:TYR:HB3	2.04	0.40
1:D:35:PRO:O	7:D:101[A]:PG4:H32	2.22	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	96/102 (94%)	95 (99%)	1 (1%)	0	100	100
1	B	96/102 (94%)	95 (99%)	1 (1%)	0	100	100
1	C	97/102 (95%)	95 (98%)	2 (2%)	0	100	100
1	D	95/102 (93%)	94 (99%)	1 (1%)	0	100	100
1	E	97/102 (95%)	95 (98%)	2 (2%)	0	100	100
1	F	98/102 (96%)	96 (98%)	2 (2%)	0	100	100
1	G	96/102 (94%)	95 (99%)	1 (1%)	0	100	100
1	H	98/102 (96%)	96 (98%)	2 (2%)	0	100	100
1	I	98/102 (96%)	97 (99%)	1 (1%)	0	100	100
1	J	97/102 (95%)	95 (98%)	2 (2%)	0	100	100
1	K	96/102 (94%)	94 (98%)	2 (2%)	0	100	100
1	L	97/102 (95%)	95 (98%)	2 (2%)	0	100	100
All	All	1161/1224 (95%)	1142 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	81/84 (96%)	80 (99%)	1 (1%)	71	77
1	B	83/84 (99%)	83 (100%)	0	100	100
1	C	84/84 (100%)	82 (98%)	2 (2%)	49	53
1	D	83/84 (99%)	82 (99%)	1 (1%)	71	77
1	E	84/84 (100%)	84 (100%)	0	100	100
1	F	81/84 (96%)	80 (99%)	1 (1%)	71	77
1	G	83/84 (99%)	83 (100%)	0	100	100
1	H	83/84 (99%)	83 (100%)	0	100	100
1	I	85/84 (101%)	83 (98%)	2 (2%)	49	53
1	J	81/84 (96%)	81 (100%)	0	100	100
1	K	78/84 (93%)	77 (99%)	1 (1%)	69	75
1	L	80/84 (95%)	79 (99%)	1 (1%)	69	75
All	All	986/1008 (98%)	977 (99%)	9 (1%)	81	84

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	C	44	ARG
1	C	49	ARG
1	D	95	ARG
1	F	95	ARG
1	I	49[A]	ARG
1	I	49[B]	ARG
1	K	95	ARG
1	L	61	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	32	GLN
1	K	28	ASN
1	K	66	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

94 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PPI	G	601	-	4,4,4	0.96	0	4,4,4	1.10	0
3	GOL	L	603	-	5,5,5	0.87	0	5,5,5	0.98	0
4	CAD	G	607	-	1,4,4	2.93	1 (100%)	2,6,6	1.15	0
5	GLY	B	1202	-	3,3,4	0.60	0	0,2,4	-	-
2	PPI	E	604	-	4,4,4	0.96	0	4,4,4	1.04	0
2	PPI	G	606	-	4,4,4	0.95	0	4,4,4	1.09	0
2	PPI	J	301	-	4,4,4	0.93	0	4,4,4	1.10	0
6	1PE	F	506	-	9,9,15	0.11	0	8,8,14	0.14	0
4	CAD	L	601	-	1,4,4	3.08	1 (100%)	2,6,6	1.29	0
3	GOL	B	1204	-	5,5,5	0.93	0	5,5,5	0.94	0
3	GOL	B	1208	-	5,5,5	0.88	0	5,5,5	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PPI	E	605	-	4,4,4	0.96	0	4,4,4	1.10	0
7	PG4	D	101[B]	-	12,12,12	0.52	0	11,11,11	0.34	0
2	PPI	F	503	-	4,4,4	0.94	0	4,4,4	1.12	0
2	PPI	G	605	-	4,4,4	0.95	0	4,4,4	1.10	0
3	GOL	H	508	-	5,5,5	0.90	0	5,5,5	0.96	0
2	PPI	K	205	-	4,4,4	0.96	0	4,4,4	1.09	0
2	PPI	A	402	-	4,4,4	0.94	0	4,4,4	1.04	0
6	1PE	K	201	-	15,15,15	0.11	0	14,14,14	0.10	0
2	PPI	D	104	-	4,4,4	0.95	0	4,4,4	1.19	0
2	PPI	L	608	-	4,4,4	0.97	0	4,4,4	1.05	0
2	PPI	C	408	-	4,4,4	0.94	0	4,4,4	1.03	0
2	PPI	D	103	-	4,4,4	0.96	0	4,4,4	1.00	0
2	PPI	E	603	-	4,4,4	0.94	0	4,4,4	1.17	0
2	PPI	A	405	-	4,4,4	0.94	0	4,4,4	1.09	0
2	PPI	C	406	-	4,4,4	0.98	0	4,4,4	0.92	0
3	GOL	A	409	-	5,5,5	0.94	0	5,5,5	0.89	0
2	PPI	D	105	-	4,4,4	0.95	0	4,4,4	1.07	0
2	PPI	K	204	-	4,4,4	0.97	0	4,4,4	0.95	0
6	1PE	H	504	-	12,12,15	0.10	0	11,11,14	0.14	0
2	PPI	B	1201	-	4,4,4	0.93	0	4,4,4	1.05	0
2	PPI	A	401	-	4,4,4	0.97	0	4,4,4	1.04	0
2	PPI	A	407	-	4,4,4	0.93	0	4,4,4	1.12	0
2	PPI	H	505	-	4,4,4	0.95	0	4,4,4	1.09	0
2	PPI	D	102	-	4,4,4	0.93	0	4,4,4	1.07	0
2	PPI	H	503	-	4,4,4	0.95	0	4,4,4	1.09	0
3	GOL	B	1212	-	5,5,5	0.92	0	5,5,5	0.93	0
2	PPI	K	203	-	4,4,4	0.95	0	4,4,4	1.04	0
2	PPI	H	501	-	4,4,4	0.92	0	4,4,4	1.04	0
2	PPI	G	603	-	4,4,4	0.94	0	4,4,4	1.03	0
2	PPI	L	606	-	4,4,4	0.95	0	4,4,4	1.07	0
3	GOL	E	608	-	5,5,5	0.89	0	5,5,5	1.04	0
2	PPI	B	1210	-	4,4,4	0.96	0	4,4,4	1.05	0
3	GOL	F	501	-	5,5,5	0.91	0	5,5,5	1.02	0
2	PPI	F	508	-	4,4,4	0.92	0	4,4,4	1.15	0
2	PPI	L	604	-	4,4,4	0.93	0	4,4,4	1.09	0
4	CAD	B	1209	-	1,4,4	2.83	1 (100%)	2,6,6	1.33	0
2	PPI	F	505	-	4,4,4	0.96	0	4,4,4	1.08	0
6	1PE	D	106	-	12,12,15	0.11	0	11,11,14	0.13	0
2	PPI	J	303	-	4,4,4	0.97	0	4,4,4	1.04	0
2	PPI	C	405	-	4,4,4	0.96	0	4,4,4	1.06	0
2	PPI	A	408	-	4,4,4	0.96	0	4,4,4	1.08	0
2	PPI	A	403	-	4,4,4	0.95	0	4,4,4	1.09	0
2	PPI	L	609	-	4,4,4	0.96	0	4,4,4	1.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PPI	B	1206	-	4,4,4	0.96	0	4,4,4	1.10	0
6	1PE	B	1203	-	12,12,15	0.13	0	11,11,14	0.10	0
2	PPI	K	206	-	4,4,4	0.95	0	4,4,4	1.12	0
2	PPI	L	605	-	4,4,4	0.95	0	4,4,4	1.09	0
4	CAD	H	507	-	1,4,4	3.05	1 (100%)	2,6,6	0.68	0
2	PPI	J	302	-	4,4,4	0.97	0	4,4,4	1.08	0
2	PPI	B	1205	-	4,4,4	0.96	0	4,4,4	1.09	0
6	1PE	L	607	-	15,15,15	0.14	0	14,14,14	0.12	0
3	GOL	C	403	-	5,5,5	0.85	0	5,5,5	1.05	0
3	GOL	B	1207	-	5,5,5	0.87	0	5,5,5	0.97	0
3	GOL	G	602	-	5,5,5	0.87	0	5,5,5	1.02	0
4	CAD	I	105	-	1,4,4	3.03	1 (100%)	2,6,6	1.23	0
3	GOL	E	606	-	5,5,5	0.88	0	5,5,5	1.05	0
2	PPI	A	410	-	4,4,4	0.94	0	4,4,4	1.04	0
2	PPI	C	404	-	4,4,4	0.94	0	4,4,4	1.06	0
3	GOL	C	402	-	5,5,5	0.88	0	5,5,5	0.97	0
2	PPI	H	502	-	4,4,4	0.95	0	4,4,4	1.14	0
2	PPI	I	101	-	4,4,4	0.93	0	4,4,4	1.13	0
3	GOL	H	506	-	5,5,5	0.99	0	5,5,5	0.95	0
2	PPI	K	202	-	4,4,4	0.94	0	4,4,4	1.12	0
3	GOL	B	1213	-	5,5,5	0.89	0	5,5,5	1.02	0
2	PPI	I	106	-	4,4,4	0.95	0	4,4,4	1.14	0
4	CAD	E	602	-	1,4,4	2.89	1 (100%)	2,6,6	1.11	0
3	GOL	A	406	-	5,5,5	0.90	0	5,5,5	1.00	0
4	CAD	F	507	-	1,4,4	3.04	1 (100%)	2,6,6	1.35	0
2	PPI	G	604	-	4,4,4	1.02	0	4,4,4	1.13	0
2	PPI	A	404	-	4,4,4	0.96	0	4,4,4	1.06	0
2	PPI	L	602	-	4,4,4	0.96	0	4,4,4	1.06	0
2	PPI	I	102	-	4,4,4	0.95	0	4,4,4	1.06	0
2	PPI	E	607	-	4,4,4	0.97	0	4,4,4	1.05	0
2	PPI	B	1211	-	4,4,4	0.94	0	4,4,4	1.08	0
6	1PE	E	601	-	12,12,15	0.11	0	11,11,14	0.13	0
6	1PE	I	103	-	15,15,15	0.10	0	14,14,14	0.13	0
7	PG4	D	101[A]	-	12,12,12	0.52	0	11,11,11	0.27	0
4	CAD	A	411	-	1,4,4	2.95	1 (100%)	2,6,6	1.25	0
2	PPI	I	104	-	4,4,4	0.96	0	4,4,4	1.11	0
3	GOL	F	502	-	5,5,5	0.85	0	5,5,5	0.96	0
2	PPI	C	401	-	4,4,4	0.98	0	4,4,4	1.06	0
6	1PE	C	407	-	6,6,15	0.09	0	5,5,14	0.19	0
2	PPI	F	504	-	4,4,4	0.94	0	4,4,4	1.09	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PPI	G	601	-	-	0/2/2/2	-
3	GOL	L	603	-	-	2/4/4/4	-
5	GLY	B	1202	-	-	0/0/1/2	-
2	PPI	E	604	-	-	2/2/2/2	-
2	PPI	G	606	-	-	0/2/2/2	-
2	PPI	J	301	-	-	2/2/2/2	-
6	1PE	F	506	-	-	5/7/7/13	-
3	GOL	B	1204	-	-	2/4/4/4	-
3	GOL	B	1208	-	-	3/4/4/4	-
2	PPI	E	605	-	-	0/2/2/2	-
7	PG4	D	101[B]	-	-	5/10/10/10	-
2	PPI	F	503	-	-	0/2/2/2	-
2	PPI	G	605	-	-	0/2/2/2	-
3	GOL	H	508	-	-	2/4/4/4	-
2	PPI	K	205	-	-	0/2/2/2	-
2	PPI	A	402	-	-	2/2/2/2	-
6	1PE	K	201	-	-	7/13/13/13	-
2	PPI	D	104	-	-	0/2/2/2	-
2	PPI	L	608	-	-	2/2/2/2	-
2	PPI	C	408	-	-	1/2/2/2	-
2	PPI	D	103	-	-	2/2/2/2	-
2	PPI	E	603	-	-	0/2/2/2	-
2	PPI	A	405	-	-	0/2/2/2	-
2	PPI	C	406	-	-	2/2/2/2	-
3	GOL	A	409	-	-	0/4/4/4	-
2	PPI	D	105	-	-	0/2/2/2	-
2	PPI	K	204	-	-	0/2/2/2	-
6	1PE	H	504	-	-	1/10/10/13	-
2	PPI	B	1201	-	-	0/2/2/2	-
2	PPI	A	401	-	-	2/2/2/2	-
2	PPI	A	407	-	-	0/2/2/2	-
2	PPI	H	505	-	-	2/2/2/2	-
2	PPI	D	102	-	-	1/2/2/2	-
2	PPI	H	503	-	-	0/2/2/2	-
3	GOL	B	1212	-	-	4/4/4/4	-
2	PPI	K	203	-	-	0/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PPI	H	501	-	-	2/2/2/2	-
2	PPI	G	603	-	-	2/2/2/2	-
2	PPI	L	606	-	-	2/2/2/2	-
3	GOL	E	608	-	-	0/4/4/4	-
2	PPI	B	1210	-	-	2/2/2/2	-
3	GOL	F	501	-	-	2/4/4/4	-
2	PPI	F	508	-	-	2/2/2/2	-
2	PPI	L	604	-	-	2/2/2/2	-
2	PPI	F	505	-	-	0/2/2/2	-
6	1PE	D	106	-	-	4/10/10/13	-
2	PPI	J	303	-	-	2/2/2/2	-
2	PPI	C	405	-	-	1/2/2/2	-
2	PPI	A	408	-	-	1/2/2/2	-
2	PPI	A	403	-	-	0/2/2/2	-
2	PPI	L	609	-	-	2/2/2/2	-
2	PPI	B	1206	-	-	0/2/2/2	-
6	1PE	B	1203	-	-	1/10/10/13	-
2	PPI	K	206	-	-	2/2/2/2	-
2	PPI	L	605	-	-	1/2/2/2	-
2	PPI	J	302	-	-	0/2/2/2	-
2	PPI	B	1205	-	-	0/2/2/2	-
6	1PE	L	607	-	-	6/13/13/13	-
3	GOL	C	403	-	-	1/4/4/4	-
3	GOL	B	1207	-	-	4/4/4/4	-
3	GOL	G	602	-	-	0/4/4/4	-
3	GOL	E	606	-	-	0/4/4/4	-
2	PPI	A	410	-	-	1/2/2/2	-
2	PPI	C	404	-	-	0/2/2/2	-
3	GOL	C	402	-	-	0/4/4/4	-
2	PPI	H	502	-	-	0/2/2/2	-
2	PPI	I	101	-	-	0/2/2/2	-
3	GOL	H	506	-	-	0/4/4/4	-
2	PPI	K	202	-	-	1/2/2/2	-
3	GOL	B	1213	-	-	2/4/4/4	-
2	PPI	I	106	-	-	0/2/2/2	-
3	GOL	A	406	-	-	4/4/4/4	-
2	PPI	G	604	-	-	0/2/2/2	-
2	PPI	A	404	-	-	0/2/2/2	-
2	PPI	L	602	-	-	0/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PPI	I	102	-	-	2/2/2/2	-
2	PPI	E	607	-	-	2/2/2/2	-
2	PPI	B	1211	-	-	0/2/2/2	-
6	1PE	E	601	-	-	7/10/10/13	-
6	1PE	I	103	-	-	6/13/13/13	-
7	PG4	D	101[A]	-	-	4/10/10/10	-
2	PPI	I	104	-	-	1/2/2/2	-
3	GOL	F	502	-	-	2/4/4/4	-
2	PPI	C	401	-	-	0/2/2/2	-
6	1PE	C	407	-	-	1/4/4/13	-
2	PPI	F	504	-	-	0/2/2/2	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	601	CAD	O1-AS	3.08	1.78	1.70
4	H	507	CAD	O1-AS	3.05	1.78	1.70
4	F	507	CAD	O1-AS	3.04	1.78	1.70
4	I	105	CAD	O1-AS	3.03	1.78	1.70
4	A	411	CAD	O1-AS	2.95	1.78	1.70
4	G	607	CAD	O1-AS	2.93	1.78	1.70
4	E	602	CAD	O1-AS	2.89	1.78	1.70
4	B	1209	CAD	O1-AS	2.83	1.77	1.70

There are no bond angle outliers.

There are no chirality outliers.

All (121) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	408	PPI	O2-C1-C2-C3
3	A	406	GOL	O1-C1-C2-C3
3	A	406	GOL	C1-C2-C3-O3
3	B	1204	GOL	C1-C2-C3-O3
3	B	1207	GOL	O1-C1-C2-O2
3	B	1207	GOL	O1-C1-C2-C3
3	B	1212	GOL	C1-C2-C3-O3
3	B	1212	GOL	O2-C2-C3-O3
3	F	501	GOL	O1-C1-C2-C3
6	E	601	1PE	OH4-C13-C23-OH3
7	D	101[B]	PG4	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
7	D	101[A]	PG4	O2-C3-C4-O3
7	D	101[B]	PG4	O2-C3-C4-O3
3	A	406	GOL	O2-C2-C3-O3
7	D	101[B]	PG4	O4-C7-C8-O5
7	D	101[B]	PG4	C8-C7-O4-C6
3	B	1207	GOL	C1-C2-C3-O3
3	B	1208	GOL	C1-C2-C3-O3
3	B	1213	GOL	O1-C1-C2-C3
3	H	508	GOL	O1-C1-C2-C3
3	L	603	GOL	C1-C2-C3-O3
6	E	601	1PE	OH2-C12-C22-OH3
6	L	607	1PE	OH2-C12-C22-OH3
3	B	1204	GOL	O2-C2-C3-O3
3	L	603	GOL	O2-C2-C3-O3
6	B	1203	1PE	OH2-C12-C22-OH3
6	I	103	1PE	OH2-C12-C22-OH3
2	C	405	PPI	O2-C1-C2-C3
2	D	102	PPI	O2-C1-C2-C3
2	D	103	PPI	O2-C1-C2-C3
2	E	604	PPI	O2-C1-C2-C3
2	E	607	PPI	O1-C1-C2-C3
2	F	508	PPI	O2-C1-C2-C3
2	H	505	PPI	O2-C1-C2-C3
2	I	102	PPI	O2-C1-C2-C3
2	J	301	PPI	O2-C1-C2-C3
2	K	202	PPI	O2-C1-C2-C3
2	L	606	PPI	O2-C1-C2-C3
2	L	608	PPI	O1-C1-C2-C3
2	L	609	PPI	O2-C1-C2-C3
3	H	508	GOL	O1-C1-C2-O2
6	C	407	1PE	OH4-C13-C23-OH3
6	I	103	1PE	C14-C24-OH4-C13
3	A	406	GOL	O1-C1-C2-O2
6	D	106	1PE	OH5-C14-C24-OH4
6	D	106	1PE	C14-C24-OH4-C13
6	L	607	1PE	C13-C23-OH3-C22
6	I	103	1PE	C15-C25-OH5-C14
6	F	506	1PE	C24-C14-OH5-C25
6	K	201	1PE	C12-C22-OH3-C23
3	B	1212	GOL	O1-C1-C2-O2
3	B	1213	GOL	O1-C1-C2-O2
3	F	502	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	E	601	1PE	C14-C24-OH4-C13
6	F	506	1PE	C16-C26-OH6-C15
6	K	201	1PE	C23-C13-OH4-C24
6	D	106	1PE	C15-C25-OH5-C14
6	L	607	1PE	C25-C15-OH6-C26
2	A	402	PPI	O1-C1-C2-C3
2	A	402	PPI	O2-C1-C2-C3
2	B	1210	PPI	O1-C1-C2-C3
2	B	1210	PPI	O2-C1-C2-C3
2	C	406	PPI	O1-C1-C2-C3
2	C	406	PPI	O2-C1-C2-C3
2	D	103	PPI	O1-C1-C2-C3
2	E	604	PPI	O1-C1-C2-C3
2	E	607	PPI	O2-C1-C2-C3
2	F	508	PPI	O1-C1-C2-C3
2	G	603	PPI	O1-C1-C2-C3
2	H	501	PPI	O1-C1-C2-C3
2	H	501	PPI	O2-C1-C2-C3
2	H	505	PPI	O1-C1-C2-C3
2	I	102	PPI	O1-C1-C2-C3
2	I	104	PPI	O1-C1-C2-C3
2	J	301	PPI	O1-C1-C2-C3
2	J	303	PPI	O1-C1-C2-C3
2	K	206	PPI	O1-C1-C2-C3
2	L	604	PPI	O1-C1-C2-C3
2	L	606	PPI	O1-C1-C2-C3
2	L	608	PPI	O2-C1-C2-C3
6	F	506	1PE	C25-C15-OH6-C26
6	K	201	1PE	OH6-C15-C25-OH5
3	B	1208	GOL	O2-C2-C3-O3
3	F	501	GOL	O1-C1-C2-O2
6	K	201	1PE	C16-C26-OH6-C15
6	D	106	1PE	C24-C14-OH5-C25
6	E	601	1PE	C12-C22-OH3-C23
6	F	506	1PE	C15-C25-OH5-C14
6	L	607	1PE	C14-C24-OH4-C13
3	B	1208	GOL	O1-C1-C2-C3
6	I	103	1PE	OH4-C13-C23-OH3
3	B	1207	GOL	O2-C2-C3-O3
6	E	601	1PE	C24-C14-OH5-C25
6	K	201	1PE	OH5-C14-C24-OH4
7	D	101[A]	PG4	C5-C6-O4-C7

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Mol	Chain	Res	Type	Atoms
6	H	504	1PE	C15-C25-OH5-C14
7	D	101[A]	PG4	O3-C5-C6-O4
6	I	103	1PE	C12-C22-OH3-C23
2	A	401	PPI	O1-C1-C2-C3
2	A	401	PPI	O2-C1-C2-C3
2	A	410	PPI	O2-C1-C2-C3
2	C	408	PPI	O2-C1-C2-C3
2	G	603	PPI	O2-C1-C2-C3
2	J	303	PPI	O2-C1-C2-C3
2	K	206	PPI	O2-C1-C2-C3
2	L	604	PPI	O2-C1-C2-C3
2	L	605	PPI	O2-C1-C2-C3
2	L	609	PPI	O1-C1-C2-C3
3	C	403	GOL	O1-C1-C2-C3
3	F	502	GOL	C1-C2-C3-O3
7	D	101[B]	PG4	C5-C6-O4-C7
6	I	103	1PE	OH5-C14-C24-OH4
6	K	201	1PE	OH2-C12-C22-OH3
6	E	601	1PE	C15-C25-OH5-C14
3	B	1212	GOL	O1-C1-C2-C3
6	E	601	1PE	OH5-C14-C24-OH4
6	F	506	1PE	OH5-C14-C24-OH4
6	L	607	1PE	OH5-C14-C24-OH4
6	L	607	1PE	C15-C25-OH5-C14
6	K	201	1PE	OH7-C16-C26-OH6
7	D	101[A]	PG4	C8-C7-O4-C6

There are no ring outliers.

41 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	603	GOL	1	0
2	E	604	PPI	1	0
2	J	301	PPI	1	0
6	F	506	1PE	1	0
7	D	101[B]	PG4	2	0
2	F	503	PPI	1	0
3	H	508	GOL	1	0
6	K	201	1PE	1	0
2	D	104	PPI	1	0
2	L	608	PPI	1	0
2	C	408	PPI	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	103	PPI	2	0
2	C	406	PPI	2	0
3	A	409	GOL	5	0
2	B	1201	PPI	4	0
2	D	102	PPI	2	0
3	B	1212	GOL	1	0
2	K	203	PPI	1	0
2	F	508	PPI	1	0
2	F	505	PPI	2	0
6	D	106	1PE	2	0
2	J	303	PPI	1	0
2	A	408	PPI	1	0
2	L	609	PPI	1	0
2	B	1206	PPI	1	0
2	K	206	PPI	1	0
4	H	507	CAD	1	0
6	L	607	1PE	4	0
3	B	1207	GOL	1	0
3	G	602	GOL	1	0
2	A	410	PPI	1	0
2	C	404	PPI	2	0
2	H	502	PPI	1	0
3	H	506	GOL	1	0
2	I	106	PPI	1	0
3	A	406	GOL	1	0
2	G	604	PPI	2	0
2	I	102	PPI	1	0
6	E	601	1PE	2	0
6	I	103	1PE	1	0
7	D	101[A]	PG4	1	0

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	98/102 (96%)	-0.21	0 100 100	19, 24, 36, 55	0
1	B	97/102 (95%)	-0.15	3 (3%) 49 55	19, 24, 38, 51	0
1	C	98/102 (96%)	-0.01	3 (3%) 49 55	19, 25, 43, 53	0
1	D	97/102 (95%)	-0.05	2 (2%) 63 68	19, 28, 45, 55	0
1	E	98/102 (96%)	-0.18	2 (2%) 65 69	20, 27, 43, 54	0
1	F	99/102 (97%)	-0.07	5 (5%) 28 33	20, 26, 46, 73	0
1	G	98/102 (96%)	-0.22	0 100 100	22, 30, 47, 59	0
1	H	98/102 (96%)	-0.16	1 (1%) 82 85	23, 29, 42, 46	0
1	I	98/102 (96%)	-0.14	1 (1%) 82 85	20, 26, 44, 57	0
1	J	98/102 (96%)	0.32	3 (3%) 49 55	24, 33, 49, 57	0
1	K	98/102 (96%)	0.24	6 (6%) 21 26	26, 36, 49, 60	0
1	L	98/102 (96%)	0.23	3 (3%) 49 55	25, 35, 54, 63	0
All	All	1175/1224 (95%)	-0.03	29 (2%) 57 62	19, 29, 46, 73	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	0	GLY	3.9
1	C	0	GLY	3.8
1	K	1	MET	3.7
1	L	75	ARG	3.3
1	F	35	PRO	2.9
1	C	1	MET	2.9
1	I	49[A]	ARG	2.9
1	B	90	LEU	2.6
1	K	62	ALA	2.6
1	E	1	MET	2.4
1	J	49	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	14	ASP	2.3
1	D	90	LEU	2.3
1	K	88	LEU	2.3
1	L	21	ALA	2.3
1	F	90	LEU	2.2
1	L	33	ASN	2.2
1	C	90	LEU	2.2
1	F	89	PHE	2.2
1	B	88	LEU	2.1
1	J	90	LEU	2.1
1	E	69	ARG	2.1
1	D	35	PRO	2.1
1	K	74	ALA	2.1
1	F	1	MET	2.1
1	K	72	THR	2.1
1	F	0	GLY	2.0
1	J	0	GLY	2.0
1	B	97	GLU	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 monosaccharides 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
2	PPI	G	604	5/5	0.55	0.35	54,55,62,63	0
6	1PE	B	1203	13/16	0.62	0.28	33,46,56,57	0
5	GLY	B	1202	4/5	0.64	0.33	48,53,55,56	0
2	PPI	F	508	5/5	0.65	0.25	41,41,50,51	0
6	1PE	L	607	16/16	0.68	0.29	55,62,71,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PPI	I	104	5/5	0.70	0.26	36,40,43,57	0
2	PPI	I	102	5/5	0.70	0.26	35,38,54,59	0
2	PPI	E	605	5/5	0.71	0.21	45,51,65,67	0
3	GOL	F	502	6/6	0.71	0.20	32,49,57,57	0
3	GOL	L	603	6/6	0.71	0.24	38,40,46,50	0
3	GOL	B	1204	6/6	0.72	0.33	42,46,55,57	0
2	PPI	A	410	5/5	0.72	0.20	20,27,47,48	0
2	PPI	D	104	5/5	0.73	0.21	25,27,38,44	0
2	PPI	C	405	5/5	0.74	0.30	38,47,54,63	0
6	1PE	C	407	7/16	0.74	0.29	34,45,57,62	0
2	PPI	J	303	5/5	0.74	0.27	32,45,47,56	0
4	CAD	L	601	5/5	0.75	0.29	43,46,56,105	0
2	PPI	B	1201	5/5	0.77	0.18	23,25,49,52	0
2	PPI	L	608	5/5	0.77	0.28	45,56,61,62	0
3	GOL	C	402	6/6	0.78	0.20	29,40,51,52	0
4	CAD	F	507	5/5	0.78	0.23	26,35,40,85	5
4	CAD	I	105	5/5	0.78	0.23	31,38,44,91	5
6	1PE	H	504	13/16	0.78	0.21	42,51,55,58	0
6	1PE	K	201	16/16	0.78	0.34	51,58,65,67	0
2	PPI	I	106	5/5	0.78	0.24	27,39,47,49	0
3	GOL	H	506	6/6	0.79	0.22	29,48,52,60	0
3	GOL	H	508	6/6	0.79	0.29	39,42,47,48	0
2	PPI	A	403	5/5	0.81	0.18	33,37,50,55	0
2	PPI	A	407	5/5	0.81	0.20	43,49,51,52	0
2	PPI	A	408	5/5	0.81	0.35	22,35,45,46	0
2	PPI	G	606	5/5	0.82	0.15	49,53,58,59	0
6	1PE	D	106	13/16	0.82	0.28	30,49,56,58	0
3	GOL	A	406	6/6	0.82	0.22	32,35,36,36	0
2	PPI	L	604	5/5	0.82	0.28	39,46,46,48	0
4	CAD	H	507	5/5	0.82	0.24	78,82,90,137	0
2	PPI	C	406	5/5	0.83	0.26	30,31,41,54	0
2	PPI	K	204	5/5	0.83	0.15	36,37,45,49	0
2	PPI	G	605	5/5	0.84	0.21	48,51,58,63	0
3	GOL	G	602	6/6	0.84	0.25	35,41,45,45	0
2	PPI	L	606	5/5	0.84	0.23	25,35,41,42	0
2	PPI	K	206	5/5	0.84	0.16	46,59,62,64	0
7	PG4	D	101[A]	13/13	0.84	0.19	34,41,55,58	13
7	PG4	D	101[B]	13/13	0.84	0.19	32,42,55,58	13
6	1PE	F	506	10/16	0.85	0.23	30,39,53,56	0
2	PPI	C	408	5/5	0.85	0.15	31,33,40,41	0
4	CAD	A	411	5/5	0.85	0.19	32,43,59,95	0
3	GOL	B	1212	6/6	0.85	0.30	29,35,50,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	A	409	6/6	0.85	0.21	31,41,50,58	0
3	GOL	E	606	6/6	0.85	0.15	32,38,41,43	0
2	PPI	A	402	5/5	0.87	0.14	31,41,51,52	0
3	GOL	B	1207	6/6	0.87	0.15	26,39,46,52	0
6	1PE	I	103	16/16	0.87	0.17	39,52,66,67	0
2	PPI	D	103	5/5	0.87	0.20	27,30,42,45	0
2	PPI	F	503	5/5	0.87	0.17	29,29,32,44	0
3	GOL	C	403	6/6	0.87	0.15	33,41,43,50	0
6	1PE	E	601	13/16	0.87	0.13	39,49,56,59	0
2	PPI	D	102	5/5	0.88	0.22	23,37,48,50	0
3	GOL	E	608	6/6	0.88	0.15	28,34,40,44	0
2	PPI	B	1211	5/5	0.88	0.40	38,39,48,53	0
2	PPI	E	607	5/5	0.88	0.26	37,42,47,55	0
2	PPI	H	502	5/5	0.89	0.28	39,40,43,48	0
2	PPI	H	505	5/5	0.89	0.23	33,50,54,55	0
2	PPI	G	603	5/5	0.89	0.13	36,42,52,55	0
2	PPI	A	401	5/5	0.89	0.13	29,42,49,55	0
2	PPI	E	604	5/5	0.89	0.15	29,41,48,50	0
2	PPI	A	404	5/5	0.89	0.16	44,44,52,52	0
2	PPI	C	404	5/5	0.90	0.24	36,48,54,55	0
4	CAD	B	1209	5/5	0.90	0.22	29,31,66,81	5
2	PPI	F	505	5/5	0.91	0.13	39,42,45,57	0
2	PPI	K	202	5/5	0.91	0.13	37,43,48,55	0
2	PPI	K	203	5/5	0.91	0.13	39,41,42,44	0
3	GOL	B	1208	6/6	0.91	0.23	31,39,41,42	0
2	PPI	H	501	5/5	0.92	0.26	40,41,43,44	0
2	PPI	B	1206	5/5	0.92	0.19	41,42,52,58	0
2	PPI	B	1210	5/5	0.92	0.15	29,35,44,47	0
2	PPI	L	605	5/5	0.92	0.17	35,45,53,65	0
4	CAD	G	607	5/5	0.92	0.22	62,67,75,96	0
2	PPI	G	601	5/5	0.93	0.13	21,27,28,28	0
3	GOL	B	1213	6/6	0.93	0.24	30,40,47,49	0
2	PPI	J	301	5/5	0.93	0.20	30,33,42,44	0
2	PPI	L	609	5/5	0.93	0.13	47,49,52,62	0
2	PPI	A	405	5/5	0.93	0.13	21,22,25,27	0
4	CAD	E	602	5/5	0.94	0.30	46,60,74,95	0
2	PPI	K	205	5/5	0.94	0.13	31,34,35,35	0
3	GOL	F	501	6/6	0.95	0.20	27,32,34,37	0
2	PPI	I	101	5/5	0.96	0.10	21,23,27,32	0
2	PPI	J	302	5/5	0.96	0.09	26,27,28,30	0
2	PPI	D	105	5/5	0.96	0.12	22,28,32,32	0
2	PPI	F	504	5/5	0.96	0.17	20,24,26,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PPI	B	1205	5/5	0.96	0.10	20,23,24,27	0
2	PPI	E	603	5/5	0.97	0.09	21,24,25,27	0
2	PPI	C	401	5/5	0.97	0.13	22,23,26,28	0
2	PPI	L	602	5/5	0.97	0.11	27,30,34,39	0
2	PPI	H	503	5/5	0.98	0.11	24,26,28,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.